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MODELING SMALL-SCALE PHYSICAL NON-EQUILIBRIUM AND LARGE-SCALE PREFERENTIAL FLUID AND SOLUTE TRANSPORT IN A STRUCTURED SOIL

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The deviation of non-reactive solute transport from that predicted by classical convection-dispersion equations is usually attributed to physical non-equilibrium caused by small- and large-scale pore structures in porous media. Diffusion of fluid and solute into micropores or rock matrix may occur locally, while fluid and solutes can also be channeled preferentially through interconnected macropores or fractures. A multiple-pore-region (MPR) approach with local advective-diffusive mass exchange is adopted to simulate soil column tracer breakthrough and field-scale tracer releases in the Melton Branch Subsurface Transport Facility within the Oak Ridge Reservation, Tennessee. The soil column simulation indicates that both inter-region mass exchange and intra-region convection-dispersion contribute to small-scale solute transport in approximately the same order of magnitude. The field-scale study suggests that advective mass exchange has minor effect on subsurface hydrographs, and that large diffusive mass exchange may retain tracers near the source area. Comparison of modeling results and field data suggests that subsurface bedding planes on the field site may be the cause of large-scale heterogeneity and preferential mass transport.

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INTRODUCTION

A MPR conceptual model is composed of flow regions with different hydraulic parameters that result in discernible velocity fields exchanging fluid and solute with other flow regions. Intra-region and inter-region mass transfer are conceptualized as two separate but intermingled processes that govern the transport of mass within a flow region and across flow regions, respectively. As illustrated in Figure 1 for a three-pore-region case, each flow tube consists of a flow region, while mass exchange of various rates exists between every two flow tubes. Fluid and solute may stay in the same flow tube or detour through other flow tubes while they move to a downstream area.

Figure 1. A three-pore-region mass transfer mechanism. Increased shading indicates an increase in solute concentration and position of the concentration front. Arrows indicate mass exchange among pore regions.

Sensitivity analysis on advective and diffusive exchange is conducted to investigate the effect of mass exchange on fluid and solute transport in a macropore-mesopore-micropore soil. The Melton Branch site, which has been a study site for subsurface storm flow dynamics since the 1980's, is used to demonstrate the application of a three-dimensional multi-region flow and solute transport model. Through the aforementioned two studies, we intend to gain insight on the effect of small-scale and large-scale heterogeneities on the movement of fluid and solute under transient flow and solute transport conditions in variably-saturated soils.

MATHEMATICAL MODELS

Under the concept of overlapped continua, one can apply volume-average procedures to each of the continua or pore regions in a porous medium. The following equation is

obtained after the empirical Darcy's law is adopted to represent the intra-region isothermal fluid flow processes (Gwo, 1992).

$$F_{\alpha} \frac{\partial h_{\alpha}}{\partial t} = \nabla \cdot \mathbf{K}_{\alpha} \nabla (h_{\alpha} + z) + \theta_{\alpha} q_{\alpha} - \sum_{\substack{j=1 \\ j \neq \alpha}}^n \varepsilon_{\alpha j}^f (h_{\alpha} - h_j), \quad \alpha = 1, 2, \dots, n \quad (1)$$

where, for pore region α , F_{α} is storage coefficient, h_{α} is fluid pressure head, z is elevation head, $\mathbf{K}_{\alpha}$ is hydraulic conductivity tensor, t is time, θ_{α} is water content, q_{α} is external source or sink flow rate, and $\varepsilon_{\alpha j}^f$ is an empirical advective exchange coefficient.

The solute transport equations for the pore regions can be similarly derived, and they are (Gwo, 1992):

$$\begin{aligned} \theta_{\alpha} \frac{\partial c_{\alpha}}{\partial t} + \rho_{b\alpha} \frac{\partial s_{\alpha}}{\partial t} + \theta_{\alpha} \mathbf{v}_{\alpha} \cdot \nabla c_{\alpha} = \nabla \cdot (\theta_{\alpha} \mathbf{D}_{\alpha} \cdot \nabla c_{\alpha}) + \theta_{\alpha} q_{\alpha} c_{q\alpha}^* - \theta_{\alpha} q_{\alpha} c_{\alpha} \\ - \sum_{\substack{j=1 \\ j \neq \alpha}}^n \varepsilon_{\alpha j}^f (h_{\alpha} - h_j) c_{\varepsilon}^* - \sum_{\substack{j=1 \\ j \neq \alpha}}^n \varepsilon_{\alpha j}^i (c_{\alpha} - c_j) + \sum_{\substack{j=1 \\ j \neq \alpha}}^n \varepsilon_{\alpha j}^f (h_{\alpha} - h_j) c_{\varepsilon}, \quad \alpha = 1, 2, \dots, n \end{aligned} \quad (2)$$

