

Using the HYDRUS-1D and HYDRUS-2D Codes for Estimating Unsaturated Soil Hydraulic and Solute Transport Parameters

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Abstract. In this paper we describe a parameter estimation procedure which combines the Levenberg-Marquardt nonlinear parameter optimization method involving weighted least squares with either a one-dimensional numerical model (HYDRUS-1D) or a two- or quasi three-dimensional model (HYDRUS-2D), which solve the governing equations for water flow and solute transport in variably-saturated porous media. The procedure permits several unknown parameters in the unsaturated soil-hydraulic functions to be estimated from observed water contents, pressure heads, and/or instantaneous or cumulative boundary fluxes (e.g., infiltration or outflow data) during transient water flow by numerical inversion of the Richards equation. Additional retention or hydraulic conductivity data, as well as a penalty function for constraining the optimized parameters to remain in some feasible region (Bayesian estimation) can be optionally included in the parameter estimation procedure. Similarly, the procedure permits solute transport and/or reaction parameters to be estimated from observed concentrations and/or instantaneous or cumulative boundary solute fluxes during transient solute transport by numerical inversion of the convection-dispersion equation. The unsaturated soil hydraulic and solute transport and reaction parameters can be estimated either sequentially or simultaneously. Depending upon the quality of observed data, soil hydraulic or solute transport parameters for several soil layers can be estimated simultaneously. The parameter estimation procedure is demonstrated for several laboratory and field experiments.

INTRODUCTION

As increasingly more complicated computer models are being developed for simulating subsurface flow and transport processes, the accuracy of numerical simulations largely depends upon the accuracy with which various model parameters can be estimated. Flow and transport models for the unsaturated zone are often based on numerical solutions of the Richards equation which requires knowledge of the unsaturated soil hydraulic functions, i.e., the soil water retention curve, $\theta(h)$, describing the relationship between the water content θ and the pressure head h , and the unsaturated hydraulic conductivity function, $K(h)$, defining the hydraulic conductivity K as a function of h . Accurate measurement of the hydraulic properties is difficult because of the highly nonlinear nature of these properties, especially $K(h)$, instrumental limitations, and the extreme heterogeneity of the subsurface environment. Hence, methods for making relatively fast and reliable measurements of the unsaturated soil-hydraulic properties remain sorely needed [*van Genuchten and Leij, 1992*].

A variety of field methods are currently available for direct measurement of the hydraulic conductivity, K , or the soil water diffusivity, D , as a function of h and/or θ [*Klute and Dirksen, 1986; Green et al., 1986*]. Popular field methods include the instantaneous profile method, various unit-gradient type approaches, sorptivity methods following ponded infiltration, and the crust method based on steady water flow. While relatively simple in concept, these direct measurement methods have a number of limitations that restrict their use in practice. For

example, most methods are very time-consuming to execute because of the need to adhere to relatively restrictive initial and boundary conditions. This is especially true for field gravity-drainage experiments involving medium- and fine-textured soils. Methods requiring repeated steady-state flow situations, or other equilibrium conditions are also tedious, while linearizations and other approximations or interpolations to allow analytic or semi-analytic inversions of the flow equation may introduce additional errors. Finally, information about uncertainty in the estimated hydraulic parameters is not readily obtained using direct inversion methods.

A much more flexible approach for solving the inverse problem is the use of parameter optimization methods [Hopmans and Šimčnek, 1999]. Optimization procedures make it possible to simultaneously estimate the retention and hydraulic conductivity functions from transient flow data [Kool *et al.*, 1987]. While many possible scenarios exist for the application of parameter optimization methods, numerical inversion of the Richards equation has thus far been limited only, or nearly exclusively, to one-dimensional experiments [Kool *et al.*, 1985; Russo *et al.*, 1991], mostly in conjunction with one-step or multi-step outflow experiments [Kool and Parker, 1988; van Dam *et al.*, 1992, 1994; Eching *et al.*, 1993]. Nevertheless, other types of experiments, such as upward infiltration [Hudson *et al.*, 1996] or evaporation methods [Ciollaro and Romano, 1995; Santini *et al.*, 1995; Šimčnek *et al.*, 1998d, 1999b], were also reported. Possible multi-dimensional applications involve the use of disc tension permeameters [Perroux and White, 1988; Ankeny *et al.*, 1991, Šimčnek and van Genuchten, 1996, 1997; Šimčnek *et al.*, 1998a,c], a modified cone penetrometer [Gribb *et al.*, 1998; Kodešová *et al.*, 1998, 1999; Šimčnek *et al.*, 1999a], a multistep soil-water extraction method [Inoue *et al.*, 1998, 1999], infiltration from a furrow, and surface or subsurface drip irrigation experiments.

