Parameter Estimation Analysis of the Evaporation Method for Determining Soil Hydraulic Properties

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ABSTRACT

Soil hydraulic properties are important parameters affecting water flow in variably saturated soils. We estimated the hydraulic properties from a laboratory evaporation experiment using both a parameter estimation method and the modified Wind method. The parameter estimation method combined a one-dimensional numerical solution of the Richards equation with the Marquardt–Levenberg optimization scheme. In our study we used both numerically generated data and data measured in the laboratory. Two experiments were carried out on 10-cm-high soil cores containing two different soils. Pressure heads inside the cores were measured with five tensiometers, while evaporative water loss from the top was determined by weighing the soil samples. The objective function for the parameter estimation analysis was defined in terms of the final total water volume in the core and pressure head readings by one or several tensiometers. An analysis of numerically generated data showed that the optimization method was most sensitive to the shape factor (n) and the saturated water content (θ_s) and least to the residual water content (θ_r). Pressure heads measured close to the soil surface were found to be more valuable for the parameter estimation technique than those measured at lower locations. The optimized hydraulic parameters corresponded closely with those obtained using Wind's analysis. All optimizations gave similar results for the soil hydraulic properties within the range of measured pressure heads (0 to -700 cm). Extrapolation beyond this range involved a high level of uncertainty because of high correlation between parameters θ_r and n.

M ANY LABORATORY AND FIELD METHODS exist to determine soil hydraulic properties, especially for the unsaturated hydraulic conductivity (Klute and Dirksen, 1986; Green et al., 1986). Most methods remain relatively time consuming and costly, and are often limited to relatively narrow ranges of water content. One fairly simple laboratory method for simultaneous estimation of both retention and unsaturated hydraulic conductivity data for the past 30 yr has been the evaporation method. This method was first introduced by Gardner and Miklich (1962), who imposed a series of constant fluxes on one side of an initially equilibrated sample, and measured the pressure head response of two tensiometers. The flux needed to be sufficiently small to assume a constant hydraulic conductivity and diffusivity in the sample (Halbertsma and Veerman, 1994). Becher (1971) simplified the evaporation method by using a continuous evaporation rate. Several other modifications of the evaporation method with simultaneous measurements of evaporation rate and pressure heads at different heights in the sample have since been devel-

oped (Wind, 1968; Becher, 1971; Boels et al., 1978; Schindler, 1980; Tamari et al., 1993; Wendroth et al., 1993; Halbertsma and Veerman, 1994).

An important modification was suggested by Wind (1968), who introduced an iterative graphical procedure. He first estimated the water retention characteristic from average water content and pressure head readings at several locations in a homogeneous soil sample, and subsequently determined hydraulic conductivities from the measured pressure head profile and changes in the water content distribution. The water content profile was obtained from results of the first step. The Wind iterative method was later automated by several researchers (e.g., Boels et al., 1978; Halbertsma and Veerman, 1994). Wendroth et al. (1993) developed a method that required measurement of the pressure head at only two locations. In the traditional setup, only unsaturated hydraulic conductivities in the pressure head range from approximately -50 to -700 cm could be determined. Good estimates of the conductivity close to saturation could not be obtained because the hydraulic gradients were too small. To overcome these problems near saturation, Wendroth et al. (1993) imposed two different evaporation rates: initially a relatively high evaporation rate to obtain large pressure head gradients near saturation and, after reestablishing hydraulic equilibrium, much lower evaporation rates as controlled by the prevailing laboratory conditions. Using numerically generated data, several researchers (Tamari et al., 1993; Wendroth et al., 1993; Mohrath et al., 1997) evaluated the assumptions of the evaporation method or the effects of experimental errors.

An alternative method of analyzing transient flow during an evaporation experiment is to use parameter estimation techniques (Kool et al., 1987). Methods of this type typically involve the coupling of a numerical model for variably saturated water flow with a parameter optimization algorithm. The Levenberg–Marquardt method (Marquardt, 1963) has been especially popular for this purpose. Starting with the studies of Zachmann et al. (1981) and Dane and Hruska (1983), the parameter estimation method is increasingly being used for estimating unsaturated soil hydraulic functions. Computer models applicable to laboratory column outflow measurements have been given by Kool et al. (1985a,b) and Parker et al. (1985) for one-step outflow procedures, and by van Dam et al. (1992, 1994) and Eching and Hopmans (1993) for multistep approaches. A more general parameter estimation model applicable to transient water flow subject to less restrictive initial and boundary conditions was developed by Kool and Parker (1987). Applications to evaporation experiments have been presented by Feddes et al. (1988), Ciollaro and Romano (1995), and Santini et al. (1995). In a review, Feddes et

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al. (1988) compared hydraulic conductivities determined from an evaporation experiment using both parameter estimation and Wind's method. While quite successful, they applied their method to only one data set and did not discuss problems of identifiability, stability, and uniqueness. As part of a study of the spatial variability of soil hydraulic properties, Ciollaro and Romano (1995) used parameter estimation to determine the soil hydraulic parameters of a large number of samples. Santini et al. (1995) also used parameter estimation in connection with evaporation experiments and compared the results with independently measured retention data and saturated hydraulic conductivities, K_s. No attempts were made in these two studies to also compare estimated unsaturated hydraulic conductivities with independent data. Both Ciollaro and Romano (1995) and Santini et al. (1995) assumed that θ_r was equal to zero, and independently measured θ_s. They defined the objective function only in terms of pressure head measurements, which prevented them from estimating θ_r and θ_s directly from the evaporation experiment. In spite of these relatively promising results, Halbertsma (1996) stated that evaporation experiments are not suitable for inverse modeling because of uniqueness problems.