where, for pore region α , $\mathbf{D}_{\alpha}$ is dispersion coefficient tensor, c_{α} is solute concentration, $\mathbf{v}_{\alpha}$ is velocity, $c_{q\alpha}^*$ is the solute concentration of the incoming fluid if injecting and $c_{q\alpha}^* = c_{\alpha}$ if withdrawing, $\rho_{b\alpha}$ is bulk density of the soil, $\varepsilon_{\alpha j}^i$ is an empirical diffusive exchange coefficient, $c_{\varepsilon}^* = c_{\alpha}$ if $h_{\alpha} > h_j$, $c_{\varepsilon}^* = c_j$ if $h_{\alpha} < h_j$, and s_{α} is concentration in the sorbed phase.

Other formulations of mass exchange (e.g., Dykhuizen, 1990; and Zimmerman et al., 1993) can also be adopted to the fluid and solute exchange terms in equations (1) and (2). Equation (1) is solved using a Galerkin finite element method and has been implemented as computer codes MURF and 3DMURF. A hybrid Lagrangian-Eulerian finite element method is used to solve the solute transport equation (2) and the corresponding computer codes are MURT and 3DMURT. These computer codes have been verified (Gwo, 1992) using a fractured porous media model and a mobile-immobile model, respectively.

PARAMETER DETERMINATION

To obtain three sets of hydraulic conductivity and water retention relations for a three-pore-region soil, we divide pore regions, at -10 cm and -250 cm pressure heads, according to the classification scheme proposed by Luxmoore (1981). Both Fermi function and the van Genuchten equation (van Genuchten, 1980) are used for the $\theta(h)$

relation (Wilson et al., 1992). The following Fermi function is used to represent the water retention relation in macropores:

$$\theta_a = \frac{\theta_{sa} - \theta_{sr}}{1 + \exp[-\gamma_a (h_a - h_{\theta a})]} \quad (3)$$

where θ_a is the water content in macropores, θ_{sa} and θ_{sr} are the saturated and residual water contents of macropores, respectively, γ_a and $h_{\theta a}$ are function parameters, and h_a is the pressure head in macropores. For mesopores and micropores, the following van Genuchten equation is used:

$$\theta_\alpha = \frac{\theta_{s\alpha} - \theta_{r\alpha}}{[1 + (-\beta_\alpha h_\alpha)^{n_\alpha}]^{m_\alpha}} \quad (4)$$

where, for pore region α , θ_α is water content, $\theta_{s\alpha}$ and $\theta_{r\alpha}$ are saturated and residual water contents, h_α is pressure head, β_α , n_α , and $m_\alpha = 1 - 1/n_\alpha$ are equation parameters. The hydraulic conductivity relation used in this study, for all of the pore regions, is also a Fermi function:

$$\text{Log}_{10}(K_{a\alpha} / K_{s\alpha}) = \frac{\xi_\alpha}{1 + \exp[-\kappa_\alpha (h_\alpha - h_{k\alpha})]} - \xi_\alpha \quad (5)$$

where for region α , $K_{a\alpha}$ and $K_{s\alpha}$ are absolute and saturated hydraulic conductivities, respectively, and ξ_α , κ_α , and $h_{k\alpha}$ are function parameters.

SENSITIVITY ANALYSES ON ADVECTIVE AND DIFFUSIVE EXCHANGE

In order to understand the effect of microscopic mass exchange processes on subsurface mass transport, we conduct a sensitivity analysis on advective and diffusive exchange coefficients. The fluid flow model MURF is used to study the transient variably-saturated flow fields of a vertical soil column. The flow fields, then, are imported into the solute transport model MURT for the computation of pore-region concentration fields. A total recharge rate of 9 cm³/hr/m² is applied to the soil column at the beginning of simulations, and is terminated 5 hours later. A non-reactive tracer of relative concentration 1 is also injected at the beginning of the simulations and is terminated 2 hours later. The simulations are stopped at time = 10 hr. The advective exchange coefficients are varied by 5 orders of magnitude, and the diffusive exchange coefficients are varied by 7 orders of magnitude. The other model parameters are obtained from soil samples and a soil column collected at the Melton Branch site (Wilson et al., 1992a; Jardine et al., 1993).