In this paper we describe a parameter estimation procedure which combines the Levenberg-Marquardt nonlinear parameter optimization method involving weighted least squares with either a one-dimensional numerical model, HYDRUS-1D [Šimčnek *et al.*, 1998b], or a two- or quasi three-dimensional numerical model, HYDRUS-2D [Šimčnek *et al.*, 1996], which solve the variably-saturated water flow and solute transport equations. We demonstrate the proposed parameter estimation procedure on laboratory and field data, and briefly summarize many other applications of the HYDRUS models.

FORWARD PROBLEM

Variably-Saturated Water Flow

The governing equation for two-dimensional isothermal Darcian water flow in a variably-saturated rigid isotropic porous medium is given by the following modified form of the Richards equation:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i} \left[K (K_{ij}^A \frac{\partial h}{\partial x_j} + K_{i2}^A) \right] - S \quad (1)$$

where x_i ($i=1,2$; with $x_2=z$ being the vertical coordinate positive upwards) are the spatial coordinates, t is time, S is a sink term, K_{ij}^A are components of a dimensionless anisotropy tensor \mathbf{K}^A , and K is the unsaturated hydraulic conductivity function given as the product of the relative hydraulic conductivity, K_r , and the saturated hydraulic conductivity, K_s .

Equation (1) can be solved numerically for a given set of initial and boundary equations. The HYDRUS-1D and -2D codes implement three different types of boundary conditions: specified pressure head (Dirichlet type) conditions of the form

$$h(\mathbf{x}, t) = \psi(\mathbf{x}, t) \quad (2)$$

specified flux (Neumann type) conditions given by

$$-[K(K_{ij}^A \frac{\partial h}{\partial x_j} + K_{i2}^A)]n_i = \sigma(\mathbf{x}, t) \tag{3}$$

and specified gradient conditions (e.g., free drainage associated with a unit hydraulic gradient) as follows

$$(K_{ij}^A \frac{\partial h}{\partial x_j} + K_{i2}^A)n_i = \zeta(\mathbf{x}, t) \tag{4}$$

where ψ , σ , and ζ are the prescribed Dirichlet, Neumann, and gradient type boundary conditions, respectively, as functions of \mathbf{x} and t , \mathbf{x} is the spatial coordinate of a boundary, and n_i are the components of the outward unit vector normal to boundary.

The above boundary conditions can be implemented in HYDRUS-1D and -2D in several ways: as (a) constant boundary conditions (either flux or head), (b) variable boundary conditions (again either flux or head), (c) seepage faces, (d) atmospheric boundaries, and (e) free or deep drainage boundaries. Boundary classes (a) and (b) represent system-independent boundary conditions, while (c), (d), and (e) are system dependent, i.e., they depend on the prevailing transient soil moisture or flux conditions. As explained later, instantaneous or cumulative boundary fluxes across any of the boundaries, and water contents and pressure heads measured anywhere in the transport domain, can be included in the objective function for purposes of parameter identification.