The objective of this study was to evaluate in more detail the potential of parameter optimization techniques for simultaneously estimating the water retention and hydraulic conductivity relationships from an evaporation experiment. We addressed the questions of identifiability, uniqueness, and stability. The sensitivity of an evaporation experiment to particular soil hydraulic parameters was investigated so as to evaluate the minimum amount of information needed to guarantee a unique solution. We also addressed the question whether or not the two-rate evaporation method of Wendroth et al. (1993) provides better information for parameter estimation than the traditional one-rate method. The first part of our study was carried out using numerically generated error-free data. Numerically generated data sets are preferred for this analysis since the true values of soil hydraulic parameters are known and since no measurement errors are present, thus causing less uncertainty in the analysis (Toorman et al., 1992). Different sources of errors could bias some of the conclusions that can be drawn from numerically generated data. We next applied the parameter estimation technique to two laboratory data sets. These data sets contained sources of errors typically present in experimental data sets, such as measurement errors, small inhomogeneities in the samples, and other sources of noise, which would make their analysis more complicated. The soil hydraulic characteristics obtained were compared with those using the simplified Wind method (Wendroth et al., 1993).

METHODS

Governing Flow Equations

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

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

where θ is the volumetric water content ($L^3 L^{-3}$), h is the soil-water pressure head (L), K is the hydraulic conductivity ($L T^{-1}$), z is a vertical coordinate (L) positive upward, and t is time (T). Initial and boundary conditions applicable to an evaporation experiment are as follows:

$$h(z, 0) = h_i(z) \qquad [2]$$

$$-K\left(\frac{\partial h}{\partial z} + 1\right) = q_{evap}(L, t) \qquad [3]$$

$$q(0, t) = -K\left(\frac{\partial h}{\partial z} + 1\right) = 0 \qquad [4]$$

where h_i is the initial soil-water pressure head (L), $q_{evap}(t)$ is the time-variable evaporation rate imposed at the soil surface ($L T^{-1}$), and L is a coordinate of the soil surface. Equation [1], subject to the above initial and boundary conditions, was solved numerically using the finite-element code HYDRUS-1D as documented by Šimůnek et al. (1997).

The unsaturated soil hydraulic properties in this study were assumed to be described by the following expressions (van Genuchten, 1980):

$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \frac{1}{(1 + |\alpha h|^n)^m} \qquad [5]$$

$$K(\theta) = K_s S_e^l \left[1 - (1 - S_e^{1/m})^m\right]^2 \qquad [6]$$

where S_e is the effective water content, K_s is the saturated hydraulic conductivity ($L T^{-1}$), θ_r and θ_s denote the residual and saturated water contents ($L^3 L^{-3}$), respectively, l is a pore-connectivity parameter, and α (L^{-1}), n, and m ($=1 - 1/n$) are empirical parameters. The predictive $K(\theta)$ model is based on the capillary model of Mualem (1976) in conjunction with Eq. [5]. The pore-connectivity parameter l in the hydraulic conductivity function was estimated by Mualem (1976) to be 0.5 as an average for many soils. The hydraulic characteristics defined by Eq. [5] and [6] contain five unknown parameters: θ_r, θ_s, α, n, and K_s. The evaporation experiment in general is a drying process, which means that the hydraulic parameters in Eq. [5] and [6] represent drying branches of the unsaturated hydraulic properties.

Wind Method

During the evaporation experiments we monitored the pressure head at selected times t_j at five different depths z_i (1, 3, 5, 7, and 9 cm) within the soil column (10-cm height), and also repeatedly measured the total weight of the soil sample. After conclusion of the experiment, the final water content was measured, from which the total amount of water, $V_{m,j}$ (L), at each time, t_j, could be calculated. A fourth-order polynomial function for $\log(h)$–θ was fitted to the pairs of average soil water content and soil water pressure head data obtained at different times according to Halbertsma and Veerman (1994). The polynomials were calculated by multiple regression. A polynomial function of fourth order was chosen since a third-order polynomial function did not always provide enough flexibility to follow the particular shape of the $\log(h)$–θ curve. The water content value $\theta_{i,j}^k$ was subsequently calculated for each pressure head reading for iteration number $k = 1$. For a given time t_j, this water content value was considered representative for the depth compartment associated with a

particular tensiometric reading. Multiplying the thicknesses of the five compartments with the respective volumetric water contents yielded water storage values, which, when summed, gave the calculated total water storage, $V_{c,j}$, at a given time. A correction factor c_j^k was determined from the ratio between the calculated amount of water and the measured total amount of water, $V_{m,j}$. This approach led to a set of j correction factors, one for each time when the weight and tensiometer readings of the sample were obtained. Assuming that the error invoked in the initial water retention curve was distributed equally to the five depth compartments, the calculated water content values $\theta_{i,j}^k$ were updated using

