Determinant of Parameters for Bimodal Hydraulic Functions by Inverse Modeling

Torsten Zurmuëhl and Wolfgang Durner*

ABSTRACT
To determine the hydraulic properties of soils, transient flow experiments on soil samples and their evaluation by parameter identification methods have become common. In the past, the feasibility of this method has been investigated for soils exclusively with unimodal pore-size distributions. In this work we investigated, both from a theoretical and from an experimental point of view, whether hydraulic properties of structured soils with bimodal pore-size characteristics can be identified by inverse simulation. Multistep outflow experiments were simulated for three hypothetical soils with different degrees of bimodality. The outflow data thus created were then used in the inverse procedure, both in the original form and with an added random error. An analysis of sensitivity coefficients for the model parameters showed that if the bimodality of the pore system is well developed, the parameters of the bimodal hydraulic functions are uncorrelated and can be identified. This was confirmed by inverse optimization runs with simultaneous optimization of up to six parameters, which consistently converged from different initial values to the true parameter values, indicating uniqueness of the inverse problem. Attempts to fit the bimodal outflow data with simulations using unimodal hydraulic functions were not successful, as expressed by systematic disagreement between fitted and "observed" data and nonuniqueness of the inverse solution. We validated these theoretical results with experimental data from an undisturbed sandy forest soil, which showed that it is possible to determine the retention parameters of bimodal hydraulic properties by inverse modeling of multistep outflow experiments.

Contamination of groundwater by hazardous substances has received increasing concern in the last decades. As the boundary conditions at the top of the soil, i.e., water infiltration and evapotranspiration, are mainly transient, water content and water flow in the soil will change with time and depth. As solutes are transported with the water phase, solute transport will also be transient. Thus the knowledge of the water flow is a prerequisite to simulate solute transport. The most important approaches to model water flow in unsaturated soils are based on the Richards equation. To solve this equation, a proper knowledge of the soil hydraulic properties, namely, the water retention characteristic and the hydraulic conductivity function, is required. The most common approaches to express the water retention curve as an analytical function are the models of Brooks and Corey (1966) and van Genuchten (1980). Van Genuchten’s parametric model is commonly used because it results in an analytical expression for the unsaturated hydraulic conductivity when it is combined with the concept of Mualem (1976). One of the drawbacks of most descriptions of hydraulic functions is that these curves imply the soil to possess a unimodal distribution of equivalent pore sizes; i.e., the derivative of the water content, θ, with respect to the logarithm of matric head, log(−ψ), is a function that has only one maximum (Durner, 1994). Natural soils, however, do not implicitly have a unimodal pore-size distribution. As an example, consider a well-aggregated soil that may have one maximum of pore-size classes in the range of intraaggregate pores and another one in the range of interaggregate pores. In order to gain more flexibility and to overcome the unimodal approach, multimodal retention functions were recently presented (Othmer et al., 1991; Durner, 1992; Wilson et al., 1992; Ross and Smettem, 1993). Zurmuëhl and Durner (1996) showed that the use of bimodal hydraulic functions not only influences the water flow but may also lead to enhanced solute transport compared with simulations using unimodal functions. The state-of-the-art method to determine unimodal soil hydraulic functions is the multistep outflow method with inverse modeling (Zachmann et al., 1982; Scotter and Clothier, 1983; Kool et al., 1985; van Dam et al., 1990). Eching and Hopmans (1993), van Dam et al. (1994), and Zurmuëhl (1996) demonstrated that the multistep method is superior to the one-step method because none of the parameters of the van Genuchten–Mualem model are correlated and therefore all of the parameters can be identified. The drawback of the more flexible multimodal hydraulic functions is the larger number of parameters. As the number of parameters to be optimized increases, the probability that two or more parameters are highly correlated will increase. High correlation of parameters means that a certain flow behavior under given boundary conditions can be equally well described by different parameter combinations. The parameters are then not identifiable by the inverse method (Yeh, 1986).

The aim of this study was to investigate whether the use of bimodal functions may improve the goodness of fit for measured outflow data and whether parameters of bimodal hydraulic functions can unambiguously be determined by the inverse modeling technique.