While different functions for the unsaturated soil-hydraulic properties may be used in the inverse problem, the expressions adopted in HYDRUS codes are those of *van Genuchten* [1980]:

$$\theta_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = (1 + |\alpha h|^n)^{-m} \tag{5}$$

$$K(\theta) = K_s \theta_e^l [1 - (1 - \theta_e^{1/m})^m]^2 \tag{6}$$

and *Brooks and Corey* [1966]:

$$\theta_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \begin{cases} |\alpha h|^{-n} & h < -1/\alpha \\ 1 & h \geq -1/\alpha \end{cases} \tag{7}$$

$$K(\theta) = K_s \theta_e^{l+2+2/n} \tag{8}$$

where θ_e is the effective water content, θ_r and θ_s denote the residual and saturated water contents, respectively, and α , n , $m (= 1 - 1/n)$, and l are empirical parameters. The hydraulic characteristics defined by (5) through (8) contain 6 unknown parameters: θ_r , θ_s , α , n , l , and K_s . Of these, θ_r , θ_s , and K_s have a clear physical meaning, whereas α , n and l are essentially empirical parameters determining the shape of the retention and hydraulic conductivity functions [*van Genuchten*, 1980].

For the hysteretic case the HYDRUS codes use the formulation of *Kool and Parker* [1987] who coupled the van Genuchten-Mualem model with a simplified scaling approach proposed by *Scott et al.* [1983] to describe the scanning curves. *Scott et al.* [1983] assumed that the shape parameters α and n for all drying scanning curves are the same as those for the main drying curve and, similarly, the shape parameters for all wetting scanning curves are the same as those for the main wetting curve. Scanning curves are then calculated by varying the residual and saturated water contents for the wetting and drying scanning curves, respectively. *Kool and Parker* [1987] further assumed that the shape parameter n is the same for both wetting and drying, thus decreasing the number of required parameters. Using the additional restrictions that θ_r and θ_s are

the same for both drying and wetting, the only additional parameter describing hysteresis is a third shape parameter α_d for the drying retention curve (we use α_w for wetting).

Equation (1) subject to initial and boundary conditions (2), (3) and (4) was solved numerically by means of the finite element method. The solution scheme was based on the mass-conservative numerical iterative scheme used by *Celia et al.* [1990]. A simple modification of this numerical scheme also permits similar mass-conservative solutions of quasi-three-dimensional axisymmetrical flow problems [*Şimçnek et al.*, 1996].

Solute Transport

We assume that solutes can exist in all three phases (liquid, solid, and gaseous) and that production and decay processes can be different in each phase. We further assume that solutes are transported by convection and dispersion in the liquid phase, as well as by diffusion in the gas phase. The partial differential equations governing the nonequilibrium chemical transport of solutes involved in a sequential first-order decay chain during transient water flow in a variably saturated rigid porous medium are taken as [*Şimçnek et al.*, 1998b]:

$$\begin{aligned} \frac{\partial \theta c_k}{\partial t} + \frac{\partial \rho s_k}{\partial t} + \frac{\partial a_v g_k}{\partial t} = \frac{\partial}{\partial x} (\theta D_k^w \frac{\partial c_k}{\partial x}) + \frac{\partial}{\partial x} (a_v D_k^g \frac{\partial g_k}{\partial x}) - \frac{\partial q c_k}{\partial x} - \\ - (\mu_{w,k} + \mu'_{w,k}) \theta c_k - (\mu_{s,k} + \mu'_{s,k}) \rho s_k - (\mu_{g,k} + \mu'_{g,k}) a_v g_k + \mu'_{w,k-1} \theta c_{k-1} \\ + \mu'_{s,k-1} \rho s_{k-1} + \mu'_{g,k-1} a_v g_{k-1} + \gamma_{w,k} \theta + \gamma_{s,k} \rho + \gamma_{g,k} a_v - S c_{r,k} \quad k \in (2, n_s) \end{aligned} \quad (9)$$