$$\theta_{i,j}^k = \frac{\theta_{i,j}^k}{c_j^k} \qquad [7]$$

to lead to new estimates of the water content, $h-\theta_{i,j}^k$. The resulting data pairs of $h-\theta_{i,j}^k$ were subsequently used to obtain an improved polynomial function for $\log(h)-\theta$. Using this function and the measured pressure heads, new water content estimates $\theta_{i,j}^{k+1}$ for iteration $k + 1$ were obtained, leading to calculated water storage values that were closer to the measured values (i.e., the correction factors c_j^k became closer to one). With each iteration, the difference between the measured and calculated total water storage values decreased. The solution was considered to converge when the maximum water content change between two iterations became insignificant (less than some small preset value). Once convergence in the water retention curve was reached, temporal changes in the water content of each of the five compartments were used to calculated water flux profiles as follows

$$q_{i,j} = \frac{V_{i,j+1} - V_{i,j}}{\Delta t_j} + q_{i+1,j} \qquad [8]$$

in which q_{ij} (L T^{-1}) denotes the flux from compartment i upward into compartment $i - 1$ (the compartment number increases with depth) during time interval $\Delta t_j = t_{j+1} - t_j$, where t_j and t_{j+1} are the beginning and the end of the time interval. The hydraulic conductivity for a compartment was subsequently derived according to Darcy:

$$K(\overline{h}_{i,j}) = \frac{q_{i,j}}{(\Delta h_{i,j}/\Delta z_i) + 1} \qquad [9]$$

where $\Delta h_{i,j}$ is the hydraulic gradient between two consecutive compartments (z_{i-1} and z_i) as estimated from tensiometer readings, and $\Delta z_i = z_{i-1} - z_i$. In Eq. [9] we used the average gradient during a given time interval, Δt_j. The K value was next plotted against the geometric mean, $\overline{h}_{i,j}$, of the pressure head values within the two compartments at the beginning and the end of the time interval involved.

Inverse Solution

The objective function Φ, which is minimized during the parameter estimation process, is defined as

$$\Phi(\mathbf{b}, \mathbf{p}) = \sum_{j=1}^{m} v_j \sum_{i=1}^{nj} w_{i,j} \, [p_j^* \, (t_i) - p_j(t_i, \mathbf{b})]^2 \qquad [10]$$

where m represents the different sets of measurements (observed pressure heads at different locations and the total water volumes in the sample), n_j is the number of measurements in a particular measurement set, $p_j^*(t_i)$ are specific measurements at time t_i for the jth measurement set, $p_j(t_i,\mathbf{b})$ are the corresponding model predictions for the vector of optimized parameters $\mathbf{b}$ (e.g., θ_r, θ_s, α, n, and K_s), and v_j and $w_{i,j}$ are weights associated with a particular measurement set or point, respectively. For an evaporation experiment, the vector $\mathbf{p}_j^*$ consists of pressure heads measured at either one or several locations,

and one value of the average water content in the soil sample, usually measured at the end of the experiment. We assumed in this study that the weighting coefficients $w_{i,j}$ in Eq. [10] are equal to one; that is, the variances of the errors inside of a particular measurement set are the same. The weighting coefficients v_j are given by (Clausnitzer and Hopmans, 1995)

$$v_j = \frac{1}{n_j \sigma_j^2} \qquad [11]$$

which shows that the objective function is defined as the average weighted squared deviation normalized by measurement variances σ^2. Since the final water volume is only one number and the variance cannot be defined, the weight for this data point is assumed to be one.

Minimization of the objective function Φ is accomplished by using the effective Levenberg–Marquardt nonlinear minimization method (Marquardt, 1963), which has become a standard in nonlinear least-square fitting among soil scientists and hydrologists (van Genuchten, 1981; Kool et al., 1985a,b, 1987). The method combines the Newton and steepest descent methods, and provides confidence intervals for the optimized parameters.

NUMERICAL EXPERIMENT

An evaporation experiment was first simulated numerically using average parameter values of the silty soil textural group as estimated by Carsel and Parrish (1988) from an analysis of a large number of soils. The soil hydraulic parameters for this hypothetical experiment are given in Table 1. The soil sample was assumed to have a height of 10 cm, with five tensiometers located in the soil core 1, 3, 5, 7, and 9 cm below the sample surface. The soil profile was divided into 100 elements for our numerical simulations using HYDRUS-1D. The thickness of the first element at the soil surface was 0.0205 cm. Subsequent elements increased linearly up to 0.1111 at the depth of the first tensiometer, below which the grid spacing remained constant throughout the sample.

As an initial condition, we assumed hydraulic equilibrium with a zero pressure head at the bottom of the soil sample. A zero-flux condition was imposed at the bottom boundary. Two scenarios were used for the upper boundary condition. For the first scenario we assumed a constant evaporation rate of 0.15 cm d^{-1} for 14.4 d. Pressure head readings at intervals of 0.1 d were used to define the objective function. In the second scenario a higher evaporation rate of 1.5 cm d^{-1} was used during the first 0.5 d, followed by a zero surface flux until 1 d, and a constant rate of 0.15 cm d^{-1} afterward until the end of the simulation at 10.4 d. Shorter measurement intervals of 0.05 d were employed for the higher evaporation rate. The second scenario was used to evaluate whether or not a two-rate evaporation experiment (Wendroth et al., 1993) could benefit the parameter optimization procedure. Both simulations were terminated when the pressure head of the uppermost tensiometer dropped below -700 cm. Pressure head readings for both scenarios are shown in Fig. 1. Notice the much faster decrease in pressure head for the second (two-step evaporation) scenario at the beginning of the experiment.