The times required to balance pore-region pressure and concentration fields are inversely related to advective and diffusive exchange coefficients, respectively. However, no apparent relation between advective exchange coefficients and the

equilibration of concentration fields has been observed. The contributions to the increase/decrease of fluid and solute mass in macropores and mesopores by intra-region advection-dispersion and inter-region advective and diffusive exchange are in the same orders of magnitude (Figure 2), while in micropores the major contribution to mass change rates is the advective and diffusive mass exchange. Because of the high flow rates in macropores and mesopores and the large porosity in micropores, these results indicate that bypassing flow is very likely to occur in the soil during moderate to high infiltration rates and that not only diffusive but also advective exchange needs to be incorporated into a fluid and solute transport model if the micropores of a soil are to be considered as an immobile pore region without an associated velocity field.

APPLICATION TO A FORESTED WATERSHED

The Melton Branch subwatershed is underlain by Conasauga shale interbedded with Maryville Limestone formation. The strata of the Conasauga group weathers to a shallow ($< 1\text{ m}$) soil, which overlies saprolite that retains the bedding and structure of the parent materials. A 2 m deep by 16 m long trench was excavated across the outflow region of the subwatershed to collect subsurface drainage. Two H-flumes equipped with Manning ultrasonic level recorders were positioned in the trench to give integrated flow rates of the soil horizons and a surface runoff collector (Wilson et al., 1992b). A buried line source of length 6 m at the depth of 0.5 m is located at the top of the eastern hillslope. In the numerical model, the subwatershed is divided into 10,500 elements and 12,090 nodes. Since each node consists of three pore regions, this requires the solving of 36,270 coupled equations simultaneously. Two series of rain storms in 1991, from February 13 to 20, are used as input to the system. The rain storms during February 13 to 14 (25 mm) lasted for 20 hours and those during February 17 to 20 (145 mm) lasted for 66 hours. The subsurface hydrograph of the former storm events is used to calibrate the model. Parameters thus obtained are used to predict the subsurface hydrograph for the latter storm events. A tracer release of 8000 mg Br/L (as MgBr_2) at a rate of $0.194\text{ m}^3/\text{h}$ was initiated on February 18 at 0950 (relative time 119 hours) over a 16.5 hour period through the buried line source near the ridge top (Wilson et al., 1992b).

For the calibration study using the rain storm events during Feb. 13-14, the peak arrival times of the simulated and measured hydrographs are in good agreement (not shown). The total outflow obtained from the simulated and measured hydrographs are also approximately the same. For the storm events during Feb. 17-20, the predicted peak arrival times agree well with those measured (Figure 3), but the predicted total flow is about 60% of the measured. Scenario studies with different advective exchange coefficients suggest that pore-scale mass exchange has little effect on subsurface hydrographs in field-scale problems. These results and the low fluid storage of the

(a) diffusive exchange and advection-dispersion

(b) advective exchange and advection-dispersion

Figure 2. Effect of mass exchange on pore-region solute mass accumulations: (a) diffusive exchange, and (b) advective exchange. The contributions of inter-region and intra-region mass transfer (ME = mass exchange, AD = advection-dispersion) in macropores and mesopores are approximately in the same order of magnitude, while in micropores inter-region mass transfer dominates.

storm flow zone suggest that large-scale heterogeneities, i.e., subsurface bedding planes that dip perpendicular to the topography, may be responsible for the differences between the predicted and measured subsurface hydrographs.

Figure 3. The calculated and measured subsurface hydrographs for the storm events during Feb. 17-20.

The peak concentrations of the predicted BTC for the C horizon (Figure 4) are about two times of those measured. The flowpath obtained during the flow simulations appears to follow the topography of the site (not shown), and the length of the flowpath is about half of the true flowpath that dips southwards along a subsurface bedding plane until it reaches the convergent zone. This large-scale feature has not yet been implemented into the numerical model.

Because hydrodynamic dispersion reaches beyond the locale of interest for storage of solutes and diffusive exchange utilizes local storage available in the micropores, high dispersivities may result in field-scale distribution of solutes, but high diffusive exchange tends to restrict solutes from moving far away from the source area. Scenario studies with various diffusive exchange coefficients suggest that micropore storage is utilized to restrain Br from moving further downstream in high diffusive exchange cases. This observation is in contrast to macroscopic dispersion that extends the area covered by the solute plume in low diffusive exchange cases.

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Figure 4. The calculated and measured Br BTCs through C horizon. The subsurface flow rate in the soil horizon is also shown.

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