T. Zurmuëhl, Inst. of Soil Science, Dep. of Soil Physics, Univ. of Hohenheim, D-70593 Stuttgart, Germany; W. Durner, Dep. of Hydrology, Univ. of Bayreuth, D-95440 Bayreuth, Germany. Received 19 June 1997. *Corresponding author (Wolfgang.Durner@uni-bayreuth.de).


THEORY

One-dimensional water flow without sinks and sources is described by the Richards equation in the mixed form as
\[
\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ K(\theta) \frac{\partial \psi}{\partial z} - K(\theta) \right]
\]
where \( \theta \) is the volumetric water content, \( t \) (T) is time, \( z \) (L) is depth with positive values pointing downward, \( K(\theta) \) \((L\cdot T^{-1})\) is the hydraulic conductivity, and \( \psi \) (L) is the matric head. As a model for the unimodal water retention curve, the parametric function of van Genuchten (1980) is used
\[
\Theta(\psi) = \frac{\theta - \theta_s}{\theta_i - \theta_s} = \left[ 1 + (\alpha|\psi|)^{n} \right]^{-m} \quad \text{for } \psi < 0
\]
\[
\Theta(\psi) = \frac{\theta - \theta_s}{\theta_i - \theta_s} = \left[ \frac{1}{1 + (\alpha|\psi|)^{n}} \right] \quad \text{for } \psi \geq 0
\]
where \( \Theta(\psi) \) is the effective saturation, \( \theta_s \) is the saturated water
content, and \( \theta, \alpha [\text{L}^{-1}], n, \) and \( m \) are empirical parameters. Mualem (1976) proposed a semiempirical model to calculate the unsaturated relative hydraulic conductivity from water retention data:

\[
K(\theta) = K_s K_r(\theta) = K_s \int_0^\theta \left[ \frac{1}{1 - \phi(s)} \right] ds
\]

where \( K_r \) (L T\(^{-1}\)) is the saturated conductivity, which scales the predicted relative conductivity function, \( K_r \), and \( \tau \) is an empirical shape parameter that accounts for tortuosity and correlation between pore sizes. Substituting Eq. [2] into [3] and using the constraint \( m = 1 - 1/n \) gives the relative conductivity function in closed form:

\[
K_r(\theta) = \theta^\tau \left[ 1 - (1 - \theta^{1/m})^n \right]^2
\]

The derivative of \( \theta \) with respect to \( \log(-\phi) \), \( d\theta/d[\log(-\psi)] \) expresses an equivalent pore-size distribution, which for the functional form of Eq. [2] always has a unimodal shape.

For aggregated soils with a multimodal pore-size distribution, a more flexible retention function is used. Durner (1992) proposed a linear superposition of van Genuchten-type subcurves to yield the following expression for a multimodal retention curve:

\[
\Theta(\psi) = \sum_{i=1}^{k} w_i \left[ 1 + (\alpha_i |\psi|)^{n_i} \right]^{-m_i} \quad \text{for } \psi < 0
\]

\[
= \sum_{i=1}^{k} w_i \left[ 1 + (\alpha_i |\psi|)^{n_i} \right]^{-m_i} \quad \text{for } \psi \geq 0
\]

where the integer \( k \) denotes the modality of the model (i.e., the number of pore-size density maxima), \( w_i \) are the weighting factors for the subcurves, subject to the constraints \( 0 < w_i < 1 \) and \( \sum w_i = 1 \), and \( \alpha_i, n_i, \) and \( m_i \) are the curve-shape parameters of the subcurves, as in the unimodal case. The conductivity function for the multimodal model is again given by the predictive model of Mualem, Eq. [3]. As Eq. [5] cannot be analytically inverted, we evaluated Eq. [3] numerically for the bimodal hydraulic functions.

