Models to Simulate Preferential/Nonequilibrium Flow and Transport in Vadose Zone.

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Summary

We present a new version of the HYDRUS codes that include various approaches for modeling preferential and nonequilibrium flow and transport in the vadose zone. Existing approaches differ in terms of their underlying assumptions and complexity. They range from relatively simplistic models to more complex physically based dual-porosity and dual-permeability type models. A relatively simple dual-porosity flow model results when the Richards equation is combined with composite equations for the hydraulic properties to account for both soil textural and soil structural effects on flow. The simplest nonequilibrium flow model, a single-porosity model, which distinguishes between actual and equilibrium water contents, is based on a formulation by Ross and Smettem (2000) that requires only one additional parameter to account for nonequilibrium. A more complex dual-porosity, mobile-immobile water flow model results when the Richards or kinematic wave equations are used for flow in the fractures, and immobile water is assumed to exist in the matrix. We also discuss various dual-permeability models, including the formulation of Gerke and van Genuchten (1993a) and the kinematic wave approach as used in the MACRO model of Jarvis (1994). These models differ mainly in the description of the flow in the macropores. Several examples and comparisons of equilibrium and various nonequilibrium flow and transport models are also provided.

A. Equilibrium Flow and Transport Models

Richards equation for variably-saturated water flow and the convection-dispersion equation for solute transport, i.e.:

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right]-S$$

$$\frac{\partial\theta c}{\partial t}+\frac{\partial\rho s}{\partial t}=\frac{\partial}{\partial z}\left(\theta D\frac{\partial c}{\partial z}\right)-\frac{\partial qc}{\partial z}-\mu(\theta c+\rho s)+\gamma(\theta+\rho)$$

Composite Retention and Hydraulic Conductivity Functions:

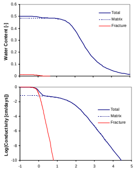
Durner et al. (1999)

$$S_e(h)=\frac{\theta(h)-\theta_r}{\theta_s-\theta_r}=\sum_{i=1}^{k}w_i\frac{1}{\left(1+|\alpha_i h|^{n_i}\right)^{m_i}}$$

$$K(\theta)=K_s\left(\sum_{i=1}^{k}w_i S_{e_i}\right)^{l}\frac{\left(\sum_{i=1}^{k}w_i\alpha_i\left[1-\left(1-S_{e_i}^{1/m_i}\right)^{m_i}\right]\right)^2}{\left(\sum_{i=1}^{k}w_i\alpha_i\right)^2}$$

Mohanty et al. (1997)

$$K(h)=K^*+K^*\left[e^{(h-h^*)\delta}-1\right]\qquad h^*<h\le 0$$



Composite models improve predictions of accelerated flow for conditions close to saturation

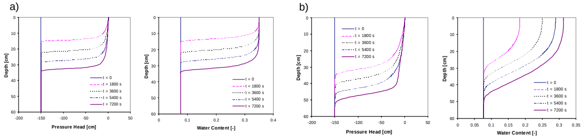
B. Nonequilibrium Flow and Transport Models

1. Single-Porosity Models

Ross and Smettem (2000): τ - an equilibration time constant

$$\frac{\partial\theta}{\partial t}=f(\theta,\theta_e)=\frac{\theta_e-\theta}{\tau}$$

$$\theta^{j+1}=\theta^{j}+\left(\theta_e^{j+1}-\theta^{j}\right)\left[1-\exp\left(-\Delta t/\tau\right)\right]$$



Pressure head and water content profiles calculated with the a) equilibrium and b) nonequilibrium (Ross and Smettem, 2000) water flow models.

B. Nonequilibrium Flow and Transport Models (cont.)

2. Dual-Porosity Models:

$$\theta=\theta_f+\theta_m$$

a) Richards equation based:

