SIMULATION OF GROUNDWATER RECHARGE DYNAMICS THROUGH VARIABLY SATURATED FRACTURED POROUS MEDIA

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ABSTRACT
Groundwater recharge through variably saturated fractured porous media is extremely complex. In this study, groundwater recharge dynamics were investigated using numerical simulations of variably saturated discretely fractured porous media. Infiltration simulations were performed on a simple porous matrix containing a single vertical rough-walled fracture. The influence of fracture and matrix properties as well as antecedent moisture conditions was assessed. It was shown that moisture exchange between the fracture and the matrix had a significant influence on vertical water flux during infiltration. The effects of matrix imbibition restricted the advance of the wetting front in the fracture and limited the influence of aperture variability. Vertical fluxes were highly sensitive to matrix properties and antecedent moisture conditions. In all cases, vertical tracer migration was controlled by the fracture flux.

RÉSUMÉ
La recharge des aquifères à travers un milieu poreux fracturé non saturé est un phénomène extrêmement complexe. Dans la présente étude, la dynamique de la recharge est étudiée à l'aide de simulations numériques à saturation variable dans un milieu poreux fracturé. Des simulations d'infiltration ont été effectuées sur un milieu poreux simple contenant une seule fracture verticale à parois irrégulières. L'influence des propriétés de la matrice et de la fracture ainsi que la teneur en eau initiale ont été évaluées. Il est démontré que l'échange d'eau entre la fracture et la matrice a une influence importante sur le flux vertical dans la fracture lors du processus d'infiltration. L'imbibition de la matrice a comme effet de restreindre la progression du front d'infiltration dans la fracture et de limiter l'influence de la variabilité de l'ouverture de la fracture. Les flux verticaux sont très sensibles aux propriétés de la matrice ainsi qu'à la teneur en eau préexistante. Dans tous les cas, la migration verticale des traceurs est contrôlée par le flux dans la fracture.

1. INTRODUCTION

Understanding groundwater recharge is critical for managing groundwater resources and evaluating the vulnerability of aquifers to contamination. In previously glaciated terrain, including much of southern Ontario, groundwater recharge often occurs through till or other fine-grained surficial deposits. Groundwater recharge processes in these settings can be extremely complex, often as a result of the presence of macropores, such as fractures, rootholes, and animal burrows. Previous research has shown that fractures and other large macropores have a significant influence on groundwater flow and contaminant transport, particularly through low permeability porous media (Beven and Germann, 1982; e.g., Gerber et al., 2001; Jorgensen et al., 2002; McKay et al., 1993). Preferential flow through fractures affects groundwater recharge flux (Wood et al., 1997), contaminant migration rates (Jorgensen et al., 2002; Kelly and Pomes, 1998), and the response of watersheds to rainfall events (McGlynn et al., 2002). There is increasing evidence that flow along preferential paths is the rule more often than the exception in these types of sediments and can represent a significant portion of the total flow system (Flury et al., 1994; Jury and Wang, 2000).

The current understanding of flow and transport processes in the fractured vadose zone is limited. Issues such as capillarity, film flow, flow instability, fracture geometry, and matrix-fracture interactions result in complex flow phenomena in partially saturated, fractured porous media (National Research Council, 2001). The response of the flow system to groundwater recharge events is dependent upon antecedent moisture conditions, precipitation intensity and duration, and the properties of both the porous matrix and fractures. The relative importance of these various factors is not well understood, which makes prediction of groundwater recharge in partially saturated fractured porous media extremely difficult.

Small-scale physical processes are expected to have a significant influence on groundwater recharge dynamics. Under saturated conditions, fractures in low permeability sediments typically serve as preferential flow paths. Under partially saturated conditions, there is a complex relationship between pressure, saturation and relative hydraulic conductivity. As a result, either the matrix or the fractures could represent the predominant flow system depending on saturation conditions. In addition, natural fractures have rough walls that control the flow and distribution of water in the fracture plane, particularly during variably saturated conditions where capillary pressures are a function of pore (or aperture) size. Finally, there is the potential for significant imbibition of water from the fractures into the matrix during a recharge event, given the relatively large porosity and small pore sizes in the matrix compared to the fracture.

