Inverse Optimization, Calibration and Validation of Simulation Models at the Field Scale

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Abstract

An overview is given of the issues of parameter estimation, model verification, and model validation as applied to field-scale subsurface flow and transport problems. We briefly review inverse optimization methods for estimating soil hydraulic parameters from a variety of field experiments, including tension disc infiltrometry, cone penetrometry, and gravity drainage experiments. An example is presented showing calibration of the numerical HYDRUS-2D model using data of a tile-drainage experiment. The hydraulic characteristics of the layered soil profile at the site were identified based on the joined use of laboratory data, field monitoring data, and the numerical model. A split sampling technique was used to test applicability of the numerical model for this study.

Keywords: Simulation models, parameter estimation, calibration, tile-drained field

Introduction

Computer models based on numerical solutions of the flow and solute transport equations are increasingly being used for a wide range of applications in research and management. Application of the models is enhanced by the ever increasing power of personal computers, and the development of more accurate and numerically stable numerical techniques. Precision of the obtained predictions depends to a large extent upon the accuracy of the available model input parameters, and on a successful description of the actual physical system, including soil heterogeneity and the possible presence of nonequilibrium flow and transport conditions such as preferential flow. Parameters in the soil hydraulic functions characterizing the water retention and permeability properties are the most important input variables for models based on numerical solutions of the variably-saturated flow (Richards) equation. These hydraulic parameters directly influence the mobility of various chemical species through their effect on pore-water flow velocities and water contents. Transport and chemical parameters additionally affect the rate of spreading of chemicals and their distribution between mobile and immobile phases.

Water flow and solute transport models are increasingly being applied to natural subsurface systems. While a major purpose of their application is to provide future predictions, they are more often used also to interpret the complex interactions found in laboratory and field data (Steefel & Van Cappellen, 1998). Models are also often used to study the sensitivity of natural systems to selected variables and processes, and to determine the uncertainties in predictions. The results of a sensitivity analysis can provide insight into the relative importance of individual model parameters, and thus help guide the allocation of resources for further laboratory and field investigations (Šimůnek & Valocchi, 2000).

There have been more efforts lately to test the reliability of model predictions, in part motivated by the widespread use of numerical models for management purposes. It is still an open question whether we ultimately can use water flow and solute transport models as true predictive tools to make with confidence quantitative forecasts necessary for practical purposes. At present, there is even controversy regarding the predictive capability of simpler models of saturated water flow and single component transport (e.g., Konikow & Bredehoeft, 1992; de Marsily et al., 1992; Anderson & Woessner, 1992; Mazoszewski & Zuber, 1992; Oreskes et al., 1994). Attempts to deal with the problem of reliability of model predictions has spurred the introduction in the literature of a long list of terms that are often only loosely defined and frequently substituted for each other, such as model verification, validation, confirmation, and calibration. In this paper we give first brief definitions of the most relevant terms as used in the above references, and provide a short summary of ongoing discussions on model validation. Next we will review inverse optimization as used for estimating soil hydraulic parameters from field experiments, and conclude with a calibration of the numerical HYDRUS-2D model using field data collected as part of a tile-drainage experiment.

Reliability of Model Predictions

A model is 'a representation of a real system or process' (Konikow & Bredehoeft, 1992). The word model can represent many things, such as conceptual (or process-based) model, mathematical model (deterministic or stochastic), numerical or analytical model, physical model (analog), and many others. *A conceptual model* is a 'hypothesis for how a system or process operates' (Konikow & Bredehoeft, 1992) or 'a qualitative description of a system and its representation relevant to the intended use of the model' (OECD/NEA, 1990). *A mathematical model* is a representation of a conceptual model with objects, forces and events replaced with mathematical expressions. A majority of the mathematical models used today to simulate water flow and solute transport in both saturated and variably saturated systems are *deterministic mathematical models* that generally solve a set of partial differential equations representing conservation of mass, momentum, and energy. Since most practical problems cannot be simplified and/or idealized to the point so that analytical solutions exist, most models use various numerical techniques to solve the governing equations subject to appropriate initial and boundary conditions. Implementation of a numerical algorithm that solves the governing equation(s) results in a computer code that can be considered a *generic model*. A generic model applied to a particular geographical area with given (optimized or calibrated) parameters and initial conditions, represents a *site-specific model* (Konikow & Bredehoeft, 1992).

The term *verification* can refer to the governing equation, the code or the model (Anderson & Woessner, 1992). *Verification of the governing equation* involves demonstration that the equation in the model accurately describes the simulated process. While it is generally accepted that Darcy's law combined with conservation of mass accurately describes saturated groundwater flow, the applicability of the Richards equation to flow in the unsaturated zone and the convection-dispersion equation to solute transport at the field scale is often questioned (Jury & Flħhler, 1992). *Verification of a numerical code* consists of showing that the results generated by the model for simpler problems are consistent with available analytical solutions, or are the same, or similar, as results generated with other numerical codes. The latter procedure is often also called *benchmarking*. Verification of a code should ensure that the equations constituting the mathematical model are correctly encoded and solved. However, verification of a code does not mean verification of the governing equation, nor does it imply absolute certainty that the numerical solution is implemented correctly. Also, available analytical solutions are often limited to idealized transport domains, homogeneous and isotropic media, and uniform initial and constant boundary conditions. The very reason for developing numerical models is to go beyond the range of available analytical solutions, i.e., to allow irregular transport domains, nonhomogeneous and anisotropic media, variable boundary conditions, and nonlinear processes, i.e. to use them for situations or conditions for which they can not be verified. Verification in such conditions is often accomplished using approximate tests of having internal consistency and accuracy, such as mass conservation, global mass-balance errors, and sensitivity to changes in mesh size and time steps.