where for simplicity the one-dimensional formulation is used. In (9) c , s , and g are solute concentrations in the liquid, solid and gas phases, respectively; q is the volumetric flux density, $\mu_{w,k}$, $\mu_{s,k}$, and $\mu_{g,k}$ are first-order rate constants for solutes in the liquid, solid and gas phases, respectively; $\mu'_{w,k}$, $\mu'_{s,k}$ and $\mu'_{g,k}$ are similar first-order rate constants providing connections between individual chain species, γ_w , γ_s , and γ_g are zero-order rate constants for the liquid, solid and gas phases, respectively; ρ is the soil bulk density, a_v is the air content, S is the sink term in the flow equation (1), c_r is the concentration of the sink term, D^w is the dispersion coefficient for the liquid phase, and D^g is the diffusion coefficient for the gas phase. The subscripts w , s , and g correspond with the liquid, solid and gas phases, respectively; subscript k represents the k th chain number, and n_s is the number of solutes involved in the chain reaction. The nine zero- and first-order rate constants in (9) may be used to represent a variety of reactions or transformations including biodegradation, volatilization, and precipitation.

The HYDRUS codes may be used to simulate nonequilibrium interactions between the solution (c) and adsorbed (s) concentrations, and equilibrium interaction between the solution (c) and gas (g) concentrations of the solute in the soil system. The equilibrium adsorption isotherm relating s and c is described by a generalized nonlinear equation of the form

$$s = \frac{k_s c^\beta}{1 + \eta c^\beta} \quad (10)$$

where k_s , β and η are empirical coefficients. The Freundlich, Langmuir, and linear adsorption equations are special cases of (10). The concentrations g and c are related by a linear expression of the form

$$g = k_g c \quad (11)$$

where k_g is an empirical constant, often referred to as Henry's constant.

The concept of two-site sorption [*Selim et al.*, 1977; *van Genuchten and Wagenet*, 1989] is implemented in the HYDRUS codes to permit consideration of nonequilibrium adsorption-desorption reactions. The two-site sorption concept assumes that the sorption sites can be divided

into two fractions. Sorption, s^e , on one fraction of the sites (the type-1 sites) is assumed to be instantaneous, while sorption, s^k , on the remaining (type-2) sites is considered to be time-dependent. The mass balance equation for the type-2 sites in the presence of production and degradation is given by

$$\frac{\partial s^k}{\partial t} = \omega \left[(1-f) \frac{k_s c^\beta}{1 + \eta c^\beta} - s^k \right] - (\mu_s + \mu'_s) s^k + (1-f) \gamma_s \quad (12)$$

where ω is the first-order rate constant and f is the fraction of exchange sites assumed to be in equilibrium with the solution phase.

The HYDRUS models also implement the concept of two-region, dual-porosity type solute transport [van Genuchten and Wierenga, 1976] to permit consideration of physical nonequilibrium transport. The two-region concept assumes that the liquid phase can be partitioned into mobile (flowing), θ_m , and immobile (stagnant), θ_{im} , regions and that solute exchange between the two liquid regions can be modeled as a first-order process, i.e.,

$$\left[\theta_{im} + \rho (1-f) \frac{k_s \beta c_{im}^{\beta-1}}{(1 + \eta c_{im}^\beta)^2} \right] \frac{\partial c_{im}}{\partial t} = - \left[\theta_{im} (\mu_w + \mu'_w) + \rho (\mu_s + \mu'_s) (1-f) \frac{k_s c_{im}^{\beta-1}}{1 + \eta c_{im}^\beta} \right] c_{im} + \omega (c - c_{im}) + \gamma_w \theta_{im} + (1-f) \rho \gamma_s \quad (13)$$

where c_{im} is the concentration in the immobile region and ω is the mass transfer coefficient.

By selecting certain values of the $\gamma_w, \gamma_s, \gamma_g, \mu_w, \mu_s, \mu_g, \mu_w', \mu_s', \mu_g', \eta, k_s, k_g, f, \theta_m, \beta$ and ω in (9) through (13), the entire system can be simplified significantly.

FORMULATION OF INVERSE PROBLEM

The inverse problem may be carried out using several direct and indirect methods [Neuman, 1973]. Direct methods treat the model parameters as dependent variables in a formal inverse boundary value problem [Yeh, 1986]. Indirect approaches, such as the one used in this paper, attempt to minimize a suitable objective function which expresses the discrepancy between observed and predicted system response. Initial estimates of the assumed unknown hydraulic and transport parameters are then iteratively adjusted and improved upon during the minimization procedure until a desired precision is obtained.