**Numerical Solution of the Direct Problem**

The Richards equation is solved in the mixed form following the method of Celia et al. (1990). For practical use, the hydraulic conductivity is numerically computed at 150 \( K(\psi) \) and \( K(\theta) \) values and stored in tabular form. These values are subsequently used as base values for rational spline interpolation. In this way, the bimodal hydraulic conductivity can be treated as a “closed-form” function in the simulations. To verify the numerical integration of Eq. [3] and the accuracy of the spline interpolations, simulations using the unimodal model with closed-form prediction of the hydraulic conductivity, Eq. [4], were compared with simulations using a numerical evaluation of Eq. [3] followed by spline interpolation. The initial and boundary conditions were those for the outflow experiment, given below. An excellent agreement between the two simulations was found (Fig. 1).

**Numerical Solution of the Inverse Problem**

To estimate the unknown hydraulic parameters, a nonlinear least-squares optimization approach based on the Levenberg-Marquardt method is used (Kool and Parker, 1988). The objective function, \( S(\mathbf{b}) \), which has to be minimized, is given by

\[
S(\mathbf{b}) = (\mathbf{Y}_m - \mathbf{Y}_c)^T W (\mathbf{Y}_m - \mathbf{Y}_c)
\]

\[
= \sum_{i=1}^{n} w_i (Y_{m_i} - Y_{c_i})^2
\]

where \( \mathbf{b} \) represents the vector of unknowns containing \( p \) adjustable parameters \( b_j \) (\( j = 1, ..., p \)); \( \mathbf{Y}_m \) is the vector of measured values and \( \mathbf{Y}_c \) the one containing the calculated values, which depend on time and depth and on the parameters of the hydraulic functions, i.e., \( Y_m = Y_m(t, z, \mathbf{b}) \); \( W \) is the weighting matrix, which is of diagonal form for uncorrelated measurements; and \( N \) is the number of measurements. Water content, matric head, and/or cumulative water outflow at some given depths could be used for the objective function. In this study, we focused only on cumulative water outflow. Minimizing \( S(\mathbf{b}) \) with respect to \( \mathbf{b} \) leads to \( p \) nonlinear equations for the \( p \) unknown parameters, which have to be solved iteratively. At the \( j \)th iteration, the correction vector \( \Delta \mathbf{b} \) is evaluated according to the following linear equation:

\[
\mathbf{b}^{j+1} = \mathbf{b}^j + \Delta \mathbf{b} \quad \Delta \mathbf{b} = -(\mathbf{J}^T \mathbf{W} \mathbf{J} + \lambda \mathbf{D}^T \mathbf{D})^{-1} \mathbf{J}^T \mathbf{W} \mathbf{r}
\]

where \( \lambda \) is a positive scalar, \( \mathbf{D} \) is a diagonal scaling matrix, \( \mathbf{J} \) is the \( N \times p \) Jacobian or sensitivity matrix, and \( \mathbf{r} = \mathbf{Y}_m - \mathbf{Y}_c \) is the vector containing the residuals. The elements of the sensitivity matrix are the derivatives of the calculated model outputs with respect to the parameters (\( J_{ij} = \partial Y_m/\partial b_i \)). They are approximated by finite differences according to

\[
\frac{\partial Y_m}{\partial b_i} = \frac{Y_m(x, t, b_1, ... , b_i + \Delta, ... , b_p) - Y_m(x, t, b_1, ... , b_i, ... , b_p)}{\Delta b_i}
\]

\( \Delta \) was set to 0.01 for all parameters except for \( b_1 < 0.1 \times 10^{-5} \). In this case \( \Delta b_i \) is set to 0.01. Details of the solution procedure can be found in Kool and Parker (1988).

**MATERIAL AND METHODS**

To study identifiability of parameters, three hypothetical soils, A, B, and C, with bimodal hydraulic functions were chosen (Fig. 2). The parameters are given in Table 1. Note that the values of \( \theta, K_s, \) and \( \tau \) are equal for all three soils. Soil C has a narrow textural pore-size distribution with a distinct secondary pore system at larger pore sizes. In Soil A, the secondary pore system is less pronounced and shifted toward smaller pores than in Soil C. In Soil B, the bimodality of the hydraulic functions is weak and the two pore systems are hard to distinguish. This soil might be described approximately as well by unimodal hydraulic functions.