Table 1. Parameter spacings used for the parameter planes of the hypothetical evaporation experiment.

Parameter	True value	Lower parameter value	Parameter step value	Upper parameter value
θ_r	0.034	0.00	0.0035	0.1015
θ_s	0.46	0.307	0.007	0.51
α, cm^{-1}	0.016	0.002	0.002	0.06
n	1.37	1.02	0.02	1.6
K_s, cm d^{-1}	6.0	0.00001	1.0	30.0

Evaporation losses during the first 5 d for the first scenario were about equal to the evaporation loss during the first day for the second scenario; pressure head readings afterward were almost identical except for the time difference of 4 d.

Two-rate evaporation experiments have two important advantages compared with more traditional one-rate experiments. First, by initially increasing the evaporation rate, the total amount of time required for the experiment can be decreased (e.g., by 4 d in our example). Second, higher evaporation rates require higher fluxes inside the soil sample, and correspondingly higher pressure head gradients. By increasing the pressure head gradients, the effects of experimental errors associated with the pressure head readings can be reduced substantially (Wendroth et al., 1993). This is especially important when hydraulic conductivities are calculated directly from pressure head gradients, as is the case with the Wind method or its modifications. The question remains whether or not adapting two-rate evaporation experiments will also benefit numerical inversions, which use only pressure head readings and do not require the estimation of gradients from measured data. If such a benefit exists, then the sensitivity of pressure head readings to the unknown soil hydraulic parameters would have to increase significantly during the high-evaporation stage of a two-rate evaporation experiment. We first studied this problem by means of a sensitivity analysis.

Sensitivity Analysis

In general, an experiment should be designed such that measurements are made that yield the most information about the unknown parameters to be optimized, i.e., measurements that are most sensitive to changes in the unknown parameters. One could expect that different locations of the tensiometers and measurements taken at different times will provide different degrees of information for the parameter estimation method. The optimal positions of the tensiometers are best evaluated by means of a sensitivity analysis.

Sensitivity coefficients, $s(z,t,b_j)$, for the hypothetical experiment were calculated from (Šimůnek and van Genuchten, 1996)

Fig. 1. Simulated pressure heads h for a silty soil for (a) one- and (b) two-step evaporation experiments.

$$s(z,t,b_j) = 0.01b_j \frac{\partial h(z,t,b_j)}{\partial b_j} \approx 0.01b_j \frac{h(\mathbf{b} + \Delta\mathbf{b}e_j) - h(\mathbf{b})}{1.01b_j - b_j}$$

$$= h(\mathbf{b} + \Delta\mathbf{b}e_j) - h(\mathbf{b}) \qquad [12]$$

where $s(z,t,b_j)$ is the change in the variable h (the pressure head) corresponding to a 1% change in parameter b_j, $\mathbf{e}_j$ is the jth unit vector, and $\Delta\mathbf{b} = 0.01\mathbf{b}$. Equation [12] allows a comparison of the sensitivities to different parameters, independent of the invoked units or their absolute values. We stress here that Eq. [12] calculates sensitivity coefficients, which characterize the behavior of the objective function at a particular location in parameter space, presumably in the vicinity of the true parameter values. A high sensitivity in this respect means that the minimum is well defined, and that one should be able to estimate the parameters with relatively high precision once the global minimum is identified. The approach, however, does not give any information about possible local minima in the objective function elsewhere in parameter space.

Figure 2 shows sensitivity coefficients for all five hydraulic parameters as calculated with Eq. [12] for five different tensiometer locations in the soil core. Results are for the constant-evaporation case; similar results were obtained also for the two-rate evaporation experiment (data not shown here). Results for both scenarios, as in Fig. 1, have similar shapes in terms of the time translation of 4 d. The sensitivity coefficients for both scenarios increased substantially as the experiments progressed in time, suggesting that long-duration experiments will provide much more information for the parameter optimization process. The second scenario, however, shows only a relatively insignificant bump during the first day when the evaporation rate is high. These slightly higher sensitivity coefficients are not expected to have an important effect on the overall parameter estimation procedure, except for short-duration experiments.

The absolute sensitivity of the pressure head readings to all soil hydraulic parameters increased with time as the soil profile became drier. With the exception of α, Tensiometer 1 yielded much higher sensitivity coefficients to changes in the hydraulic parameters than the other tensiometers. Figure 2 indicates that the pressure head is most sensitive to the parameter n, followed by θ_s. Sensitivities to θ_r, α, and K_s are, by comparison, much smaller. The results presented in Fig. 2 also suggest that the longer the measurements are taken, the more valuable the information becomes.