When measurement errors follow a multivariate normal distribution with zero mean and covariance matrix V , the likelihood function can be written as [Bard, 1974]

$$L(\mathbf{b}) = (2\pi)^{-n/2} \det^{-1/2} \mathbf{V} \exp \left\{ -\frac{1}{2} [\mathbf{q}^* - \mathbf{q}(\mathbf{b})]^T \mathbf{V}^{-1} [\mathbf{q}^* - \mathbf{q}(\mathbf{b})] \right\} \quad (14)$$

where $L(\mathbf{b})$ is the likelihood function, $\mathbf{b} = \{b_1, b_2, \dots, b_m\}$ is the vector of unknown parameters ($\theta, \theta_s, \alpha, n, l, K_s, \lambda, \mu_w, \mu_s, \beta, \eta$, and/or others), m is the number of parameters to be estimated, $\mathbf{q}^* = \{q_1^*, q_2^*, \dots, q_n^*\}$ is a vector containing the observations (e.g., observed pressure heads, water contents, concentrations, and/or cumulative and actual water or solute infiltration or outflow rates), $\mathbf{q}(\mathbf{b}) = \{q_1, q_2, \dots, q_n\}$ is a vector of corresponding model predictions obtained with the unknown parameters, and n is the number of observations. The maximum likelihood estimate is that value of the unknown parameter vector \mathbf{b} that maximizes the value of the likelihood function.

Assuming that the covariance matrix \mathbf{V} is diagonal, i.e., the measurement errors are uncorrelated, the problem of maximizing the likelihood function simplifies in a weighted least-squares minimization problem

$$\Phi(\mathbf{b}) = \sum_{i=1}^n w_i [q_i^* - q_i(\mathbf{b})]^2 \quad (15)$$

where w_i is the weight assigned to a particular measured value.

If something about the distribution of the fitted parameters is known before the inversion, that information can be included into the parameter identification procedure by multiplying the likelihood function with the prior probability density function (pdf), $p_0(\mathbf{b})$, which summarizes the prior information. Estimates which make use of prior information are known as Bayesian estimates, and lead to the maximization of a posterior pdf, $p^*(\mathbf{b})$, given by

$$p^*(\mathbf{b}) = c L(\mathbf{b}) p_0(\mathbf{b}) \tag{16}$$

in which c is a constant. The posterior density function is proportional to the likelihood function when the prior distribution is uniform

The objective function Φ to be minimized during the parameter estimation process in both HYDRUS models is defined as [Šimunek et al., 1998b,c]:

$$\begin{aligned} \Phi(\mathbf{b}, \mathbf{q}, \mathbf{p}) = & \sum_{j=1}^{m_q} v_j \sum_{i=1}^{n_{qj}} w_{i,j} [q_j^*(\mathbf{x}, t_i) - q_j(\mathbf{x}, t_i, \mathbf{b})]^2 + \\ & \sum_{j=1}^{m_p} v_j \sum_{i=1}^{n_{pj}} w_{i,j} [p_j^*(\theta_i) - p_j(\theta_i, \mathbf{b})]^2 + \sum_{j=1}^{n_b} \hat{v}_j [b_j^* - b_j]^2 \end{aligned} \tag{17}$$