Model verification has often been used synonymously with *model validation* (Anderson & Woessner, 1992). We agree with the suggestions by Narasimhan (1987) to associate model verification with the accuracy of the invoked numerical solution schemes and the coding of a model, and model validation with the inherent capability (or the degree of validity) of a model in describing a set of processes (in our case subsurface flow and transport processes). Many definitions have been used for the term model validation; still, much controversy remains of what it means and whether model validation can be truly achieved (Oreskes et al., 1994). For example, the International Atomic Energy Agency defines a validated model as one that gives 'a good representation of the actual processes occurring in a real system' (IAEA, 1982). Similarly, the U.S. Department of Energy defines a validated model as one that 'reflects the behavior of the real world' (US DOE, 1986). Another definition states that model 'validation is a process of obtaining assurance that a model is a correct representation of the process or system for which it is intended' (OECD/NEA, 1990; Mazoszewski & Zuber, 1992). Regulatory agencies often request scientists and model developers to validate their models or to show that the models were independently validated. This did lead to several international projects for the purpose of addressing the issues of verification and validation of hydrogeological models assessing nuclear waste repositories. These included projects INTRACOIN (the International Nuclide Transport Code Intercomparison Study, SNPI, 1986), INTRAVAL (an International Project to Study Validation of Geosphere/Transport Models, SNPI, 1987), and HYDROCOIN (Hydrologic Code Intercomparison Study, OECD/NEA, 1990).

Model validation remains a contentious topic among soil and groundwater hydrologists and scientists. For example, the journal Advances in Water Resources devoted in 1992 two special issues to the topic of 'Validation of Geo-hydrological models' (Hassanizadeh & Carrera, 1992). Konikow & Bredehoeft (1992), in their enlightening contribution entitled 'Ground-water models cannot be validated', suggest that since groundwater models are embodiment of scientific hypothesis they cannot be proven or validated, similarly as any scientific hypothesis or theory, but only tested and invalidated. They also argue that 'the terms validation and verification are misleading and their use in groundwater science should be abandoned in favor of more meaningful model-assessment descriptors'. In a comment on the latter article, de Marsily et al. (1992) first disagreed with that notion, but later offered a compromise statement by stating that 'we do not validate our models, but we try to show that they are not invalidated by the data!', which does not seem to contradict the arguments of Konikow and Bredehoeft. Similarly as Konikow & Bredehoeft (1992), Oreskes et al. (1994) also argue that verification and validation of numerical models of natural systems is impossible since such systems are never closed and model results are always non-unique.

Model calibration is generally defined as the process of tuning a model for a particular problem or case by manipulating the input parameters (e.g., hydraulic conductivities), and initial or boundary conditions, within reasonable ranges until the simulated model results closely match the observed variables (e.g., pressure heads, water contents, fluxes). The general approach in model calibration is to select some merit or objective function that is a measure of the agreement between measured and modeled data, and that is directly or indirectly related to the adjustable parameters. The best-fit parameters are obtained by minimizing the objective function. Model calibration, i.e., minimization of the merit function, can be achieved by trial and error or, as is becoming more popular, by using an automated minimization or parameter estimation technique. A model is considered calibrated when it reproduces data within some subjectively acceptable level of precision (Konikow & Bredehoeft, 1992). Model calibration is often also called *history matching*. When the ultimate goal of model calibration is not merely to calibrate a model, but rather to optimize unknown parameters in that model, the process is often called *parameter optimization* or *parameter estimation*.

A two-step calibration scheme or *split sampling* has sometimes been used for the model calibration process, or instead of model validation (if one accepts the notion that models cannot be formally validated). The existing data set is then divided into two parts with the first (calibration) part being used to calibrate the model and to estimate all necessary parameters, while the second (validation or verification) part of the data set serves to compare predicted and measured data values using the parameters calibrated against the first part of the data set. Although successful performance of the model during the second part does not constitute a rigorous validation of the model, it is often accepted that the model is validated if it predicts the system response during this second phase within acceptable limits (Anderson & Woessner, 1991). A two-step calibration process of this type is sometimes called *historical validation*.

The most rigorous test of the performance of a model is the *postaudit* or *predictive validation* (Anderson & Woessner, 1992). The calibrated model in this case is first used to make a prediction of the future behavior of the system; only after the modeling study is completed are new data collected and compared against the model predictions. A literature study by Anderson & Woessner (1992) revealed five modeling studies that underwent a rigorous postaudit test. None of the models was found to accurately predict the future behavior of the system. This was partly due to errors in the conceptual model of the hydrogeological system and partly due to failure to correctly predict future boundary conditions. Anderson & Woessner (1992) concluded that the issue of model validation is mainly a regulatory one, not a scientific one. A model can never be proven valid from a scientific standpoint because our understanding of a system will always be incomplete. Accepting the argument that models cannot be validated experimentally and can be verified mathematically only in a limited sense, we now discuss the problems of parameter estimation and model calibration.