Numerical simulations were used in this study to examine the dynamics of groundwater recharge in the fractured vadose zone and evaluate the nature of matrix-fracture interactions. The results of transient infiltration simulations utilizing a three-dimensional discrete fracture flow and transport model are presented herein. A discrete fracture approach was used in order to incorporate the small-scale physical processes that are thought to control fracture flow and influence fracture-matrix interaction. In particular, variable fracture apertures were incorporated into the model to examine their influence on flow. The influence of varying fracture and matrix properties and antecedent moisture conditions on vertical fluid flux is examined.

2. NUMERICAL METHOD

The numerical model employed in this study, designated HydroSphere (Therrien et al., 2004), is a three-dimensional fully integrated subsurface and overland flow and solute transport model. The subsurface component of the model is built upon the three-dimensional variably saturated flow code of Therrien and Sudicky (1996), which is capable of simulating discretely fractured porous media. A modified form of Richards equation is used to describe transient subsurface flow. The model uses a common node approach, where fractures are discretized on the face of matrix blocks and they share common nodes. This ensures the continuity of hydraulic head at the fracture-matrix interface and no fluid leakage terms are required to account for mass exchange between fracture and matrix.

Simulations were performed on a simple three-dimensional domain measuring 2.0 m high by 0.5 m wide by 0.5 m deep. A single vertical fracture was generated through the middle of the domain at y = 0.25 m (see Figure 1). The finite difference mesh was discretized into elements 0.02 m by 0.02 m by 0.02 m in size. The mesh was refined near the fracture plane, where a nodal spacing of 0.002 m was used adjacent to the fracture in the y-direction and the spacing was gradually increased to a maximum of 0.02 m further from the fracture. This resulted in a domain with a total of 91,910 nodes and 85,000 elements, including 2,500 fracture elements. All lateral boundaries in the model were assigned a no-flow boundary condition. Infiltration along the upper boundary was simulated using a constant flux equivalent to the applied rainfall rate. The bottom boundary was assigned a constant head to simulate the presence of a static water table either beneath or within the flow domain. Top and bottom boundary conditions for the simulations are provided in Tables 1 and 2. Equilibrium initial conditions were employed for all simulations by setting the initial hydraulic head within the model domain equal to the hydraulic head at the bottom boundary.

Detailed analysis of rainfall-runoff relationships were beyond the scope of this study, however, overland flow was incorporated into the simulations to enable ponding and possible overland flow of water applied in excess of the infiltration rate.

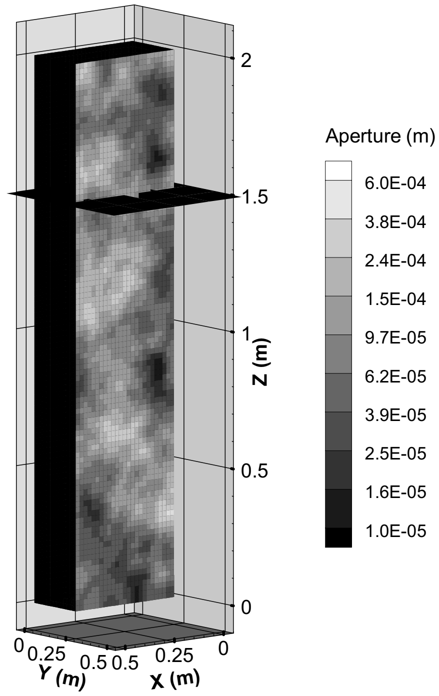

Figure 1. Model half-domain shown with spatial aperture distribution in the fracture plane. Vertical water fluxes are calculated at the location of the horizontal slice (z = 1.5 m).

2.1 Porous Media Properties

Hydraulic properties for the porous media were selected to be representative of silt or silty till materials that are common in glacial deposits in southern Ontario. These sediments are fine-grained and typified by a low to moderate permeability. A saturated hydraulic conductivity, K_{sat}, value of 0.01 m/d (1.2×10^{-7} m/s) was selected for the porous media for the Base Case. The porous media properties used in the simulations are listed in Tables 1 and 2.