One can expect the sensitivity of tensiometer readings to increase with time. As the soil becomes drier, the retention curve becomes steeper, resulting in larger changes in pressure head with small changes in parameter values and water contents. Figure 3 shows sensitivity coefficients expressed in terms of the water content for all five hydraulic parameters for five different locations in the soil core. Notice that sensitivity coefficients, again, increased with time for all parameters except **α** for the location closest to the soil surface. The increase is, however, less steep due to the nonlinear nature of the retention curve. Sensitivity coefficients at other locations also increased initially, but reached a maximum at about 10 to 12 d, after which they remained more or less constant.

Response Surfaces

We tested whether data measured conventionally during an evaporation experiment (i.e., pressure head readings at several locations and average water contents) provide enough information to enable the identification of a unique set of soil hydraulic parameters from the inverse problem. We approached this question in a similar way as was done previously by Toorman et al. (1992) and Šimůnek and van Genuchten
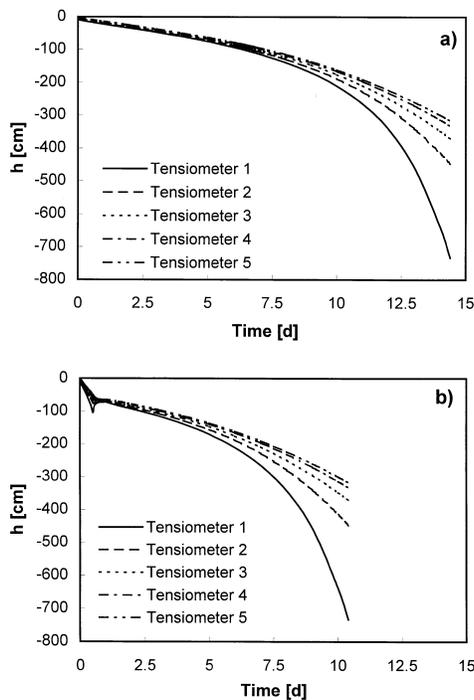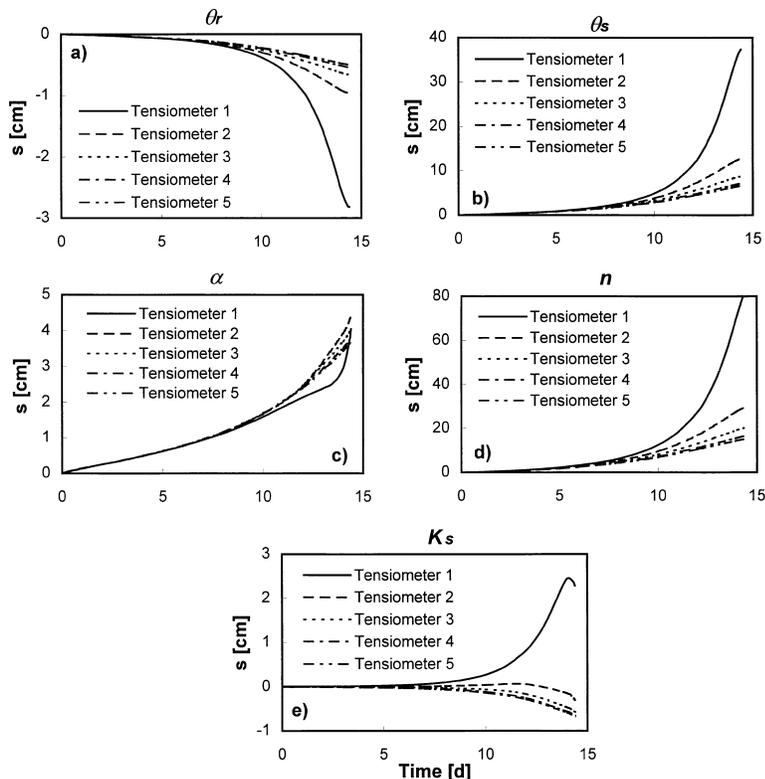
Fig. 2. Sensitivity of the pressure head h to parameters (a) residual soil water content, θ_r, (b) saturated water content, θ_s, (c) α, (d) n, and (e) saturated hydraulic conductivity, K_s, as a function of time for a silty soil assuming a one-step evaporation experiment.
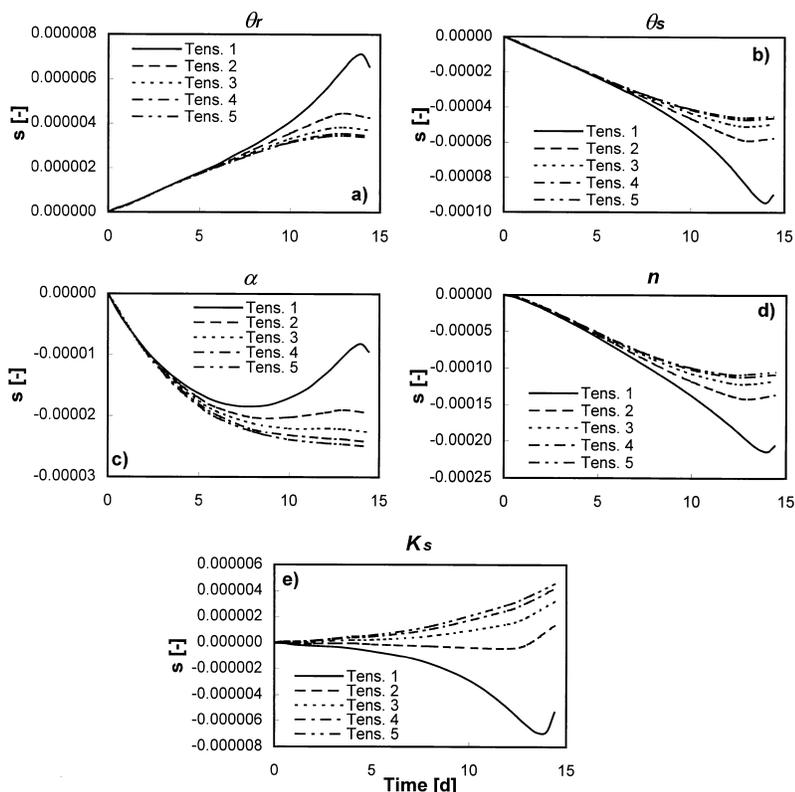
Fig. 3. Sensitivity of the water content θ to parameters (a) residual soil water content, θ_r, (b) saturated water content, θ_s, (c) α, (d) n, and (e) hydraulic conductivity, K_s, as a function of time for a silty soil assuming a one-step evaporation experiment.