Parameter Estimation

Objective Function

The general approach in parameter estimation is to select a merit or objective function that is a measure of the agreement between measured and modeled data, and which is directly or indirectly related to the adjustable parameters. The merit function is often based on a *maximum likelihood estimator*, which simplifies to a *weighted least-squares* problem for uncorrelated measurement errors (Bard, 1974):

$$\Phi(\boldsymbol{\beta}) = \sum_{i=1}^{n} w_i [q_i^* - q_i(\boldsymbol{\beta})]^2 \tag{1}$$

where $\boldsymbol{\beta} = \{\beta_1, \beta_2,...,\beta_m\}$ is the vector of optimized parameters, m is the number of optimized parameters, $\boldsymbol{q}^* = \{q_1^*, q_2^*,..., q_n^*\}$ is the vector of observations, $\boldsymbol{q}(\boldsymbol{\beta}) = \{q_1, q_2,..., q_n\}$ is the corresponding vector of model predictions as a function of the unknown parameters being optimized, n is the number of observations, and w_i is the weight of a particular measured point. The weighted least-squares estimator (1) is a maximum-likelihood estimator as long as the weights, w_i, contain the measurement error information such that

$$w_i = \frac{1}{\sigma_i^2} = \frac{1}{\text{variance of measurement error of } q_i^*} \tag{2}$$

The robustness of the least-squares criterion for the estimation of model parameters has recently been questioned by Finsterle & Najita (1998). They pointed out that the least-squares criterion causes outliers to strongly influence the final values of optimized parameters. Hence, outliers (e.g., individual data points with large measurement errors as is often the case with field measurements) can introduce a significant bias in the estimated model parameters. Finsterle & Najita (1998) studied several other more robust estimators with different error distributions that reduce the effect of outliers on the optimized parameters. For example, they suggest using as an alternative the least absolute deviates or L1-estimator for a double exponential distribution of errors:

$$\Phi(\boldsymbol{\beta}) = \sum_{i=1}^{n} \frac{1}{\sigma_i} \left| q_i^* - q_i(\boldsymbol{\beta}) \right| \tag{3}$$

or the maximum-likelihood estimator for measurement errors following a Cauchy distribution:

$$\Phi(\boldsymbol{\beta}) = \sum_{i=1}^{n} \log\left(1 + \frac{1}{2} w_i [q_i^* - q_i(\boldsymbol{\beta})]^2\right) \tag{4}$$

The vector of optimized parameters $\boldsymbol{\beta}$ typically contains parameters describing the unsaturated soil hydraulic properties (i.e., soil water retention and unsaturated hydraulic conductivity functions), and/or such solute transport parameters as the dispersivity and selected adsorption or decay coefficients. The vector of observations typically contains measured variables such as pressure heads, positions of the groundwater table, water contents, concentrations, infiltration rates, and/or drainage fluxes.

The weighted least-squares estimator (1), as well as the presumably more robust estimators (3) and (4), can be easily modified to accommodate additional information, such as prior information about the optimized parameters, and/or known data points of the retention and hydraulic conductivity functions. For example, the objective function in the HYDRUS models describing variably-saturated flow and transport (Šimůnek et al., 1998b, 1999b) is defined as the sum of three components:

$$\Phi(\boldsymbol{\beta}, \boldsymbol{q}, \boldsymbol{p}) = \sum_{j=1}^{m_q} v_j \sum_{i=1}^{n_{qj}} w_{i,j} \, [q_j^*(\boldsymbol{x}, t_i) - q_j(\boldsymbol{x}, t_i, \boldsymbol{\beta})]^2 + \sum_{j=1}^{m_p} \overline{v}_j \sum_{i=1}^{n_{pj}} \overline{w}_{i,j} \, [p_j^*(\theta_i) - p_j(\theta_i, \boldsymbol{\beta})]^2 + \sum_{j=1}^{n_b} \hat{v}_j \, [\beta_j^* - \beta_j]^2 \tag{5}$$

where the first term on the right-hand side represents deviations between the measured and calculated space-time variables such as observed pressure heads, h, water contents, θ, and/or concentrations, c, at different locations and/or time in the flow domain, or actual or cumulative fluxes versus time across certain boundaries. 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, $q_j^*(\boldsymbol{x},t_i)$ represents specific measurements at time t_i for the jth measurement set at location $\boldsymbol{x}(r,z)$, $q_j(\boldsymbol{x},t_i,\boldsymbol{\beta})$ represents the corresponding model predictions for the vector of optimized parameters $\boldsymbol{\beta}$, and v_j and $w_{i,j}$ are weights associated with a particular measurement set or point, respectively. The second term on the right-hand side of (5) represents differences between independently measured and predicted soil hydraulic properties (e.g., retention, $\theta(h)$, and/or hydraulic conductivity, $K(\theta)$ or $K(h)$, data), while the terms m_p, n_{pj}, $p_j^*(\theta_i)$, $p_j(\theta_i, \boldsymbol{\beta})$, $\overline{v}_j$ and $\overline{w}_{ij}$ have similar meanings as for the first term but now for the soil hydraulic properties. The last term of (5) represents a penalty function for deviations between prior knowledge of the soil hydraulic parameters, β_j^*, and their final estimates, β_j, with n_b being the number of parameters with prior knowledge and $\hat{v}_j$ representing pre-assigned weights. The best-fit parameters are obtained by minimizing this objective function using any minimization technique, such as the Marquard-Levenberg method, the simplex method, or others (Šimůnek & Hopmans, 2000).

Water Flow

Water flow in variably-saturated flow models is typically described using a mixed formulation of the Richards equation:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i}\left[K(h)\left(K_{ij}^A \frac{\partial h}{\partial x_j} + K_{iz}^A\right)\right] \tag{6}$$

where θ is the water content (L^3L^{-3}), h is the pressure head (L), K is the hydraulic conductivity (LT^{-1}), $\boldsymbol{K^A}$ is the anisotropy tensor, t is time (T), and x_i is the spatial coordinate (L). The soil hydraulic properties can be described using the van Genuchten-Mualem model (van Genuchten, 1980):

$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \frac{1}{(1 + |\alpha h|^n)^m} \tag{7}$$

$$K(\theta) = K_s S_e^l \left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \quad (8)$$

where S_e is effective fluid saturation (-), K_s is the saturated hydraulic conductivity (LT^{-1}), θ_r and θ_s denote the residual and saturated water contents (-), respectively; l is the pore-connectivity parameter (-), and α (L^{-1}), n (-), and m (= 1 - 1/n) (-) are empirical shape parameters. The above hydraulic functions contain 6 unknown parameters: θ_r, θ_s, α, n, l and K_s.