Γ_w - transfer rate for water from inter- to intra-aggregate pores

$$\frac{\partial\theta_f}{\partial t}=\frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right]-S_f-\Gamma_w$$

$$\frac{\partial\theta_m}{\partial t}=-S_m+\Gamma_w$$

b) Kinematic equation based:

r - macropore sorbance
q - volumetric flux density
C - kinematic wave velocity

$$\frac{\partial q}{\partial t}+C\frac{\partial q}{\partial z}+cr\theta_f=0$$

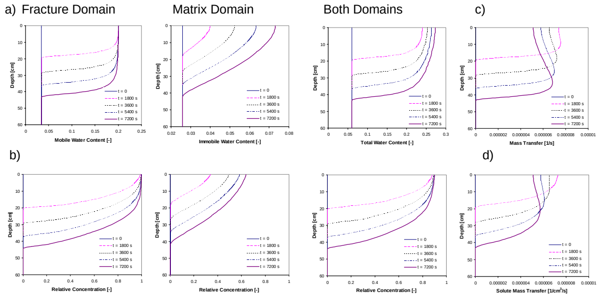
$$q=b\theta_f^a$$

$$C=\frac{\partial q}{\partial\theta_f}$$

Solute transport:

$$\frac{\partial\theta_f c_f}{\partial t}+\frac{\partial f\rho s_f}{\partial t}=\frac{\partial}{\partial z}\left(\theta_f D_f\frac{\partial c_f}{\partial z}\right)-\frac{\partial qc_f}{\partial z}-\phi_f-\Gamma_s$$

$$\frac{\partial\theta_m c_m}{\partial t}+\frac{\partial(1-f)\rho s_m}{\partial t}=-\phi_m+\Gamma_s$$



Water content (a) and concentration (b) profiles in the fracture domain, matrix domain, and both domains combined, as well as water (c) and solute (d) mass transfer terms calculated with the dual-porosity model.

3. Dual-Permeability Models:

a) Richards equation based:

Gerke and van Genuchten (1993a)

$$\frac{\partial\theta_f}{\partial t}=\frac{\partial}{\partial z}\left(K_f\frac{\partial h_f}{\partial z}+K_f\right)-S_f-\frac{\Gamma_w}{w}$$

$$\frac{\partial\theta_m}{\partial t}=\frac{\partial}{\partial z}\left(K_m\frac{\partial h_m}{\partial z}+K_m\right)-S_m+\frac{\Gamma_w}{1-w}$$

b) Kinematic equation based

Jarvis (1994): MACRO

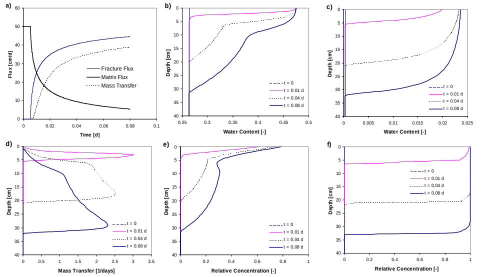
$$q=b\left(\frac{\theta_f}{\theta_{sf}}\right)^a=b\left(S_e^f\right)^a$$

Solute transport:

$$\frac{\partial\theta_f c_f}{\partial t}+\frac{\partial f\rho s_f}{\partial t}=\frac{\partial}{\partial z}\left(\theta_f D_f\frac{\partial c_f}{\partial z}\right)-\frac{\partial qc_f}{\partial z}-\phi_f-\frac{\Gamma_s}{w}$$

$$\frac{\partial\theta_m c_m}{\partial t}+\frac{\partial(1-f)\rho s_m}{\partial t}=\frac{\partial}{\partial z}\left(\theta_m D_m\frac{\partial c_m}{\partial z}\right)-\frac{\partial qc_m}{\partial z}-\phi_m-\frac{\Gamma_s}{1-w}$$

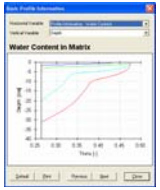
3. Dual-Permeability Models (Cont.):



Infiltration and mass exchange fluxes (a), water contents in the matrix (b) and fracture (c) domains, water mass exchange rates (d) and concentrations in the matrix (e) and fracture (f) domains calculated with the dual-permeability model of Gerke and van Genuchten (1993).

Implementation in HYDRUS:

versions 3



Applications:

a) Analyses of solute transport column studies (steady-state or transient water flow):

1. Equilibrium Solute Transport Model in the Two Pore Regions
2. Mobile-Immobile Nonequilibrium Solute Transport Model in the Two Pore Regions
   (Mobile and immobile water in the matrix, mobile water in the fracture)
3. Two-Site Sorption Nonequilibrium Solute Transport Model in the Two Pore Regions
   (Kinetic and equilibrium sorption in two mobile regions, or in mobile and immobile regions)

b) Analyses of transient water flow and solute transport studies involving nonequilibrium/preferential flow or transport

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