(1997) in studies of the one-dimensional one-step outflow method and the axisymmetrical three-dimensional tension infiltrometer experiment, respectively.

The uniqueness of the inverse problem was evaluated in terms of two-dimensional response surfaces of the objective function as a function of pairs of soil hydraulic parameters. Response surfaces were obtained by changing two selected soil hydraulic parameters around their true values, while keeping other parameters constant at their true values. The objective function used for this purpose is given by Eq. [10]. We calculated the objective functions for 10 parameter planes (i.e., α–n, α–K_s, n–K_s, α–θ_s, n–θ_s, K_s–θ_s, α–θ_r, n–θ_r, K_s–θ_r, and θ_r–θ_s) for all data combined (i.e., five tensiometer readings and the final average water content) and for each tensiometer separately combined with the final average water content. The response surfaces were calculated on a rectangular grid with parameter values given in Table 1. Each parameter domain was discretized into 30 discrete points, resulting in 900 grid points for each response surface.

We emphasize that the different parameter planes given below represent only cross sections of the full five-dimensional parameter space. The behavior of the objective function in these parameter planes can only suggest how the objective function might behave in the five-dimensional continuum. For example, local minima of the objective function Φ could exist and not show up in the cross-sectional planes (Šimůnek and van Genuchten, 1996). Nevertheless, the response surfaces provide a useful approximate view of the behavior of the objective function in the entire parameter space. The inverse parameter estimation technique is expected to be unsuccessful if response surfaces do not display a clearly defined global minimum in the two-dimensional parameter planes.

Contours of the objective function Φ in 10 parameter planes are presented in Fig. 4. The objective function Φ was defined in terms of all five tensiometer measurements and the final total water volume in the sample. All response surfaces, with the exception of the n–θ_r parameter plane (Fig. 4h), show relatively well-defined global minima, and no additional local minima. The structure of the response surfaces is very consistent with plots of the sensitivity coefficients presented above. Because of the high sensitivity of the pressure head to the saturated water content (Fig. 2), θ_s yields well-defined minima in all parameter planes (Fig. 4d, 4e, 4f, and 4j). By comparison, the sensitivity to K_s was relatively low (Fig. 2), with the response surfaces showing also less certainty toward this parameter (Fig. 4b, 4c, and 4f). While the different minima for K_s are still relatively well defined, many of the contours away from the minima are nearly parallel with the K_s axis, especially at the higher K_s values. This suggests that initial estimates of K_s for parameter optimization should be relatively small. Pressure head measurements were also quite sensitive to n, with this parameter again yielding relatively well-defined minima (Fig. 4a, 4c, and 4e). One exception is the n–θ_r parameter plane (Fig. 4h), mainly because of uncertainty in θ_r, toward which the measurements showed the lowest sensitivity. The parameters n and θ_r were found to be highly correlated, as will be discussed below.

Inverse Solutions

We next examined whether the global minimum of the response surfaces could be identified numerically via inverse simulation using the Levenberg–Marquardt optimization method. We defined the objective function of Eq. [10] in terms of the final total water volume in the soil sample and either

(i) all available pressure head data (at five locations and for each time), (ii) only one tensiometer reading at a time, or (iii) data from two tensiometers (1 and 5). For each case we chose three different sets of initial estimates. For the one-rate evaporation experiment, all three optimizations converged when all five or two tensiometers were used; for optimizations using only one particular tensiometer data set, at least two runs were always successful. The results were slightly worse for the two-rate evaporation experiment in that only two of the three optimizations converged toward the true parameters for all simulations with different definitions of the objective function. The value of the objective function for unsuccessful optimizations was about four orders of magnitude higher than for the successful runs, while the parameter values also yielded physically unrealistic values. Failure in the optimization was caused primarily by uncertainty in the parameters θ_r and n, and partially in K_s. When θ_r was fixed at its true value, or when one (θ,h) pair for $h = -150$ m was included in the objective function (Kool et al, 1985b), all optimizations for both scenarios converged rapidly to the true parameter values.