Field Applications

While inverse methods in subsurface hydrology were initially used almost exclusively for saturated flow problems (e.g., see review of Yeh, 1986); they are now also increasingly applied to the analysis of unsaturated zone experiments (e.g., Kool et al., 1987). Except for an early study by Dane & Hruska (1983), parameter estimation techniques in soil hydrology were first used with laboratory experiments, such as for one-step or multi-step type outflow, upward infiltration, and evaporation experiments (see Hopmans et al., 2000, for references on these particular methods) for which the initial and boundary conditions and homogeneity of the soil sample could be readily controlled. The application of inverse methods to field experiments is more complex due to soil heterogeneity, possible anisotropy, and uncertainty associated with the initial and boundary conditions. Examples are ponded infiltration (e.g., Russo et al., 1991), the instantaneous profile method (Dane & Hruska, 1983; Kool et al., 1987; Romano, 1992), tension disc infiltrometers (Šimůnek & van Genuchten, 1996, 1997; Šimůnek et al., 1998c, 1999c), cone penetrometers (Gribb, 1996; Gribb et al., 1998; Kodešová et al., 1998, 1999; Šimůnek et al., 1999a), water flow to a ceramic cup tensiometer (Timlin & Pachepsky, 1998), and the extraction method (Inoue et al., 1998). Contrary to laboratory methods, field experiments do not provide exact control, or often do not even permit precise knowledge, of the total amount of water or solute in the selected transport domain. Also, the use of the prior information is much more complicated. For example, in the laboratory one can generally estimate with relatively great precision the saturated water content from bulk density or porosity measurement. Such information is much less useful in field studies where the soil seldom if ever reaches full saturation, even after development of positive pressure heads.

The Instantaneous Profile Method

The inverse parameter estimation problem was probably first applied to field data by Dane & Hruska (1983), who successfully optimized the parameters in van Genuchten's (1980) soil hydraulic functions from transient drainage field data. A similar drainage problem was studied by Kool et al. (1987) for a 6-m deep lysimeter, and later by Romano (1992) in attempts to quantify soil hydraulic spatial variability along a 50 m-long transect.

The Tension Disc Infiltrometer Method

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 estimates of the steady-state infiltration rate for two different supply pressure heads, and assumes applicability of an exponential function for $K(h)$. Šimůnek & van Genuchten (1996) suggested the combined use of transient infiltration data obtained during a

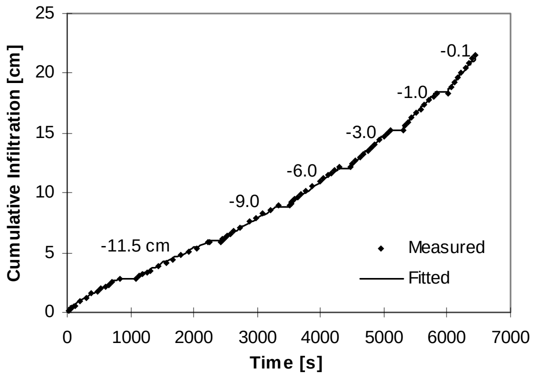

Figure 1. Measured and optimized cumulative infiltration curves for a tension disc infiltrometer experiment carried out on a sandy soil in the Sahel region.

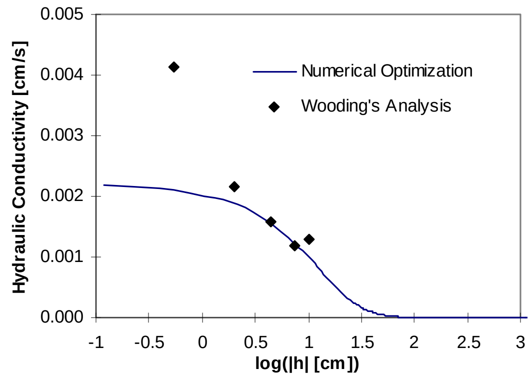

Figure 2. Unsaturated hydraulic conductivities calculated using Wooding's analytical solution, and the complete function obtained with numerical inversion.

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. They later revised this method by using multiple tension infiltration experiments in combination with knowledge of the initial and final water contents (Šimůnek & 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 (Šimůnek & van Genuchten, 1997).

Numerical inversion was later used to estimate the soil hydraulic properties of a two-layered crusted soil system in the Sahel region of Africa (Šimůnek et al.*,* 1998a). Here we will report only results for the sandy subsoil obtained with a tension disc diameter of 25 cm and for supply tensions of 11.5, 9, 6, 3, 1, and 0.1 cm. Figure 1 shows measured and optimized cumulative infiltration curves. The small breaks in the cumulative infiltration curve were caused by brief interruptions to resupply the infiltrometer with water, and to 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 2 compares the parameter estimation results against results obtained with Wooding's analysis. Both methods gave almost identical unsaturated hydraulic conductivities for pressure heads in the interval between -2 and -10.25 cm. However, the hydraulic conductivity obtained with Wooding's analysis at the highest pressure head overestimated the inverse results by a factor of two. Additional applications of inverse modeling to transient tension disc infiltration data are given by Šimůnek et al. (1998c, 1999c).