The constitutive relation between capillary pressure, saturation and relative hydraulic is required in order to simulate variably saturated flow in porous media. Two of the more common empirical models used to describe these relations are the van Genuchten (1980) and Brooks-Corey (1964) models. In this study, the capillary pressure-saturation relationship of van Genuchten (1980) was used and is given by:

$$S_e = \left(1 + \left|\alpha\psi_c\right|^n\right)^{-m} \qquad [1]$$

where ψ_c is the capillary pressure head, α, n and m are empirical fitting parameters, and S_e is the effective saturation given by:

$$S_e = \frac{S - S_r}{1 - S_r} \quad [2]$$

where S is water saturation and S_r is residual saturation, which is often used as another fitting parameter. Additionally, applying the Mualem-based theory (Mualem, 1976) yields m = 1 - 1/n.

The van Genuchten relation for relative hydraulic conductivity can induce numerical instability for very small values of the fitting parameter n (i.e., n < 1.3), which are typical of relatively fine-grained soils. Thus, the Brooks-Corey model (1964) was implemented for the capillary pressure-relative hydraulic conductivity relation to increase model stability. The relationship for relative hydraulic conductivity, K_r, is given by:

$$K_r = \left(\frac{\psi_{ae}}{\psi_c}\right)^{2.5\lambda+2} \quad \text{for } \psi_c \geq \psi_{ae} \quad [3]$$

where ψ_c is the capillary pressure head, ψ_{ae} is the air entry pressure head, and λ is an empirical pore size distribution fitting parameter. van Genuchten (1980) showed that for Mualem-based theory (Mualem, 1976) the Brooks-Corey parameters ψ_{ae} and λ are the equivalent of 1/α and (n-1) for the van Genuchten parameters. Parameter values used for the simulations are listed in Tables 1 and 2.

2.2 Fracture Properties

Fracture roughness was incorporated into the model by assigning a fracture with spatially variable apertures within the fracture plane. Fracture apertures were generated stochastically using Fourier transform techniques developed by Robin et al. (1993). The aperture distribution was assumed to follow a spatially correlated log-normal distribution. A log-normal distribution was chosen because it matches reasonably well with measured aperture distributions on rock fractures (Gale, 1987; Keller, 1998) and is consistent with earlier modelling studies (Abdel-Salam and Chrysikopoulos, 1996; Kueper and McWhorter, 1991; Vandersteen et al., 2003). The aperture field was mapped onto to the fracture plane, with each fracture element assigned an aperture that was assumed to be constant for that element (i.e., a local parallel-plate approximation). Figure 1 shows a single realization of the aperture field within the fracture plane.

Fracture saturation and hydraulic conductivity parameters were assigned on an element-by-element basis as functions of the elemental aperture. The Brooks-Corey model (1964) was used to describe the constitutive relations for the fracture. The capillary pressure-saturation relationship is given by:

$$S_e = \left(\frac{\psi_{ae}}{\psi_c}\right)^{\lambda} \quad \text{for } \psi_c \geq \psi_{ae} \quad [4]$$

Table 1. Model input parameters for the Base Case.

Parameter	Value
Water table depth	3.0 m
Applied rainfall rate	0.05 m/d
Rainfall duration	5 d
Porous Matrix	
Matrix K_{sat}	0.01 m/d
Specific storage	1×10^{-4} m^{-1}
Porosity	0.4
Residual saturation	0.2
α, van Genuchten parameter	1.0 m^{-1}
n, van Genuchten parameter	1.5
Fracture	
Geometric mean	100 µm
Variance of ln(b)	0.64
Spatial correlation length	0.10 m
Residual saturation	0.05
λ, Brooks-Corey parameter	4.0
Fluids	
Density, ρ_w	1000 kg/m^3
Viscosity, μ_w	1.124×10^{-3} N·s/m^2
Air-water interfacial tension, σ	0.07183 N/m
Solute Transport	
Free solution diffusion coefficient	1.73×10^{-4} m^2/d
Rainfall input concentration, C_o	1.0 kg/m^3
Longitudinal dispersivity, α_L	0.01 m
Transverse dispersivity, α_T	0.01 m

Table 2. Model input parameters for sensitivity analyses.