Table 2 presents a correlation matrix for the optimized parameters when all tensiometer readings were used for the one-rate evaporation experiment. Note the high correlation between n and θ_r, which corresponds well with our findings for the response surfaces (Fig. 4h). Because of this high correlation, these two parameters show a high level of uncertainty. The uncertainty in θ_r is due to the fact that within the range of measurement (0 to -700 cm) for the silty soil used here, the effective water content (S_e) dropped only to about 0.40, still far from the residual water content. As will be shown below for our laboratory data, several combinations of n and θ_r can yield similar retention curves within the range of measurements. Although the optimized parameters describe the retention curve well within the measurement range, extrapolation beyond this range will introduce a high level of uncertainty. A similar problem was also encountered by Parker et al. (1985) when analyzing one-step outflow data. They found that using only cumulative outflow data resulted in satisfactory results within the range of water contents observed in the experiment, but not for much lower θ. Including the water content at $h = -150$ m into the objective function extended the range of validity of the predicted properties to the dry end with only minor effects on the predictions at high θ values (Parker et al., 1985). One alternative solution for this problem is to estimate the parameter θ_r independently, such as by independent measurement or even using pedotransfer functions (Schaap et al., 1998), and then to treat θ_r as a known parameter. If estimated in this way, θ_r can then also be included into the objective function and the solution can be penalized for any deviations from this value (Russo et al., 1991). This technique yields Bayesian estimates of θ_r (e.g., Bard, 1974; Yeh, 1986; Šimůnek and van Genuchten, 1996). Inclusion of the true value of θ_r in the objective function always resulted in response surfaces with clearly defined minima in terms of θ_r (results not further shown), while also all optimizations converged accurately and rapidly toward the true parameter values.

Not addressed in this study is the effect on the optimization results of using initially different estimates of the parameters. For our optimizations we selected three sets that were known to be physically realistic for the soils used in our numerical experiments.

LABORATORY EXPERIMENT

Two undisturbed soil core samples with a height of 10 cm and inside diameter of 10 cm were placed on a ceramic plate
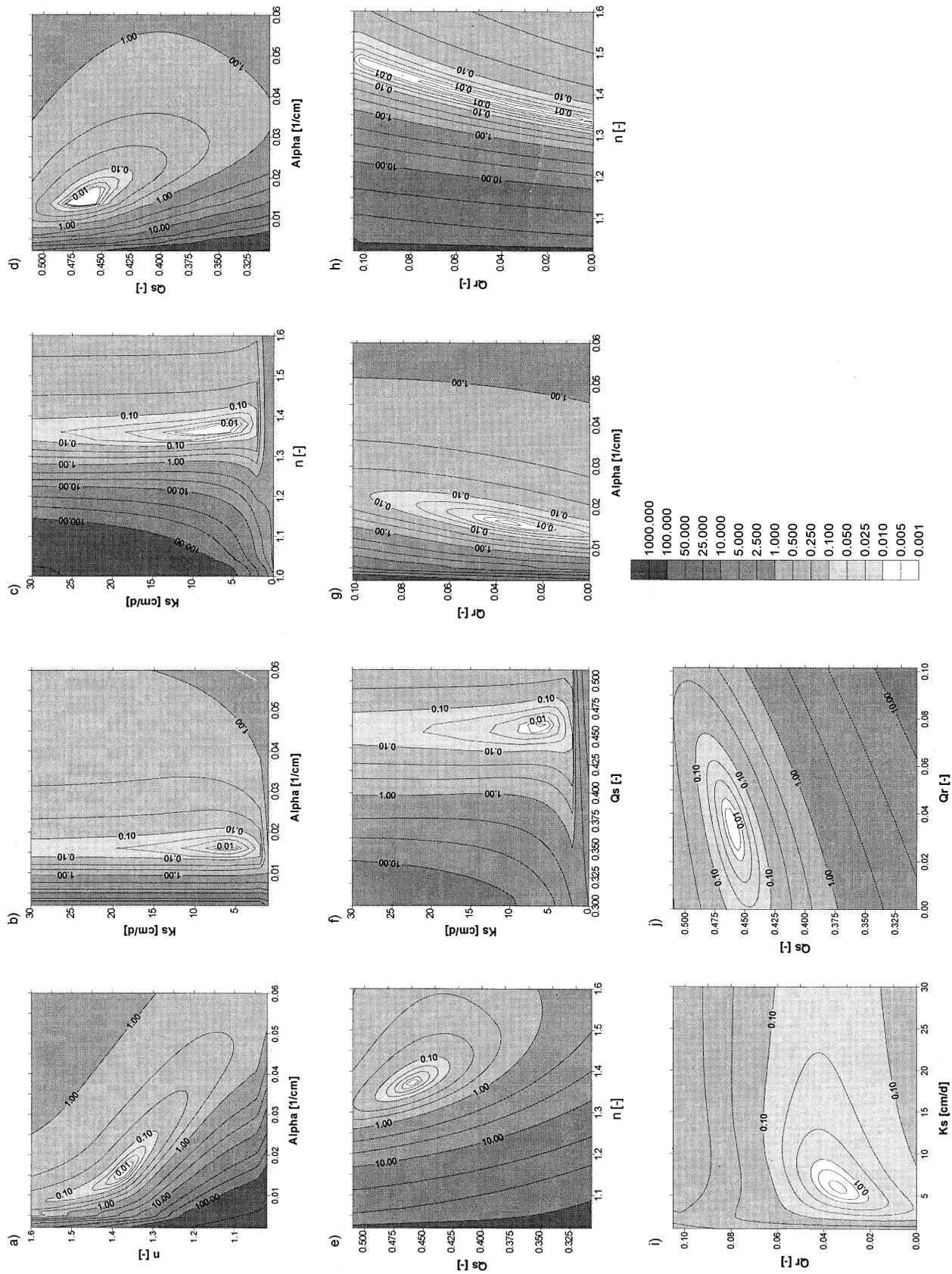
Fig. 4. Contours of the objective function Φ in the (a) α–n, (b) α–K_s, (c) n–K_s, (d) α–θ_s, (e) n–θ_s, (f) K_s–θ_s, (g) α–θ_r, (h) n–θ_r, (i) K_s–θ_r, and (j) θ_r–θ_s parameter planes. A dot represents the true value of parameters.