The Cone penetrometer method

While tension infiltrometer experiments provide relatively quick estimates of the hydraulic properties, they can be used only at the soil surface. By comparison, a new cone penetrometer method currently under development (Gribb, 1996; Gribb et al., 1998; Kodešová et al., 1998, 1999; Šimůnek et al., 1999a) can be used at depth. To obtain the hydraulic properties, a modified cone penetrometer was instrumented with a porous filter close to the penetrometer tip and two tensiometer rings 5 and 9 cm above the filter. The device is pushed into a soil to the desired depth, and a constant positive head is applied to the 5-cm filter. The volume of water imbibed into the soil is monitored, as are tensiometer ring readings registering the advancement of the wetting front. After measured pressure heads in the soil stabilize, the water source is shut off, and the redistribution of water in the soil profile is further monitored with tensiometers. Cumulative infiltration and the measured pressure heads are used to define the objective function to be minimized.

Gribb (1996) gave a detailed numerical analysis of this experiment, including a study of the identifiability of the soil hydraulic parameters. The method was subsequently used to estimate the hydraulic parameters of a sandy soil in a laboratory aquifer system measuring 5 x 5 x 3 m (Gribb et al., 1998; Kodešová et al., 1998) using the wetting part of the experiment. Šimůnek et al. (1999a) and Kodešová et al. (1999) later examined both the wetting and redistribution parts of cone permeameter experiments to find the wetting and drying branches of the soil hydraulic properties. The study by Kodešová et al. (1999), carried out under field conditions, also evaluated the impact of having one or two steps in the applied pressure head on estimates of the wetting soil hydraulic properties. The soil hydraulic properties estimated in this way corresponded reasonably well with those obtained using more standard techniques.

Model Calibration

Variably-saturated water flow and solute transport models are increasingly being applied to natural systems. Recent applications include studies of flow and transport in tile-drained fields by de Vos (1997), de Vos et al. (1999a, b), and Mohanty et al. (1998a, b), among many others. The soil hydraulic and transport parameters in these studies were either obtained independently of the model (Mohanty et al., 1998a, b) or were optimized by also considering the independently measured prior information (de Vos, 1997; de Vos et al., 1999a, b). Here we will briefly summarize the "split sampling" calibration of the HYDRUS-2D flow/transport model (Šimůnek et al., 1999b) to a tile-drained, layered silt loam soil (de Vos, 1997; de Vos et al., 1999a, b).

Case Study

The study was carried out at an experimental farm near Marknesse in the Noordoostpolder in the Netherlands. The calcareous silt loam profile showed strong stratification (Figure 3) and was drained using tile drains spaced 12 m apart and located at depths between 90 and 105 cm. The soil profile was divided into three main horizons (topsoil between 0 and 25 cm, a 25-40 cm intermediate layer, and a 40-200 cm subsoil layer), and also contained drain trench with slightly different hydraulic properties. Within the intermediate and subsoil layers, distinctions were made between different sub-layers in terms of the saturated hydraulic conductivity. Tensiometers, observation wells, piezometers, and a drainage water sampling device were installed in the field to monitor the hydrological conditions, the drain discharge rate, and nitrate concentrations in the drainage water.

Laboratory analyses included the hanging column method for measuring retention curves, the constant head method for the saturated hydraulic conductivities, and the crust method and the hot-air method for unsaturated hydraulic conductivities. Measured soil-hydraulic parameters are given by De Vos (1997) and de Vos et al. (1999b). Field water retention curves were obtained by matching the field pressure head and water content measurements. Measured retention curves and unsaturated hydraulic conductivities were used in the simulations to be discussed

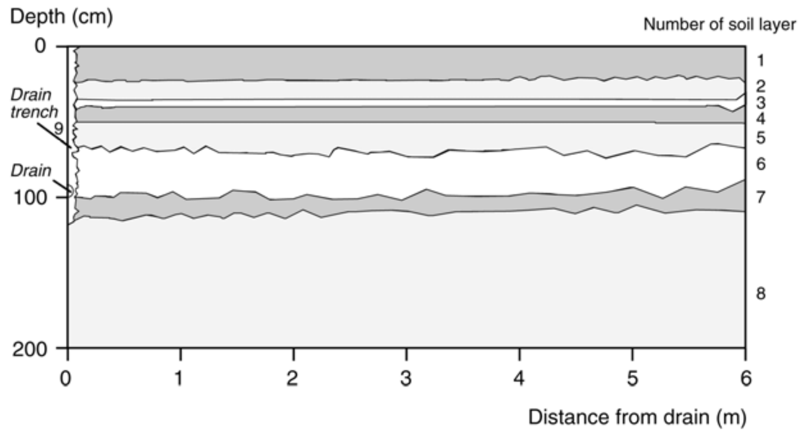

Figure 3. Distribution of different soil layers in the flow domain, including the location of a drain trench above and below the drain.

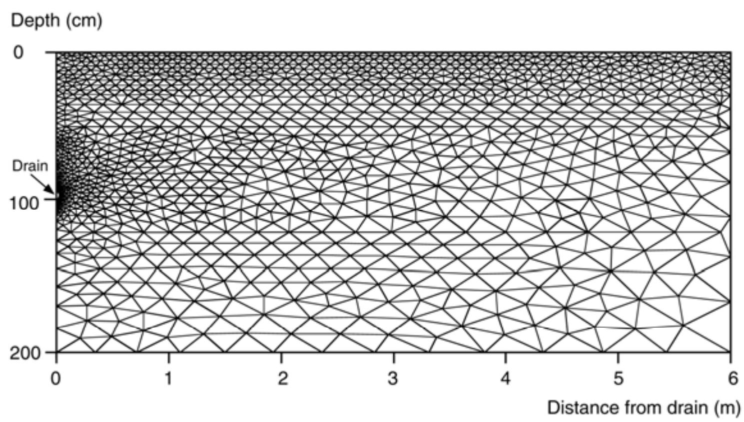

Figure 4. Finite element grid in the flow domain representing half the drain spacing. The grid system consists of 2563 triangles and 1352 nodes.

below. Since the saturated hydraulic conductivity varied by about two orders of magnitude within any particular layer, values used for model simulations were obtained by using the calibration procedure described below. A linear distribution of hydraulic conductivities was assumed between saturation and the pressure head of h= -20 cm.