For these soils the cumulative water outflow of an initially saturated homogeneous soil column with a length of 15 cm was simulated. No flux across the top of the column was
Fig. 3. Cumulative water outflow with (symbols) and without (lines) an equally distributed error of 0.05 cm for the different soils. The thin dashed line indicates the matric head at the lower boundary, $\psi_l$.

the same shape, a high correlation between these parameters exists. In this case a change of one parameter may be balanced by a corresponding change of the correlated parameter. Different parameter combinations thus may lead to the same model output, i.e., these parameters cannot be independently determined by the inverse method.

To test the uniqueness of the inverse method, parameter estimation runs were carried out using different parameter combinations as starting values. Two different starting values for $a_1, n_1, \theta_1, \sigma_2, n_2,$ and $w_1$ were combined with each other, resulting in 64 runs for each soil (Table 2). Since $\theta_1$ and $K_s$ are typically independently measured, we did not optimize these parameters. Further, $\tau = 0.5$ was kept constant. A uniformly distributed random error of 0.05 cm was overlaid on the deterministic outflow data to investigate the sensitivity of the inverse optimization to random errors in the observed data (Fig. 3). All runs were carried out with the error-free outflow data and with the data including the random error. The FORTRAN code ESHPIM was developed that solves the inverse problem for unimodal and bimodal functions (this program is available on request). The iteration was stopped when one of the following criteria was met:

$$\frac{\Delta b_i^{+1}}{b_i^*} < 10^{-4}; \quad \frac{S(b_i^{+1}) - S(b_i)}{S(b_i)} < 10^{-5};$$

for all $b_i, \quad i = 1, \ldots, p \tag{10}$

To explore the capability of unimodal hydraulic functions to simulate the outflow calculated with the bimodal functions, parameter estimation runs were conducted with different unimodal parameter combinations as starting values (see Table 3). For greater flexibility in the fitting process, we additionally allowed the conductivity parameters $K_s$ and $\tau$ to vary. Two values for $a, n, \theta, K_s,$ and $\tau$ were combined with each other, yielding 32 different runs. The bimodal outflow values without error were used as “measured” data.

To validate the results from the numerical analysis, the inverse procedure was tested with a soil column outflow experiment in the laboratory. The columns consisted of a 12.0-cm

Table 1. Parameters of the bimodal hydraulic functions for the three soils.

<table>
<thead>
<tr>
<th>Soil</th>
<th>$a_1$ (cm$^{-1}$)</th>
<th>$n_1$</th>
<th>$\theta_1$</th>
<th>$\sigma_2$</th>
<th>$K_s$ (cm h$^{-1}$)</th>
<th>$w_1$ (cm)</th>
<th>$a_2$ (cm$^{-1}$)</th>
<th>$n_2$</th>
<th>$\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.10</td>
<td>2.7</td>
<td>0.03</td>
<td>0.36</td>
<td>10.0</td>
<td>0.3</td>
<td>0.01</td>
<td>1.9</td>
<td>0.5</td>
</tr>
<tr>
<td>B</td>
<td>0.15</td>
<td>1.8</td>
<td>0.03</td>
<td>0.36</td>
<td>10.0</td>
<td>0.4</td>
<td>0.02</td>
<td>1.3</td>
<td>0.5</td>
</tr>
<tr>
<td>C</td>
<td>0.50</td>
<td>4.0</td>
<td>0.03</td>
<td>0.36</td>
<td>10.0</td>
<td>0.1</td>
<td>0.01</td>
<td>1.8</td>
<td>0.5</td>
</tr>
</tbody>
</table>
Table 2. Starting values of the parameters for the optimization runs with bimodal hydraulic functions for the three different soils.