Case No.	Sensitivity Tested	Value
1a	Matrix K_{sat} Decreased 0.1x*	0.001 m/d
1b	Matrix K_{sat} Increased 10x	0.1 m/d
2a	Fracture Aperture Decreased 0.5x	50 µm
2b	Fracture Aperture Increased 2x	200 µm
3a	Shallower water table	1.0 m
3b	Deeper water table	5.0 m

*0.1x indicates that parameter was multiplied by a factor of 0.1 compared to the Base Case

while the relative hydraulic conductivity expression is given in Eq. 3 above. If we have assume that fracture aperture is constant at the local scale, the air entry pressure for two parallel plates can be related to fracture aperture by the following equation:

$$\psi_{ae} = \frac{2\sigma \cos\theta}{b\rho g} \quad [5]$$

where ψ_{ae} is the capillary air entry pressure head for the fracture segment, σ is the interfacial tension between air and water, θ is the contact angle measured through the wetting phase, b is the fracture aperture, ρ is water density, and g is acceleration due to gravity. For all simulations, the contact angle, θ, was assumed to be zero (i.e., water is perfectly wetting).

When capillary pressure head exceeds this critical air entry value, the fracture will begin to drain. For idealized parallel plates, the fracture would theoretically drain instantly once the air entry pressure is exceeded, effectively reducing the saturation and relative hydraulic conductivity to zero. This free drainage situation seems unlikely for natural rough-walled fractures. In a natural fracture, water will remain held under capillary forces in micro-scale roughness within the fracture leading to steadily declining saturation and relative hydraulic conductivity with increasing capillary pressure (i.e., decreasing water pressure). Using the Brooks-Corey model, the λ parameter is considered to represent the micro-scale roughness at a scale below the level of fracture discretization. This conceptualization is consistent with the work of Kueper and McWhorter (1991). The resulting constitutive relations for the fracture are qualitatively very similar to the more physically rigorous liquid configuration model of Or and Tuller (2003). Fracture parameter values used in the simulations are listed in Tables 1 and 2.

2.3 Tracing Infiltrating Water

A numerical tracer technique was implemented to investigate the movement of infiltrating water from ground surface. A hypothetical conservative tracer with a specified concentration of 1.0 kg/m^3 was applied with the rainfall on the upper boundary. The initial tracer concentration throughout the model domain was set as 0.0 kg/m^3. In this way, we are able to differentiate between infiltrating rainfall and antecedent soil moisture. The solute transport parameters implemented within HydroSphere are listed in Table 1.

2.4 Simulation Scenarios

A large number of infiltration simulations were performed to evaluate the sensitivity of various input parameters during a hypothetical groundwater recharge event. The results of three cases with varying fracture and matrix properties and antecedent moisture conditions (i.e., water table depth) are presented here.

All simulations were referenced to a standard Base Case with input parameters listed in Table 1. Simulation parameters for the Base Case were chosen to be representative of realistic hydrologic and soil conditions encountered in southern Ontario. Whenever possible, realistic field measured values or "average" values published in the literature were selected. Given that published fracture geometry parameters for unconsolidated materials did not exist, these parameter values were selected from published fractured rock experiments.

Selected model input parameters were varied in the sensitivity analyses for the remaining cases. The input parameters were systematically varied about the "average" values used in the Base Case, within a reasonable range. The input values used for sensitivity analysis are shown in Table 2.

All simulations represent continuous rainfall for a period of five days. This represents a rather extreme rainfall event for southern Ontario that is approximately consistent with a 100-year return period.

3. RESULTS AND DISCUSSION

3.1 Base Case

Tracer concentrations within the matrix and fracture for the simulated Base Case are shown in Figure 2. The results demonstrate the infiltration of water from surface. Up to a time of one day, the majority of infiltrating water enters the matrix. The tracer concentration profile within the fracture plane (y = 0.25 m) at one day is relatively uniform, showing little influence of aperture variability. At 2.5 days, a large portion of the upper 0.5 m of the fracture has become saturated, and the infiltrating water has clearly begun to preferentially flow down the fracture. The infiltration pattern within the fracture is uneven because of fracture aperture variability. At the end of the simulation (5.0 days), the infiltrating water has nearly reached the bottom boundary of the model at 2.0 m depth, while it has only reached a depth of approximately 0.35 m within the matrix. It should be noted that the plots shown in Figure 2 represent the front of infiltrating rainwater, which does not necessarily coincide with the wetting or saturation front, as demonstrated below.

