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INVESTIGATION OF EPISODIC FLOW EVENTS FROM UNSATURATED SAND MEDIA INTO MACROPORES

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ABSTRACT

Episodic or intermittent flow has been observed under a number of scenarios in unsaturated flow systems under constant influx boundary conditions. Flow systems characterized by a sand media underlain by a macropore, as well as discrete fracture networks, have been cited in recent literature as examples of systems that can exhibit episodic outflow behavior. Episodic outflow events are significant because relatively large volumes of water can move rapidly through an unsaturated system, carrying water and possibly contaminants to depth greatly ahead of a diffusive wetting front. In this study, we examine the modeled behavior of water flow through a sand column underlain by a vertical capillary tube in order to assess to potential for rapid vertical water movement, and compare the results to conventional modeling approaches and with experimental data from the literature. Capillary pressure relationships were developed for the macropore domain that capture the complex interrelationships between the sand materials above and control the flow out of the system. Modeling results using the new relative permeability and capillary pressure functions capture the behavior observed in laboratory experiments remarkably well. while simulations using conventional relative permeability and capillary pressure functions fail to capture some of the observed flow dynamics.

INTRODUCTION

Episodic, intermittent, or pulsating flow behavior in the vadose zone has been receiving considerable attention in the recent literature. This flow behavior can be caused by wetting front instability, the build up and release of fluid caused by the competition between capillary and gravitational forces (Wood et al., 2005), or small changes in boundary conditions (e.g. pressure or temperature [Glass et al., 2003]), and has been observed to occur under both constant head and constant flux boundary conditions (Podgorney at al., 2000). Recent examples of this behavior occurring in single fractures (Ghezzehei and Or, 2005; Su et al., 1999), fracture networks (Glass et al., 2003; Wood et al., 2004; Glass et al., 2002), mixed sand/macropore systems (Tofteng et al., 2002), and has been inferred from field scale observations (Faybishenko et al., 2000; Faybishenko et al., 2001) suggests that this behavior may pose a significant control on the downward migration of fluids in fractured or otherwise strongly heterogeneous vadose zones.

Fractured rocks constitute a significant portion of the vadose zone at many contaminated and potential waste repository sites, making flow processes that may lead to rapid downward migration of fluid and contaminants, particularly important to capture in conceptual and numerical models.

In this paper, we examine the potential for rapid downward migration of fluids in a strongly heterogeneous flow system consisting of a sand medium underlain by a macropore using TOUGH2 (Pruess at al., 1999). In order to carry out the evaluation, capillary pressure relationships were developed that coupled the sand domain with the underlying macropore, such that the capillary suction in the macropore is not a function of the moisture content but is related to the flux rate of the water entering the domain and the macropore length. For purposes of this discussion, a macropore is any conduit for rapid vertical fluid flow (e.g., a fracture in competent rocks or a worm burrow or root channel in unconsolidated materials). In our simulations, the macropore was conceptualized as a capillary tube. We tested our capillary pressure relationships by comparing results of simulations with experimental data taken from the literature.

Laboratory Experiments

In a set of laboratory experiments, Tofteng et al. (2002) demonstrated episodic flow between a 20-cm diameter sand column overlying a capillary tube.

The laboratory setup consisted of a peristaltic pump providing water at various constant rates to the top of the sand column, a number of tensiometers embedded within the sand, and a scale to track the outflow from the experiments. The experimental setup is shown on Figure 1.



Figure 1. Experimental setup used for collection of episodic flow datasets, from Tofteng et al. (2002).

A number of experiments were conducted using 50 cm long capillary tubes of 3, 4, and 6 mm diameters and influx rates of 1.2, 2.2, 12, and 18.5 mm/hr, with the majority of the experiments using the 3 and 4 mm capillary tubes exhibiting episodic outflow (Figure 2). Data from a 3 mm experiment were used to test the numerical formulation developed for capillary pressure relationships implemented in TOUGH.



Figure 2. Experimental data from a sand column overlying a 3 mm macropore demonstrating episodic flow behavior, modified from Tofteng et al. (2002).

