One-dimensional Coupled Modeling of Unsaturated Water, Heat, and Solute Transport in Layered Soil

Juyoul Kim, Byungchul Lee, and Thomas C. Harmon*

FNC Technology Co. Main Bldg. 516, SNU Research Park, San4-2, Bongcheon7-dong, Gwanak-gu, Seoul

*School of Engineering, University of California, Merced, P.O. Box 2039, Merced, CA 95344

gracemi@fnctech.com

Coupled modeling of unsaturated water, heat, and solute transport in multi-layered soil is important to understand the long-term safety performance of engineered cover system for the planned near surface disposal of Low- and intermediate-level waste (LILW). In the present paper, one-dimensional infiltration in unsaturated layered soil is numerically modeled and verified with analytic solutions using Richards' equation for water flow, advection-dispersion equation (ADE) for solute transport, and simultaneous conductive and advective equation for heat transport.

Variably-saturated water flow in porous media is usually described using the Richards' equation. The one-dimensional, vertical flow equation can be written as

$$\frac{\partial\theta(z,t)}{\partial t}=\frac{\partial}{\partial z}\left(k(\theta,z)\frac{\partial h(\theta,z)}{\partial z}-k(\theta,z)\right)-S(h) \qquad (1)$$

where θ is volumetric moisture content (cm^3/cm^3), z is vertical coordinate assuming positive downward (cm), t is time (hr), $k(\theta,z)$ is unsaturated hydraulic conductivity (cm/hr), $h(\theta,z)$ is soil water matric pressure head (cm), and $S(h)$ is the root water extraction (cm^3/cm^3/hr). The Richards equation can be solved numerically when the initial and boundary conditions are prescribed and two constitutive relations, i.e., the unsaturated hydraulic conductivity curve, $k=k(h)$, and the soil water retention curve, $\theta=\theta(h)$ are specified. The soil hydraulic function $k(h)$ and $\theta(h)$ are described by the Mualem-van Genuchten model:

$$k(h)=k_s\,Se^{\lambda}[1-(1-Se^{1/m})^m]^2 \qquad (2)$$

$$Se(h)=\frac{\theta(h)-\theta_r}{\theta_s-\theta_r}=\frac{1}{(1+|\alpha h|^n)^m} \qquad (3)$$

where θ_s and θ_r are the saturated and residual volumetric water contents, respectively. Se is effective saturation, k_s is saturated hydraulic conductivity, and λ (-), α (cm^{-1}), n and $m(=1-1/n)$ are fitting parameters.

The transport of chemical substance in the unsaturated zone is commonly described by the general advection-dispersion equation (ADE):

$$R\frac{\partial(\theta C)}{\partial t}=\frac{\partial}{\partial z}\left[\theta D_e\frac{\partial C}{\partial z}\right]-\frac{\partial}{\partial z}(\bar{v}\theta C)-\lambda R\theta C \qquad (4)$$

where $R=1+\frac{K_d\rho_b}{\theta}$ is a retardation factor (-), K_d linear Freundlich sorption coefficient, ρ_b dry bulk density (g/cm^3), θ volumetric water content (cm^3/cm^3). C is the liquid-phase concentration of substance (mg/L), D_e is an effective combined molecular and mechanical dispersion coefficient of the substance in the pore water.

D_e is given by the relation $D_e = D_o + \varepsilon|\bar{v}|$, where D_o (cm²/hr), ε (cm), and $\bar{v}$ (cm/hr) are molecular diffusion of substance in the soil, soil dispersivity, and mean pore water velocity ($\bar{v} = q/\theta$). λ is removal rate (g/cm³/hr) of the substance associated with biodegradation and root uptake.

One-dimensional simultaneous conductive and advective heat transport equation is written as:

$$\frac{\partial(\theta C_w + (1-\phi)C_s)T}{\partial t} = \frac{\partial}{\partial z}\left[(K_T(\theta) + \theta C_w D_H(\theta))\frac{\partial T}{\partial z}\right] - C_w\frac{\partial(qT)}{\partial z} - C_w ST \quad (5)$$

where C_w is heat capacity of water (J/m³°C), C_s heat capacity of the dry solid (J/m³°C), θ volumetric water content, ϕ porosity of medium, K_T thermal conductivity of the water and solid matrix ($K_T = \theta K_w + (1-\phi)K_m$, W/m°C), D_H hydrodynamic dispersion tensor (m²/s), $q = \theta\bar{v}$ Darcian water flux (cm/s), and S energy uptake by plant roots associated with root water uptake. Using continuity equation defined by $\frac{\partial\theta}{\partial t} = -\frac{\partial q}{\partial z} - S$, Eq. (5) can be reduced as:

$$\left[\theta C_w + (1-\phi)C_s\frac{\partial T}{\partial t}\right] = \frac{\partial}{\partial z}\left[K_a(\theta)\frac{\partial T}{\partial z}\right] - C_w q\frac{\partial T}{\partial z} \quad (6)$$

where K_a is an apparent thermal conductivity coefficient which entails both the heat conduction of the medium and the dispersion by advective flow.

$$K_a(\theta) = K_T(\theta) + \theta C_w D_H = K_T(\theta) + C_w \beta_t |q| \quad (7)$$

The following figure shows an infiltration modeling in layered soil for a sand-sandy loam-sand textural structure.