In order to assess groundwater recharge potential, the vertical flux of water was estimated as a function of time. At each model time step, the vertical volumetric water flux crossing a horizontal slice at a depth of 0.5 m below ground surface (see Figure 1) was calculated. Graphs showing the variation in water flux at 0.5 m depth for the Base Case and Cases 1 through 3 are shown in Figure 3. The vertical fluxes are separated into porous matrix and fracture components.

The plots on the left side of Figure 3 represent the simulation results for the Base Case. The shape of the curves represents a complex interaction between the fracture and the matrix. In early time there is no flow at 0.5 m depth in either the matrix or the fracture. Above 0.5 m, the majority of infiltrating water enters the matrix causing an increase in saturation and pressure heads. At approximately 0.5 days, water is just beginning to saturate the smallest aperture regions near the entrance to the fracture. At this same time, the leading edge of the matrix wetting front reaches 0.5 m depth, causing the matrix flux to increase. Note that the matrix wetting front is comprised of antecedent soil water that is driven downward by infiltrating rainwater. As noted above, rainwater infiltrating through the matrix does not reach 0.5 m depth during the 5 day simulation period. Although not shown, ponding of water at surface begins to occur at approximately 1.0 days. From approximately 1 day to 2.3 days the matrix flux reaches a plateau as the matrix gradually approaches saturation. Over this same period, fracture flux remains low as the fracture wetting front, which is much sharper than the matrix wetting front due to matrix imbibition, is just reaching 0.5 m depth. After 2.3 days, there is a sharp increase in fracture flux and an associated decrease in matrix flux. Fracture flux increases due to a large increase in hydraulic conductivity of portions of the fracture that become saturated. Within the matrix, fluxes decline since the matrix hydraulic conductivity is at or near its saturated peak value and the vertical hydraulic gradient gradually begins to decrease. After both the matrix and fracture wetting fronts pass the 0.5 m depth, the fracture and matrix fluxes asymptotically approach steady-state values. At the end of five days infiltration, the fracture flux constitutes approximately 79% of the total vertical flux at 0.5 m depth.

The influence of the fracture on vertical water fluxes is not as great as might have been expected, given five days of continuously applied rainfall at a rate (0.05 m/d) five times greater than the saturated hydraulic conductivity of the matrix (0.01 m/d). After 5 days of infiltration, the leading edge of the wetting front within the fracture is only beginning to reach the lower boundary of the model (i.e., 2 m depth). Also, a large portion of the fracture, consisting of the larger aperture regions, remains below 70% saturation even after the wetting front has passed. It appears the porous matrix has a large capacity for imbibing and storing water that flows down the fracture. The simulation results suggest that fracture flow may only become significant once the surrounding matrix becomes nearly saturated.

3.2 Sensitivity Analyses

In order to assess parameter sensitivity, the transient vertical flux of water is compared for different simulations (Figure 3). From Figure 3a it can be seen that the saturated hydraulic conductivity, K_{sat}, of the matrix has a significant influence on the flow system. Decreasing K_{sat} by one order of magnitude (Case 1a) compared to the Base Case causes the fracture flow system to dominate. With a reduction in K_{sat}, the matrix is less effective at imbibing fluid from the fracture, creating a greater disequilibrium between the fracture and the matrix. Conversely, increasing K_{sat} by one order of magnitude (Case 1b) causes fracture fluxes to become negligible since the matrix K_{sat} exceeds the applied rainfall rate. This implies a much faster transport of contaminants from surface in the lower hydraulic conductivity material.