<table>
<thead>
<tr>
<th>Soil</th>
<th>$\alpha_1$</th>
<th>$n_1$</th>
<th>$\theta_1$</th>
<th>$w_1$</th>
<th>$\alpha_2$</th>
<th>$n_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.50</td>
<td>3.5</td>
<td>0.001</td>
<td>0.5</td>
<td>0.05</td>
<td>2.5</td>
</tr>
<tr>
<td></td>
<td>0.01</td>
<td>2.0</td>
<td>0.100</td>
<td>0.1</td>
<td>0.002</td>
<td>1.5</td>
</tr>
<tr>
<td></td>
<td>0.05</td>
<td>1.5</td>
<td>0.100</td>
<td>0.1</td>
<td>0.005</td>
<td>1.2</td>
</tr>
<tr>
<td>B</td>
<td>0.50</td>
<td>3.0</td>
<td>0.001</td>
<td>0.5</td>
<td>0.100</td>
<td>2.0</td>
</tr>
<tr>
<td></td>
<td>0.05</td>
<td>1.5</td>
<td>0.100</td>
<td>0.1</td>
<td>0.005</td>
<td>1.2</td>
</tr>
<tr>
<td>C</td>
<td>0.90</td>
<td>5.0</td>
<td>0.001</td>
<td>0.4</td>
<td>0.05</td>
<td>2.5</td>
</tr>
<tr>
<td></td>
<td>0.05</td>
<td>2.0</td>
<td>0.100</td>
<td>0.05</td>
<td>0.002</td>
<td>1.5</td>
</tr>
</tbody>
</table>

Table 3. Starting values of the parameters for the optimization runs with unimodal hydraulic functions for the three different soils.

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$n$</th>
<th>$\theta$</th>
<th>$K_s$</th>
<th>$\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>cm$^{-1}$</td>
<td>cm$^{-1}$</td>
<td>cm h$^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.008</td>
<td>1.5</td>
<td>0.001</td>
<td>1.0</td>
<td>-0.5</td>
</tr>
<tr>
<td>0.05</td>
<td>4.0</td>
<td>0.100</td>
<td>20.0</td>
<td>0.5</td>
</tr>
</tbody>
</table>

RESULTS AND DISCUSSION

Sensitivity Analysis

Sensitivity coefficients for $\alpha_1$, $n_1$, $w_1$, $\alpha_2$, $n_2$, and $\theta_1$ are shown in Fig. 4 for the three soils. The $T_{ij}$ values are given as a function of the row of the Jacobian matrix, because the columns of the Jacobian matrix have to be linearly independent in order to get uncorrelated parameters. The rows of the Jacobian matrix reflect the time steps in the measurements. Since, in an intelligent experimental design, the measurement times are not equally spaced, the axis in Fig. 4 is stretched in comparison to the time axis when fast changes and high flow rates occur, and is compressed when changes are slow. The fluctuations in the $T_{ij}$ values are due to the different pressure steps at the lower boundary. It is obvious that $\alpha_1$ and $n_1$ have their highest sensitivity at small numbers of Jacobian row, i.e., early times, because the secondary pore system associated with the first subcurve drains first. The highest sensitivity for $\alpha_2$ and $n_2$ consequently is at later times, thus $\alpha_1$ and $\alpha_2$ as well as $n_1$ and $n_2$ are not correlated for all three soils. Furthermore there are no linear dependencies between $\alpha_1$ and $n_1$ or between $\alpha_2$ and $n_2$. The sensitivity of $n_1$ for Soil C, however, is close to zero except at a limited range of rows from 5 to 30. Also the sensitivity of $\alpha_2$ for Soil B is quite low in comparison with the other soils. The weighting coefficient $w_1$ has its maximal value in the pressure range that lies in the region between the two maxima of the bimodal pore-size distribution. The sensitivity values of $\theta_1$ are inversely proportional to the water outflow, because the difference from the fixed value of $\theta_1$ determines the amount of water that can flow out of the soil column. For Soil B, a correlation between $n_1$ and $w_1$ and a weak linear dependence between $\alpha_1$ and $\theta_1$ can be observed. Thus for this soil the parameters are expected to be determined with large uncertainties. We conclude that if the bimodality of the hydraulic functions is weak, the risk of getting correlated parameters that cannot be independently identified increases.
Table 4. Number of runs that failed to find the true parameter values for the different bimodal soils with and without error in the “experimental data”.