where the first term on the right-hand side represents deviations between the measured and calculated space-time variables (e.g., observed pressure heads, water contents, and/or concentrations at different locations and/or time in the flow domain, or actual or cumulative fluxes versus time across a boundary of specified type). In this term, m_q is the number of different sets of measurements, n_{qj} is the number of measurements within a particular measurement set, $q_j^*(\mathbf{x}, t_i)$ represents specific measurements at time t_i for the j th measurement set at location \mathbf{x} , $q_j(\mathbf{x}, t_i, \mathbf{b})$ represents the corresponding model predictions for the vector of optimized parameters \mathbf{b} (e.g., $\theta, \theta_s, \alpha, n, l, K_s, D_l, k_g, \dots$), and v_j and w_{ij} are weights associated with a particular measurement set or point, respectively. The second term on the right-hand side of (17) represents differences between independently measured and predicted soil hydraulic properties (e.g., retention, $\alpha(h)$, and/or hydraulic conductivity, $K(\theta)$ or $K(h)$, data), while the terms $m_p, n_{pj}, p_j^*(\theta), p_j(\theta, \mathbf{b}), v_j$ and w_{ij} have similar meanings as for the first term but now for the soil hydraulic properties. The last term of (17) represents a penalty function for deviations between prior knowledge of the soil hydraulic parameters, b_j^* , and their final estimates, b_j , with n_b being the number of parameters with prior knowledge and v_j representing pre-assigned weights. We note that the covariance (weighting) matrices which provide information about the measurement accuracy, as well as any possible correlation between measurement errors and/or parameters, are assumed to be diagonal in both models. The weighting coefficients v_j may be used to minimize differences in weighting between different data types because of different absolute values and numbers of data involved, and are given either by [Clausnitzer and Hopmans, 1995]:

$$v_j = 1 / n_j \sigma_j^2 \tag{18}$$

which causes the objective function to become the average weighted squared deviation normalized by the measurement variances σ_j^2 , or by

$$v_j = \frac{1}{q_j} \min \left(\frac{\sum_{i=1}^{n_j} q_i n_i}{q_j}; \frac{n_j}{\sum_{i=1}^{n_j} n_i} \right) \tag{19}$$

where q_j is the mean of a particular measurement set, or can be specified independently as input.

SOLUTION OF THE INVERSE PROBLEM

Many techniques are available for solving the nonlinear minimization/maximization problem [Bard, 1974; Yeh, 1986; Kool *et al.*, 1987]. Most methods are iterative by starting first with a given initial estimate \mathbf{b}_i of the unknown parameters to be estimated, followed by a study of how the objective function $\Phi(\mathbf{b})$ behaves in the vicinity of the initial estimate. Based upon this behavior one selects a direction vector \mathbf{v}_i such that the new value of the unknown parameter vector, i.e.,

$$\mathbf{b}_{i+1} = \mathbf{b}_i + \rho_i \mathbf{v}_i \quad (20)$$

decreases the value of the objective function:

$$\Phi_{i+1} < \Phi_i \quad (21)$$

where Φ_i and Φ_{i+1} are the objective functions at the previous and current iteration level, and ρ_i is a scalar which insures that the iteration step is acceptable. Methods based on (20) are called gradient methods. Differences among the various gradient methods presented in the literature (e.g., steepest descent, Newton's method, directional discrimination, Marquardt's method, Gauss type methods, variable metric methods, and interpolation-extrapolation methods) are a result of differences in choosing the step direction \mathbf{v}_i and/or the step size ρ_i [Bard, 1974]. In the HYDRUS models we use Marquardt's [1963] method which has proven to be very effective in many applications involving nonlinear least-square fitting. The method represents a compromise between the inverse-Hessian and steepest descent methods by using the steepest-descent method when the objective function is far from its minimum, and switching to the inverse-Hessian method close to the minimum.

HYDRUS-1D EXAMPLES

Because of a very general formulation of the inverse problem and the possibility to use different combinations of boundary conditions, the HYDRUS models can be used for a wide variety of parameter optimization problems. Typical applications include onestep [Kool *et al.*, 1985] and multistep [van Dam *et al.*, 1992, 1994; Eching *et al.*, 1993] outflow experiments, upward infiltration [Hudson *et al.*, 1996], and evaporation experiments [Ciollaro and Romano, 1995; Santini *et al.*, 1995; Šimčnek *et al.*, 1998d, 1999b]. Below we demonstrate the use of HYDRUS-1D for estimating the soil hydraulic parameters from multistep outflow data, and a horizontal infiltration experiment followed by redistribution. The latter example demonstrates the use of HYDRUS-1D for evaluating water flow involving hysteresis. We will also use HYDRUS-1D here to estimate nonlinear parameters for solute transport involving Freundlich adsorption by analyzing a measured breakthrough curve.