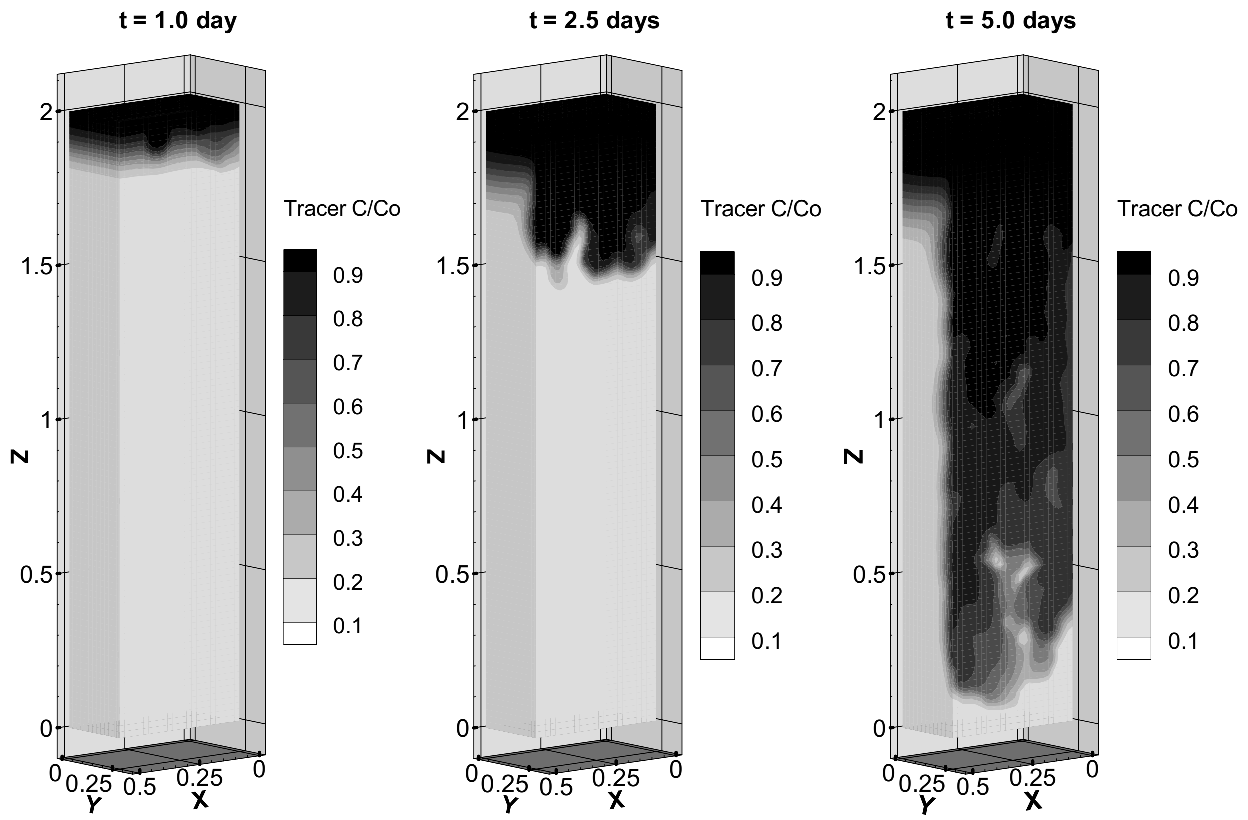

Figure 2. Base Case simulation results showing the tracer concentration within the model half-domain after 1.0 days (left), 2.5 days (middle), and 5.0 days (right) of continuous infiltration. The fracture plane is shown at y = 0.25 m.

The simulation results are less sensitive to variations in fracture parameters than porous matrix parameters. Figure 3b illustrates the influence of mean aperture variation on the fluid fluxes. Decreasing the mean aperture (Case 2a) does not change the timing of the fluxes observed at 0.5 m depth, but it causes a reduction in the magnitude of the fracture flux. Since the transmissivity, T, of a saturated fracture segment is related to the aperture according to the cubic law ($T \propto b^3$), a small reduction in aperture can significantly lower the saturated transmissivity of the fracture.

Somewhat surprisingly, an increase in mean fracture aperture (Case 2b) did not significantly change the flow