<table>
<thead>
<tr>
<th>Soil</th>
<th>( \alpha_1, n_1, \theta_1, w_1, \alpha_2, n_2 )</th>
<th>( \alpha_1, n_1, \theta_1, w_1, \alpha_2, n_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>without error</td>
<td>with error</td>
<td>without error</td>
</tr>
<tr>
<td>A</td>
<td>3/64 (4.7%)</td>
<td>6/64 (9.4%)</td>
</tr>
<tr>
<td>B</td>
<td>15/64 (23.4%)</td>
<td>28/64 (43.8%)</td>
</tr>
<tr>
<td>C</td>
<td>6/64 (9.4%)</td>
<td>10/64 (15.6%)</td>
</tr>
</tbody>
</table>

Test of Uniqueness

Table 4 gives the number of runs with different starting values that failed to find the true minimum with and without some error in the outflow data. No significant differences can be found between optimizing six parameters or only five, fixing the value of \( \theta_0 \). If the data without error are examined, for Soils A and C the portion of runs that failed to converge to the global minimum is <10%, whereas it is in the range of 25% for Soil B. Imposing a random error of 0.05 cm on the outflow data leads to an increase in unsuccessful runs for all three soils. For Soils A and C, however, the percentage of runs that failed is still in the range of 10 to 15%, whereas it is in the range of 40% for Soil B. The higher number of runs that failed to converge to the global minimum for Soil B is consistent with the sensitivity analysis, which showed (i) small sensitivity of \( \alpha_2 \) and (ii) a correlation between \( n_1 \) and \( w_1 \) for this very weakly bimodal soil.

Testing Unimodal Functions

Figure 5 shows the “measured” bimodal outflow data and the best-fit outflow curves calculated with unimodal hydraulic functions, Eq. [2] and [4], optimizing \( \alpha, n, \theta_0, K_s, \) and \( \tau \). It is obvious that the fitted unimodal curves exhibit large systematic deviations from the measured ones, especially for Soils A and C. Furthermore it was found that the unimodal fittings were not unique, i.e., the iterations with different starting values lead to different local minima. Figure 6 shows all 32 hydraulic functions for all three soils obtained from the 32 parameter starting combinations, as given in Table 3. Both the water retention curve and the hydraulic conductivity show a large scatter, which for the hydraulic conductivity curve is mainly produced by different values of \( K_s \). Also the shape factors \( \alpha \) and \( n \) are not unique. Thus although the parameters of the unimodal van Genuchten–Mualem model can all be identified, as was shown by Zurmühl (1996), the inverse problem is not unique because the measured data cannot be described reasonably well with the unimodal model. This demonstrates that identifiability is a necessary but not a sufficient condition for well-posedness, i.e., existence, uniqueness, and stability of the inverse problem. This further implies that a failure to converge to a global minimum can be caused by an inadequacy of a chosen representation of the hydraulic functions for a given soil.

Examination of Experimental Outflow Data

Figure 7 shows the measured and fitted cumulative outflow data for the Rastatt sand in the upper part and the deviations between measured and optimized data.
ZURMUÈHL & DURNER: PARAMETERS FOR BIMODAL HYDRAULIC FUNCTIONS

In the lower part. Figure 8 gives the corresponding hydraulic functions. The data were fitted with bimodal and unimodal hydraulic functions, with $K_s$ set to the measured value. For the unimodal functions, an additional optimization was performed where $K_s$ was allowed to vary in order to increase the flexibility. It is obvious from Fig. 7 that only the bimodal functions lead to an acceptable agreement between the observed and fitted outflow data of the Rastatt soil. Particularly the fit of the unimodal model with $K_s$ set to the measured value shows large and systematic deviations. Not only the amount of outflow, but also the shape of the outflow curve deviates from the observations considerably, particularly at early times. The simulated outflow reacts to each pressure change very fast and reaches equilibrium far earlier than the observed data. This behavior is caused by the unsaturated hydraulic conductivity curve, which remains near the saturated value until the air-entry point at about $\log(\psi) = 1.5$ (Fig. 8). In contrast, the bimodal conductivity function shows an early drop after the drainage of a structural pore system, and then an additional drop at the air entry of the matrix pore system. If $K_s$ is included in the unimodal parameter optimization, the agreement between simulation and measurements is improved. This is achieved by a reduction of $K_s$ to a value that brings the unsaturated conductivity in the range $\log(-\psi) = 0.5$ to 1.5 close to that of the bimodal function. Although the main part of the observed drainage curve is better matched by this reduction, the large deviations at the first two pressure steps, caused by the early water loss from the structural pore system, are still obvious. This example again demonstrates the problem of matching the unimodal conductivity function with a measured saturated conductivity value. The use of bimodal hydraulic functions makes it possible to simulate the significant outflow at early times and the low fluxes at later times by a drop in the hydraulic conductivity near saturation. This indicates that the Rastatt soil has a secondary pore system of larger pores that cannot be described by unimodal hydraulic functions.