A flow domain 6 m wide, representing half the drain spacing, and 2 m deep was used in the numerical simulations. The drain was located at a depth of 97.5 cm, and was described as a half circular hole of 5 cm diameter having a seepage face boundary condition. A stratified triangular finite element grid was generated in accordance with the layered soil profile (Figure 4).

Drain discharge rate - groundwater level data, $q(h_{GWL})$ (Figure 5), measured in the field, were used to calibrate saturated hydraulic conductivities, K_s, of different layers. Values of K_s, conditioned to remain within the range of measured values, were adjusted for different constant upper boundary fluxes until the HYDRUS-2D simulation results corresponded with the measured $q(h_{GWL})$ data. To estimate K_s for the subsoil, the calibration procedure started with a relatively low uniform infiltration rate at the soil surface (0.5 mm d^{-1}), which corresponded to a

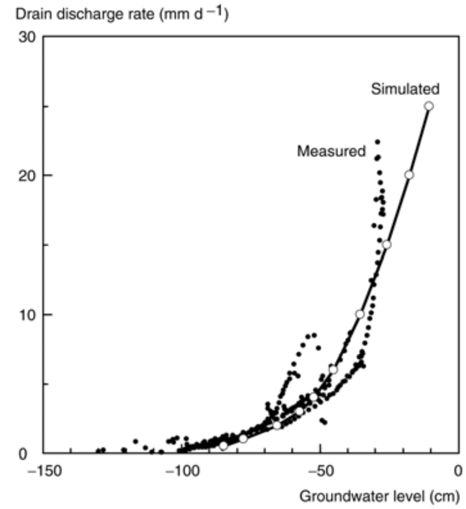

Figure 5. Measured and simulated data of the relationship between drain discharge rate and groundwater level for the leaching period from 17 December 1991 to 25 May 1992 (0<t<160 d). The groundwater data represent the position midway between two drains, i.e., at 6 m from the drain. The simulated data were obtained for steady state flow conditions.

very low drain discharge rate. By increasing the infiltration rate, the phreatic surface rose to cause shallower soil layers to become saturated, and allowing their K_s values to be calibrated. The calibration of the shallower layers depended on the results of the underlying layers. This method of calibration assumes that the saturated zone below the phreatic surface dominates water flow to the drain. We used a trial-and-error approach for calibration, since an automatic calibration procedure was beyond the computational means of our PC's due to long computational times for each simulation. The model was further calibrated against a period of 40 days starting December 17, 1991. Additional adjustments were made to the retention curve of the topsoil on the basis of field-measured water retention curves (de Vos et al., 1999a).

The HYDRUS-2D model was subsequently used to simulate water flow and nitrate transport for a period of several years (up to April 94). Pressure heads and nitrate concentrations measured on December 17, 1991 were used as initial condition. Figure 6 shows results of the simulation for the first 160 days, including the first 40 days of the calibration period. Measured and simulated groundwater levels at 6-m distance from the drain, drain discharge rates, and NO_3 concentrations in the drainage water are presented. Notice that the modeling results correspond equally well with the measured data during the calibration and validation parts of the experiment.

Conclusions

Recently developed variably-saturated water flow and solute transport models (e.g., HYDRUS-2D) can be extremely useful for analyzing a broad range of transient in-situ field flow and transport experiments, because of their inverse capabilities and generality (in terms of defi-