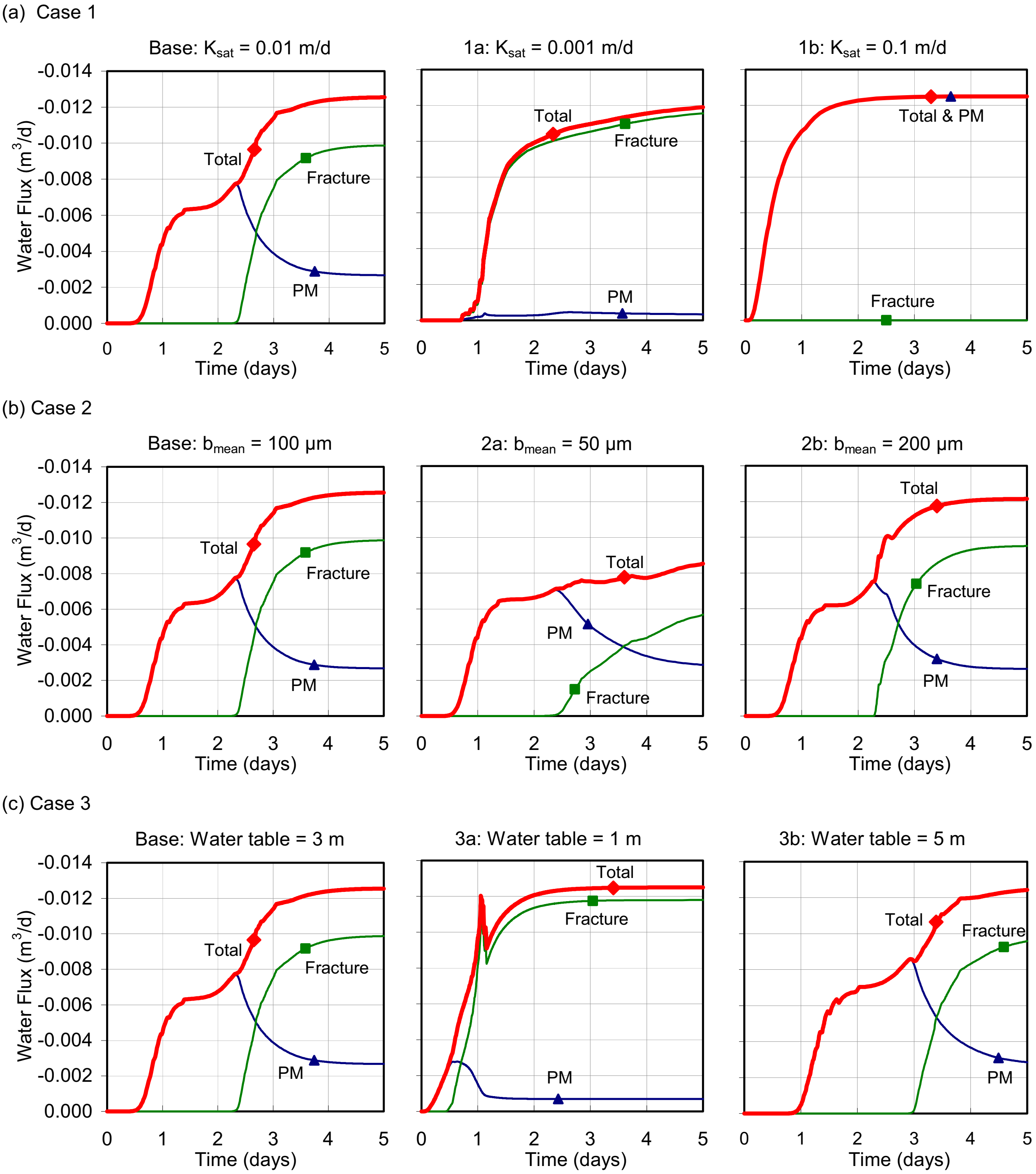

Figure 3. Vertical water fluxes at 0.5 m depth as a function of time for variations in porous matrix properties (Cases 1 and 2) and fracture properties (Cases 3 and 4). Negative flux values indicate downward flow.

system response compared to the Base Case. Figure 3b demonstrates that the timing and magnitude of the fluxes for both the 100 μm and 200 μm mean apertures were very similar. This can be explained by considering the relationship between aperture, saturation, and hydraulic conductivity. Smaller aperture regions are more likely to reach full saturation, but they have a much lower saturated transmissivity than larger aperture regions. Larger aperture segments have the potential for a much greater transmissivity based on the cubic law. However, larger aperture segments have a lower air entry pressure causing them to preferentially remain unsaturated, which in turn significantly lowers the relative transmissivity of the fracture. In the simulations presented here, flow within the fracture plane is concentrated in regions with apertures ranging between 50 μm and 150 μm. This range of apertures appears small enough to saturate under the pressure heads experienced and yet the apertures are large enough to contribute significantly to the overall flow. Even though the mean fracture aperture increased from 100 μm to 200 μm, there was still a sufficient distribution of apertures in the 50 μm to 150 μm range for the flow system to respond in a similar manner.