Inverse Analysis of a Multistep Outflow Experiment

In this test example we analyze a multistep outflow experiment with simultaneous measurement of the pressure head inside the soil sample [Hopmans, personal communication]. The experimental setup consisted of a 6-cm long soil column in a Tempe pressure cell modified to accommodate a microtensiometer-transducer system. A tensiometer was installed, with the cup centered 3 cm below the soil surface. The soil sample was saturated from the bottom and subsequently equilibrated to an initial soil water pressure head of -25 cm at the soil surface. Pressures of 100, 200, 400, and 700 cm were subsequently applied in consecutive steps at 0, 12.41, 48.12, and 105.92 hours, respectively. Figure 1 compares the measured and optimized cumulative outflow curves for the soil sample, while Figure 2 compares measured and optimized

pressure heads. Excellent agreement was obtained for both variables. The final fit for the optimized soil hydraulic parameters ($\theta=0.197$, $\theta_s=0.438$, $\alpha=0.0101 \text{ cm}^{-1}$, $n=1.43$, $l=3.80$, and $K_s=0.521 \text{ cm h}^{-1}$) had an r^2 of 0.9995.

Fig. 1. Measured and optimized cumulative bottom flux during a multistep outflow experiment.

Fig. 2. Measured and optimized pressure heads in soil sample during a multistep outflow experiment.

Horizontal Infiltration Followed by Redistribution

This example demonstrates the use of HYDRUS-1D for analyzing transient hysteretic flow. Data used in this example were published by *Vachaud* [1968]. A horizontal soil column of 60 cm length and having an internal diameter of 9 cm was used. The initially air dry silty soil was subjected to a zero pressure at one end of the column for 620 minutes, after which water was allowed to redistribute. Although water contents were measured for about 25 days with a γ -ray attenuation technique at about 20 points in the column, we used data from only 10 points for the inversion. The soil hydraulic parameters in the hysteresis model of *Kool and Parker's* [1987] assuming different α values for the wetting and drying curves (α_w , α_d), were optimized. Figure 3 shows measured and fitted water contents during the entire

experiment. An excellent fit could be obtained only when hysteresis was considered. The following soil hydraulic parameters were obtained: $\theta_r=0.009$, $\theta_s=0.423$, $\alpha_d=0.0637 \text{ cm}^{-1}$, $\alpha_w=0.0910 \text{ cm}^{-1}$, $n=3.86$, $l=1.47$, and $K_s=0.0202 \text{ cm min}^{-1}$.

Fig. 3. Measured and optimized water contents at 10 locations in a soil column during horizontal infiltration followed by redistribution.

Nonlinear Solute Transport

This example demonstrates the use of HYDRUS-1D to estimate nonlinear solute transport parameters from breakthrough curves. A 10.75-cm long soil column was first saturated with a $10 \text{ mmol}_c\text{L}^{-1}$ CaCl_2 solution. The experiment consisted of applying a 14.26 pore volume pulse ($t=358.05 \text{ h}$) of a $10 \text{ mmol}_c\text{L}^{-1}$ MgCl_2 solution, followed by the original CaCl_2 solution. The adsorption isotherm was determined independently with the help of batch experiments [Selim *et al.*, 1987], and fitted with the Freundlich equation to yield $k_s=1.687 \text{ cm}^3\text{g}^{-1}$ and $\beta=1.615$.

Only the coefficients of the Freundlich isotherm (i.e., k_s and β) were optimized. Since the governing solute transport equation is nonlinear, one can not use an analytical solution in this case but must resort to a numerical model. The observed Mg breakthrough curve is shown in Figure 4, together with the fitted breakthrough curve obtained with HYDRUS-1D. The results indicate a reasonable prediction of the measured breakthrough curve for the final estimates of the optimized solute transport parameters ($k_s=0.943$, and $\beta=1.774$).