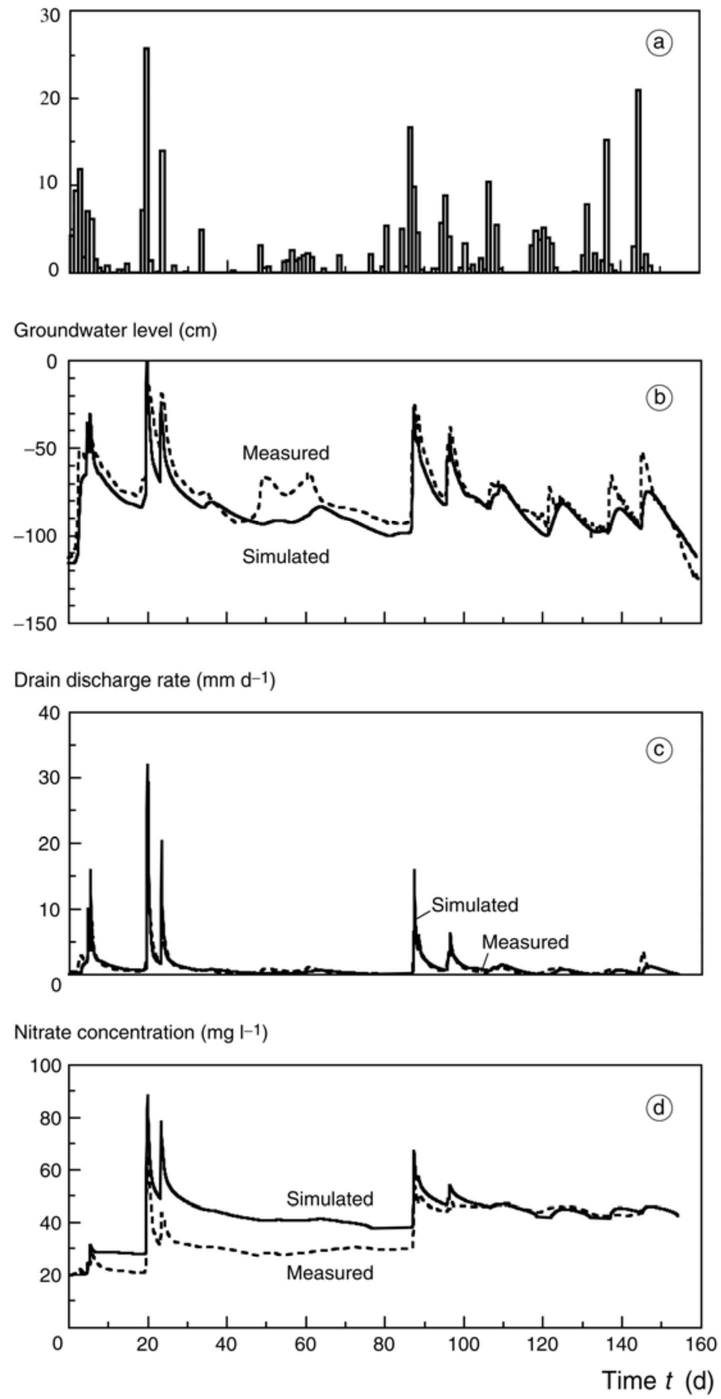

Figure 6. Precipitation amounts (a), measured and simulated groundwater levels 6-m away from the drain (b), drain discharge rates (c), and NO_3 concentrations in the drainage water (d), for the leaching period from 17 December 1991 to 25 May 1992 (0<t<160 d).

ning the objective function, possible combinations of different initial and boundary conditions, and options for considering multi-layered systems). Such models represent very powerful tools for analyzing complex environmental problems, and for developing alternative soil and water management strategies, in spite of difficulties associated with their complete (mathematical) verification and (experimental) validation. They provide a useful framework for interpreting experimental results and for understanding qualitative and quantitative trends and relationships present in observed field data. Transport models are excellent tools for integrating our knowledge of the most relevant flow and transport processes and soil properties, carrying out sensitivity analyses, and for designing, implementing and analyzing laboratory and field experiments (Steefel & Van Cappellen, 1998; de Vos et al., 1999a; Šimůnek & Valocchi, 2000). This synthesis of modeling and experimentation should lead to a more coherent and rigorous understanding of the underlying transport processes.

References

Anderson, M. P. & W. W. Woessner, 1991. Applied Groundwater Modeling, Simulation of Flow and Advective Transport. Academic Press, San Diego,CA, 381pp..

Anderson, M. P. & W. W. Woessner, 1992. The role of the postaudit in model validation. Advances in Water Resources 15 [1], 167-173.

Bard, Y., 1974. Nonlinear Parameter Estimation. Academic Press, New York, N.Y., 341pp.

Dane J. H. & S. Hruska, 1983. In-situ determination of soil hydraulic properties during drainage. Soil Sci. Soc. Am. J. 47 [3], 619-624.

de Marsily, G., P. Combes & P. Goblet, 1992. Comment on 'Ground-water models cannot be validated', by L. F. Konikow & J. D. Bredehoeft. Advances in Water Resources 15 [6], 367-369.

de Vos, J. A., 1997. Water flow and nutrient transport in a layered silt loam soil. PhD thesis, Wageningen Agricultural University, The Netherlands.

de Vos, J. A., D. Hesterberg & P. A. C. Raats, 1999a. Water flow and nitrate leaching in a layered silt loam soil. Soil Sci. Soc. Am. J., (submitted).

de Vos, J. A., J. Šimůnek & P. A. C. Raats, 1999b. Identification of the hydraulic properties of a layered silt loam. In: van Genuchten, M. Th., F. J. Leij, and L. Wu (eds.) Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media, University of California, Riverside, CA, 783-798.

Finsterle, S. & J. Najita, 1998. Robust estimation of hydrologic model parameters. Water Resour. Res. 34 [11] 2939-2947.

Gribb, M. M., 1996. Parameter estimation for determining hydraulic properties of a fine sand from transient flow measurements. Water Resour. Res. 32 [7], 1965-1974.

Gribb, M. M., J. Šimůnek & M. F. Leonard, 1998. Development of a cone penetrometer method to determine soil hydraulic properties. ASCE J. of Geotech. and Geoenviron. Eng. 124 [9], 820-829.

Hassanizadeh, S. M. & J. Carrera, (eds.) 1992. Validation of Geohydrological Models. Special issues of Advances in Water Resources 15 [1,4].

Hopmans, J. W., J. Šimůnek & N. Romano, 2000. Inverse Modeling of Transient Water Flow. In: J. H. Dane & G. C. Topp (eds.), Methods of Soil Analysis, Part 1, Physical Methods, Third edition, SSSA, Madison, WI, in press.

Inoue, M., J. Šimůnek, J. W. Hopmans & V. Clausnitzer, 1998. In-situ estimation of soil hydraulic functions using a multi-step soil water extraction technique. Water Resour. Rer. 34 [5], 1035-1050.

International Atomic Energy Agency, 1982. Radioactive waste management glossary. IAEA-TECDOC-264, Vienna.

Jury, W. A. & H. Flħhler, 1992. Transport of chemicals through soil: mechanisms, models, and field applications. Advances in Agronomy 47, 141-201.

Kodešová, R., M. M. Gribb & J. Šimůnek, 1998. Estimating soil hydraulic properties from transient cone permeameter data. Soil Science 163 [6], 436-453.

Kodešová, R., S. E. Ordway, M. M. Gribb & J. Šimůnek. 1999. Estimation of soil hydraulic properties with the cone permeameter: Field studies. Soil Science, in press.

Kool, J. B., J. C. Parker & M. Th. van Genuchten, 1987. Parameter estimation for unsaturated flow and transport models - A review. J. Hydrol. 91, 255-293.