The results of other simulations not presented here also indicated that other fracture parameters, namely the aperture variance, spatial correlation length and the Brooks-Corey λ parameter, had little influence on flow system response. In fact, simulations using a uniform parallel plate model (not shown) had nearly identical vertical water fluxes compared to the Base Case. This suggests that aperture variability is not a significant control and could potentially be neglected in larger scale, multiple fracture simulations.

3.3 Initial and Boundary Conditions

Figure 3 demonstrates the influence of varying initial and boundary conditions on the timing and magnitude of the vertical fluxes. Antecedent moisture conditions are shown to have a significant affect (Figure 3c). Higher initial matrix and fracture saturations are an outcome of shallower water table conditions due to increased pressure heads throughout the model domain. Under these conditions (Case 3a), both the fracture and matrix reach saturation more quickly. The total vertical flux is then dominated by the fracture flux because of its much greater hydraulic conductivity. Lowering the water table (Case 3b) decreases the initial saturations, resulting in a slight lag in the system response, although the magnitude of the vertical fluxes remains similar to the Base Case.

3.4 Implications for Contaminant Migration

The results suggest that fractures have a major impact on contaminant migration. It can be seen from Figure 2 that the majority of water flowing within the fracture is comprised of infiltrating rainwater. Over the 5 day simulation period, fracture flow accounted for 53% of the water flux passing 0.5 m depth, yet it accounted for 94% of the tracer mass. Water infiltrating into the matrix displaces existing interstitial water downward. Thus, the vertical water flux through the matrix is comprised primarily of water contained in the system prior to the infiltration event. The fracture has a much smaller porosity and water infiltrating from surface quickly displaces any interstitial water. The total flux of surface applied tracer is therefore controlled by fracture flow. In field situations, this could have significant implications for the rate at which contaminants, notably colloids, are transported through fractured porous materials. For more details on water quality impacts the reader is referred to Cey et al., 2004.

4. CONCLUSIONS

Groundwater recharge dynamics were simulated by applying rainfall to the surface of a variably saturated porous matrix block containing a single variable aperture fracture. Simulations indicated that the vertical water flux through the system was complex due to a high degree of fracture-matrix interaction and the non-linear relationship between pressure, saturation, and relative hydraulic conductivity. Mass transfer of water from the fracture into the matrix limited the advance of the wetting front in the fracture. Significant fracture flow began only after near saturated conditions were generated within the matrix, diminishing the influence of matrix imbibition. However, once initiated, the vertical water flux through the fracture significantly exceeded the flux through the matrix.

The response of the flow system was highly sensitive to matrix properties. Vertical water flux at 0.5 m depth switched from entirely fracture dominated flow to entirely matrix dominated flow when matrix K_{sat} was increased by two orders of magnitude. Considering the heterogeneous hydraulic conductivity distribution of most geologic deposits, one might expect substantial variability in fracture flow observations in the field. Antecedent moisture conditions also had a considerable impact on both the timing and magnitude of water fluxes through the system.

Fracture properties had a comparatively minor influence on flow system dynamics. As in other studies (Mendoza, 1992; Steele and Lerner, 2001), the mean fracture aperture had the greatest influence on fracture hydraulic properties. A range of apertures between 50 μm and 150 μm appeared to contribute the majority of the fracture flux. Thus, the influence of varying the mean aperture was relatively minor as long as an interconnected network of fractures within this range was present. Exchange of water between the fracture and the matrix during infiltration reduced the influence of aperture variability and other parameters related to small-scale fracture roughness (i.e., λ). This result implies that fracture aperture variability could possibly be neglected in larger-scale models of groundwater recharge. Since information on fracture geometry at field scales is extremely difficult to obtain or verify, this would be highly advantageous.

In all simulations, transport of a surface applied tracer was controlled by flux through the fracture. This could have serious implications for migration of surface applied solutes, such as agricultural fertilizers and chemicals. The influence of fractures is expected to be even more important for the transport of colloids, such as bacteria and viruses, which are less prone to matrix diffusion.

5. ACKNOWLEDGEMENTS

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