The sensitivity of the hydraulic conductivity function near saturation is by principle very low for any outflow experiment that is performed on relatively short soil columns. Accordingly, experience shows that the optimized values of the $K_s$ parameter is often considerably lower than an independently measured value and must be seen as a pure fitting parameter. As demonstrated above, fixing the $K_s$ parameter to the measured value can lead to a worse overall fit if unimodal functions are used to describe a soil that actually has a secondary pore system. The use of the more flexible bimodal function solves part of the problem. Fixing the $K_s$ parameter hardly affects the optimization result for the unsaturated portion of the hydraulic functions because the hydraulic model can account for the conductivity drop near saturation. Still, if $K_s$ is to be estimated by the inverse method, the parameter value is subject to great uncertainty due to its low sensitivity.

CONCLUSIONS

In this study the capability of the multistep outflow method with inverse modeling to determine the parameters of bimodal hydraulic functions was studied with three hypothetical soils. The bimodal water retention curve was assumed to be given by a superposition of van Genuchten subcurves, following Durner (1994). The hydraulic conductivity was calculated numerically using the concept of Mualem (1976). Sensitivity coefficients have been used as a suitable tool to examine identifiability of the parameters. It was shown that if the bimodality, expressed by two distinct pore systems, is well developed, the parameters of the different subcurves are not correlated, i.e., they could be determined independently. Evaluation of optimization runs with different starting values consistently showed that the inverse
problem is unique if the derivative of the water retention curve, $\partial \theta / \partial \log (-\psi)$, has two distinct maxima. Fitting unimodal functions to the bimodal calculated outflow data for the hypothetical soils indicated that outflow obtained from soils with bimodal functions cannot be reproduced with unimodal functions. Not only was the agreement of “measured” and fitted values bad, but also the inverse problem using unimodal functions was not unique. Thus if the underlying constitutive relationships are not an appropriate description of the hydraulic properties of a soil, different starting parameter combinations may converge to several local minima. The practical use of bimodal hydraulic functions was demonstrated with measured outflow data of an undisturbed soil column, consisting of a sandy forest soil. The measured data could be successfully fitted only by using bimodal functions. Thus the increased number of parameters, which is the price for more flexibility, does not impose problems to an inverse parameter optimization with outflow data, as long as the bimodality is well developed. The number of parameters that may be optimized simultaneously with the outflow method is not limited to a fixed number as, e.g., stated by Mous (1992). It depends on the type of pore system and thus the required complexity of its hydraulic functions on the one hand, and on the boundary conditions of the parameter identification experiment on the other hand.

In nature, undisturbed soils will often show some degree of aggregation, which causes their pore systems to deviate more or less from the idealized $\pm \log$-normal-shaped pore-size distribution, which is intrinsically assumed when a unimodal function is used for the hydraulic description. In practice, it may be best to perform the inverse procedure first with a simple classical hydraulic model. If the agreement between simulated and measured data is bad, the procedure can be repeated with a more flexible model. Dependent on the kind of observed disagreement, van Genuchten’s function with an unconstrained parameter $m$, or a bimodal or even a multimodal function, may be the most suitable model. From this point of view, the bimodal approach is a refinement rather than a replacement of the currently used method. Dependent on soil properties, measurement precision, and experimental conditions, even more flexible descriptions of the hydraulic functions (e.g., splines) can be appropriate. Summarizing, the decision about the adequate degree of flexibility of hydraulic functions used in an inverse optimization must be based on a careful comparison of fitted vs. observed outflow data and on examination of the correlation matrix of the sensitivity coefficients.

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