METHODS

In order to examine to the dynamics observed in the laboratory experiments with a numerical model, we first simulated the experiment using a conventional approach, analogous to a capillary barrier. The macropore domain was simulated as a high permeability sand media, using a permeability value calculated with the Hagen-Poiseuille law (Bird et al., 1960). The van Genuchten (1980) model was used for relative permeability and capillary pressure functions. Values used for the relative permeability and capillary pressure functions were consistent with those determined experimentally for natural fractures (Reitsma and Kueper, 1994). Parameters for the sand were taken directly from Tofteng et al. (2002) or were calculated from information presented by the authors. This simulation serves as a comparison case for the macropore simulations performed using our function for the macropore capillary pressure. For convenience in the discussion that follows, the comparison simulations will be referred to as VG simulations while the simulations using our capillary pressure functions will be referred to as MP simulations.

For the MP simulations, the properties for the sand were identical to those used for the VG simulations described above. The macropore domain was treated in a semi-analytical fashion, with all flow leaving the sand domain entering a boundary element whose relative permeability was envisioned as a step function controlled by the capillary pressure in the sand domain. The relative permeability can be considered to be 0 until the matrix was sufficiently saturated to overcome the air entry pressure of the macropore, at which time the relative permeability changes to 1 allowing flow from the sand domain. For the MP simulations, this change was implemented manually.

The capillary pressure of the initially dry macropore was calculated from Laplace's equation (Selker et al., 1999) and the radius of the capillary tube used in the experiment. Once flow was initiated into the macropore domain, the capillary pressure of the macropore/capillary tube was adjusted by tracking the cumulative flux entering the macropore and calculating the equivalent length of a water filled column in the capillary tube. In this way, the moisture content of the macropore was also conceptualized as a step function, similar to that of the relative permeability. The macropore was at full saturation behind the wetting front and completely dry in advance of the wetting front. The length of the saturated macropore is equated to the pressure of a hanging water column of that equivalent length, which is then added to the initial capillary pressure value in the macropore domain. Thus, the capillary

pressure in the macropore is related to the flow leaving the sand domain and the radius of the capillary tube, and not to the moisture content within the macropore domain itself. The maximum capillary pressure allowed in the macropore domain was controlled by specifying the length of the capillary tube used in the experiments. For the 3 mm capillary tube the minimum capillary pressure was approximately -5000 Pa.

Table 1 summarizes a number of the initial material properties used in the simulations.

 Table 1. Selected material properties used in the macropore simulations.

Data Type	Sand	Macropore.
Permeability (m ²)	2.0 X 10 ⁻¹¹	2.8 X 10 ⁻⁷
Air Entry Pressure (Pa)	2942	97
Porosity (-)	.42	.95

RESULTS AND DISCUSSION

The results of the simulations showed some marked differences between the VG case and the MP simulations. In general, the MP simulation was in general agreement with the laboratory data with only minor modifications to the sand domain permeability values, which were increased in the horizontal directions by approximately one order of magnitude. All other parameters were unchanged in the simulations. The VG simulation was re-run using the updated permeability field from the macropore simulations to ensure consistency between the simulations.

In the sections that follow, a comparison of the time for macropore flow to begin, as well as the capillary pressures in the sand domain, will be made. The macropore capillary pressures will be presented for the time period after flow was initiated. The velocity of the flow in the macropore will also be discussed.

It should be noted that no attempts were made to refine and calibrate the VG simulation to the experimental data, as the VG simulation was strictly for comparison purposes.

Time to Flow Initiation

Figure 3 shows the simulated cumulative flux into the macropore domain for both the MP and the VG simulations. As one can see on the figure, flow began to enter the macropore domain much earlier in the VG simulation (\sim 1.2 10³ sec) than in the MP simulation (2.18 X 10⁴ sec). In both cases, the cumulative flux of approximately 0.5 liters was similar, with the MP simulation discharging slightly more water. The total simulation time was approximately 2.2 X 10⁴ seconds.



Figure 3. Comparison of the capillary barrier type (VG) and the macropore (MP) simulation cumulative outflux results.

Figure 4 compares the capillary pressure at the bottom of the matrix domain 2.5-cm away from the connection to the macropore element. Both simulations started with initial conditions of a gravity-capillary equilibrated moisture content of 10% and an influx rate of 12.0 mm/hr, uniformly distributed over the entire top of the domain. The wetting front arrived at the bottom slightly sooner in the MP simulation, but both simulation cases returned a similar trend through early and mid simulation times. As the simulations progressed past approximately 1.5×10^4 seconds, the capillary pressure in the MP simulation begins to increase above the capillary pressure in the VG simulation, until a value exceeding the air entry pressure in the macropore domain is reached at 2.18×10^4 seconds, and flow is then allowed to exit the sand domain. In contrast, the capillary pressure in the VG simulation stays relatively constant past 1.5 X 10⁴ seconds, indicating a small continuous flux out the bottom of the sand domain.