Fig. 4. Measured and optimized breakthrough curve for a nonlinear solute transport problem.
HYDRUS-2D EXAMPLES

Similarly as HYDRUS-1D, HYDRUS-2D [Šimčnek *et al.*, 1996] can be used for a broad range of inverse problems. Recent applications with HYDRUS-2D include estimating soil hydraulic parameters from data collected with a tension disc infiltrometer [Šimčnek and van Genuchten, 1996, 1997; Šimčnek *et al.*, 1998a,c], a modified cone penetrometer [Gribb *et al.*, 1998; Kodešová *et al.*, 1998, 1999; Šimčnek *et al.*, 1999a], and using multistep soil water extraction device [Inoue *et al.*, 1998, 1999]. Below is an example of the use of HYDRUS-2D for analyzing tension disc infiltrometer data.

Tension Disc Infiltrometer Example

Tension infiltrations are increasingly being used for evaluating saturated and unsaturated hydraulic conductivities, and for quantifying the effects of macropores and preferential flow paths on infiltration. A relatively standard way for estimating unsaturated hydraulic conductivities from tension infiltrometer data has been to invoke Wooding's [1968] analytical solution. This approach requires steady-state infiltration rates for two different supply pressure heads, and assumes applicability of an exponential function for $K(h)$. Šimčnek and van Genuchten [1996] suggested the combined use of transient infiltration data obtained during a single tension infiltration experiment, and tensiometer or TDR data measured in the soil below the disc, to estimate the unknown soil hydraulic parameters via parameter estimation. We later revised this method by using multiple tension infiltration experiments in combination with knowledge of the initial and final water contents [Šimčnek and van Genuchten, 1997]. This modification avoided the cumbersome use of tensiometers and TDRs. An evaluation of the numerical stability and parameter uniqueness using numerically generated data with superimposed stochastic and deterministic errors showed that a combination of multiple cumulative tension infiltration data, a measured final water content, and an initial condition expressed in terms of the water content, provided the most promising parameter estimation approach for practical applications [Šimčnek and van Genuchten, 1997].

The numerical inversion method was later used to estimate the soil hydraulic characteristics of a two-layered crusted soil system in the Sahel region of Africa [Šimčnek *et al.*, 1998c]. Here we will report only results for the sandy subsoil obtained with a tension disc diameter of 25 cm and with supply tensions of 11.5, 9, 6, 3, 1, and 0.1 cm. Figure 5 shows measured and optimized cumulative infiltration curves. The small breaks in the cumulative infiltration curve were caused by brief removal of the infiltrometer from the soil surface to resupply the instrument with water and adjust the tension for a new time interval. Very close agreement between the measured and optimized cumulative infiltration curves was obtained; the largest deviations were generally less than 60 ml, which was only about 0.5% of the total infiltration volume. Figure 6 shows a comparison of the parameter estimation results against results obtained with Wooding's analysis. Both methods give almost identical unsaturated hydraulic conductivities for pressure heads in the interval between -2 and -10.25 cm. However, the hydraulic conductivity in the highest pressure head interval was overestimated by a factor of two using Wooding's analysis. Šimčnek *et al.* [1998c] further compared the numerical inversion results with hydraulic properties estimated from available soil textural information using a neural-network-based pedotransfer function approach. They reported relatively good agreement between the inverse and neural network predictions.

Fig. 5. Measured and optimized cumulative infiltration curves for a tension disc infiltrometer experiment carried out in the Sahel region.

Fig. 6. Unsaturated hydraulic conductivities calculated using Wooding's analytical solution for particular pressure heads, and the complete function obtained with numerical inversion.

CONCLUSIONS

Two numerical codes (HYDRUS-1D and HYDRUS-2D) were developed for identifying soil-hydraulic and solute transport parameters from unsaturated flow and transport data in a one-, two-, and quasi-three-dimensional porous media. The utility of the two codes was demonstrated using data typically obtained during multistep outflow experiment, horizontal infiltration followed by redistribution, a column miscible displacement (breakthrough) study, and a three-dimensional disc permeameter infiltration experiment. Because of their generality (in terms of the definition of the objective function, the possible combination of different boundary and initial conditions, and options for considering multi-layered systems), both models are extremely useful tools for analyzing a broad range of steady-state and transient laboratory and field flow and

transport experiments.

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