Konikow, L. F. & J. D. Bredehoeft, 1992. Ground-water models cannot be validated. Advances in Water Resources 15 [1], 75-83.

Mazoszewski, P. & A. Zuber, 1992. On the calibration and validation of mathematical models for the interpretation of tracer experiments in the groundwater. Advances in Water Resources 15 [1], 47-62.

Mohanty, B. P., R. S. Bowman, J. M. H. Hendrickx, J. Šimůnek & M. Th. van Genuchten, 1998a. Preferential transport of nitrate to a tile drain in an intermittent-flood-irrigated field: Model development and experimental evaluation. Water Resour. Rer. 34 [5], 1061-1076.

Mohanty, B. P., T. H. Skaggs & M. Th. van Genuchten, 1998b. Impact of saturated hydraulic conductivity on the prediction of tile flow. Soil Sci. Soc. Am. J. 62, 1522-1529.

Narasimhan, T. N., 1987. Some thoughts on model verification. In: D. D. Evans & T. J. Nicholson (eds.), Flow and Transport Through Unsaturated Fractured Rock, Geophysical Monograph 42, AGU, Washington, DC.

OECD/Nuclear Energy Agency, 1990. The International Hydrocoin Project, Level 2: Model Validation. OECD/Nuclear Energy Agency Publications No. 72957, Paris, France.

Oreskes, N., K. Shrader-Frechette & K. Belitz, 1994. Verification, validation, and confirmation of numerical models in the earth sciences. Science 263, 641-646.

Romano, N., 1992. Use of an inverse method and geostatistics to estimate soil hydraulic conductivity for spatial variability analysis. Geoderma 60, 169-186.

Russo, D., E. Bresler, U. Shani & J. C. Parker, 1991. Analysis of infiltration events in relation to determining soil hydraulic properties. Water Resour. Res. 27, 1361-1373.

Steefel, C. I. & P. Van Cappellen, 1998. Reactive transport modeling of natural systems. J. of Hydrology 209, 1-7.

Šimůnek, J. & M. Th. van Genuchten, 1996. Parameter estimation of soil hydraulic properties from the tension disc infiltrometer experiment by numerical inversion. Water Resour. Res. 32 [9], 2683-2696.

Šimůnek, J. & M. Th. van Genuchten, 1997. Estimating unsaturated soil hydraulic properties from multiple tension disc infiltrometer data. Soil Science 162 [6], 383-398.

Šimůnek, J., R. Angulo-Jaramillo, M. Schaap, J.-P. Vandervaere & M. Th. van Genuchten, 1998a. Using an inverse method to estimate the hydraulic properties of crusted soils from tension disc infiltrometer data. Geoderma 86 [1-2], 61-81.

Šimůnek, J., M. Šejna & M. Th. van Genuchten, 1998b. The HYDRUS-1D software package for simulating the one-dimensional movement of water, heat, and multiple solutes in variably-saturated media. Version 2.0, IGWMC-TPS-70, International Ground Water Modeling Center, Colorado School of Mines, Golden, CO, 186pp.

Šimůnek, J., D. Wang, P. J. Shouse & M. Th. van Genuchten, 1998c. Analysis of a field tension disc infiltrometer experiment by parameter estimation. Intern. Agrophysics 12, 167-180.

Šimůnek, J., R. Kodešová, M. M. Gribb & M. Th. van Genuchten, 1999a. Estimating hysteresis in the soil water retention function from modified cone penetrometer test. Water Resour. Res. 35 [5], 1329-1345.

Šimůnek, J., M. Šejna & M. Th. van Genuchten, 1999b. The HYDRUS-2D software package for simulating the two-dimensional movement of water, heat, and multiple solutes in variably-saturated media. Version 2.0, IGWMC-TPS-56, International Ground Water Modeling Center, Colorado School of Mines, Golden, CO, 251pp.

Šimůnek, J., O. Wendroth & M. Th. van Genuchten, 1999c. A parameter estimation analysis of the laboratory tension disc experiment for determining soil hydraulic properties, Water Resour. Res., in press.

Šimůnek, J. & J. W. Hopmans, 2000. Parameter optimization and nonlinear fitting, In: J. H. Dane & G. C. Topp (eds.), Methods of Soil Analysis, Part 1, Physical Methods, Third edition, SSSA, Madison, WI, in press.

Šimůnek, J. & A. J. Valocchi, 2000. Geochemical Transport, In: J. H. Dane & G. C. Topp (eds.), Methods of Soil Analysis, Part 1, Physical Methods, Third edition, SSSA, Madison, WI, in press.

SNPI (Swedish Nuclear Power Inspectorate), 1986. INTRACOIN Final Report, Levels 2 and 3, Model Validation and Uncertainty Analysis. SKI 86:2.

SNPI (Swedish Nuclear Power Inspectorate), 1987. INTRAVAL Project Proposal. SKI 87:3.

Timlin, D. & Y. Pachepsky, 1998. Measurement of unsaturated soil hydraulic conductivities using a ceramic cup tensiometer. Soil Sci. 163 [8], 625-635.

U.S. Department of Energy, 1986. Environmental assessment: Yucca Mountain site, Nevada Research and Development Area, Nevada. DOE/RW-0073, Vol. 2, U.S. Department of Energy, Office of Civilian Radioactive Waste Mangement, Washington, DC.

van Genuchten, M. Th., 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. J. 44, 892-898.

Wooding, R. A., 1968. Steady infiltration from large shallow circular pond. Water Resour. Res. 4, 1259-1273.

Yeh, W. W-G. 1986. Review of parameter identification procedures in groundwater hydrology: The inverse problem. Water Resour. Res. 22 [2], 95-108.