Figure 4. Matrix capillary pressure comparison of the capillary barrier type (VG) and the macropore (MP) simulations. Pressure is presented for a location 2.5 cm away from the macropore location at the bottom of the sand domain.

<u>Capillary Pressure Relationships and Flow</u> <u>Velocities</u>

Comparisons of the capillary pressure behavior and flow velocities in the macropores in the two simulation cases during the period of active flow to the macropore (Figures 5 and 6, respectively) clearly demonstrate the differences between the two approaches. Figure 4 presents the capillary pressure and flow velocity for 1.0×10^4 seconds of drainage into the macropore for the VG simulation (actual total simulation times are 1.2×10^4 to 2.2×10^4 seconds). As can be seen on the figure, both the velocity and capillary pressure vary in a smooth fashion, exhibiting an increasing trend with time.



Figure 5. Macropore capillary pressures and flow velocity in the VG simulation.

In the MP simulation (Figure 6), the capillary pressure rapidly decreases as flow enters the macropore. As the macropore fills with water, the capillary pressure drops from -97 Pa at flow initiation to ~-5000 Pa when flow reaches the bottom of the macropore. The time to fill the macropore and reduce the capillary pressure is approximately 2 seconds. After this time, the capillary pressure is maintained at ~-5000 Pa for the remainder of the drainage period. The flow velocity in the macropore reaches a maximum of approximately 0.75 m/s when the capillary pressure first reaches it minimum value, and then decreases as the matrix above drains out and the hydraulic gradient lessens. Shown on Figure 5 is the first 10 seconds of drainage in to the macropore (actual total simulation time presented begins at 2.18 $X \ 10^4$ seconds). A total of only 210 seconds were required to drain out an equivalent amount of water that drained in 1 X 10^4 seconds in the VG simulations.



Figure 6. Macropore capillary pressures and flow velocity in the MP simulation.

<u>Cumulative Flux Comparisons</u>

The simulated outflow in the MP simulation captured the experimental outflow behavior quite well, as shown on Figure 7. The cumulative flux from one episodic outflow event in the laboratory experiment totaled approximately 0.46 liters in 210 seconds, at which time flow stopped. The simulated outflux captured the overall behavior of the experimental data, while not exactly matching the shape of the experimental curve. In the MP simulation, the outflux continued past the time the flow in the experiment ceased. The saturation in the sand above the macropore remained relatively high, and the capillary pressure did not decrease to the air entry pressure of the sand, the point we originally deemed would be the point of flow cessation.

Results from the VG simulation are also shown on Figure 7. As the flux exiting over a much larger time interval in the simulation, the cumulative flux from was only on the order of 6×10^{-4} liters in the 250 seconds plotted on Figure 6.



Figure 7. Comparison of the experimentally measured outflux and the outflux simulated with the VG and MP models.

CONCLUSIONS

A capillary pressure relationship was developed for flow from a sand media overlying a macropore, represented as a capillary tube. The capillary pressure relationship was coded into the TOUGH2 simulation code (Pruess et al., 1999) and tested against experimental data and compared to simulation results obtained using the van Genuchten (1990) capillary pressure relationship.

Simulations using the macropore capillary pressure function matched the experimental data quite well, and were in general agreement for both flux and capillary pressures. Of particular importance is the time for the flux to exit the sand media into the macropore. In the MP simulations, this time was on the order of 200 seconds, while the VG simulations required nearly 1×10^4 seconds to discharge the same volume of water.

The velocity of the water moving through the macropore domain reached a maximum of nearly 0.7 m/s in the MP simulation, a value several of orders of magnitude higher than that calculated for the VG simulation. The rapid downward movement of water in the MP simulation better represents the experimental data, and provides an improved methodology to describe and predict wetting front advance in the vadose zone. The MP simulation, in the described case study, predicted the arrival of the wetting front more rapidly than current model predictions.

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