Table 2. Correlation matrix for the optimized parameters for the hypothetical evaporation experiment.

Parameter	θ_r	θ_s	α	n	K_s
θ_r	1.0				
θ_s	−0.7772	1.0			
α	−0.5425	0.4903	1.0		
n	0.9850	−0.7964	−0.6745	1.0	
K_s	−0.2318	0.2549	0.8893	−0.3871	1.0

and saturated with deionized water. Soil used in the first core sample (Experiment I) had a bulk density of 1.59 g cm^{-3}, and sand, silt, and clay fractions of 7.4, 79.3, and 13.3%, respectively. The second soil core sample (Experiment II) had a bulk density of 1.58 g cm^{-3} and sand, silt, and clay fractions of 45.2, 43.6, and 11.2%, respectively. Five tensiometers with cups of 6-cm length and 0.6-cm outside diameter were horizontally inserted into drill holes in the soil cores 1, 3, 5, 7, and 9 cm from the sample surface. The ceramic cups were connected to pressure transducers. Following previous experiments on the same soil columns with infiltrometer disks, the samples were moved onto impermeable plates for the evaporation experiment. Initial pressure heads of −15.4 cm for Experiment I and −19.3 cm for Experiment II were measured in the middle of the soil sample.

Evaporation was subsequently allowed to start. After each pressure reading, transducer wires were disconnected and the soil samples with the tensiometers weighted to determine the evaporative water loss as a function of time. At the beginning of the experiments the evaporation rate was increased to approximately 1.2 cm d^{-1} by using of a fan to blow air away from the soil surface at room temperature (Wendroth et al., 1993). Once the gradient between the tensiometers reached a value between 1.5 and 2.5 m m^{-1}, the top of the soil sample was covered to prevent further evaporation. After reestablishing hydraulic equilibrium in the samples, evaporation was allowed to continue, without the fan, at a rate of approximately 0.2 cm d^{-1}. Measurements were taken every 30 min during higher evaporation rate period, and every 4 h during the lower rates. The evaporation experiment was terminated after the upper tensiometer recorded a pressure head value below −650 cm. This limit was originally set because of the close proximity of the tensiometer measurement range, and because Wind's method requires simultaneous readings of all installed tensiometers. For the purpose of parameter optimization study, the experiment could have continued as long as at least one tensiometer was functioning. The water loss between particular measurements was used to calculate the average evaporation rate for a given time interval; this information was subsequently used as the upper boundary condition in the numerical simulations.

RESULTS AND DISCUSSION

The laboratory experiments were first analyzed using the modified Wind method as described by Wendroth

et al. (1993). We obtained 179 and 303 data pairs $\theta(h)$ and 94 and 119 data pairs $K(h)$ for Experiments I and II, respectively. The lowest tension for which we could calculate the hydraulic conductivity was 26 cm. Hence, we also included in the data sets for each experiment three $K(h)$ data points measured with a tension infiltrometer at pressure heads of −1, −5, and −10 cm. The hydraulic parameters for both soils were obtained by simultaneous fitting Eq. [5] and [6] to the resulting $\theta(h)$ and $K(h)$ data using the RETC code (van Genuchten et al., 1991). We obtained an excellent fit with $R^2 =$ 0.992 and 0.963 for Experiments I and II, respectively. There was some uncertainty in the parameters K_s and n for Experiment I because of high correlation (−0.992) between these two parameters. The final parameters for both experiments are given in Tables 3 and 4. Data obtained with Wind's method and the fitted hydraulic functions are shown in Fig. 5 and 7 for Experiments I and II, respectively.

The soil hydraulic parameters were also estimated from the evaporation experiment using parameter inversion. We used, for this purpose, the tensiometer readings as a function of time and the total water volume at the end of the experiment. All other water volume measurements were used to calculate evaporation rates needed for the upper boundary condition in the simulations. Inclusion of these measurements in the objective function would have resulted in duplicate information, without any benefit for the numerical inversion process. Only one value of the water volume (irrespective of when the measurement was made) is needed in the objective function in order to position the retention curve along the θ axis. Without this information, neither θ_s nor θ_r can be estimated because of their mutual correlation. The objective function therefore always involved the total volume of water at the end of the experiment. Three different scenarios were used for the data analysis (Tables 3 and 4). Pressure head measurements of all five tensiometers were included in the objective function for the first scenario. Only one tensiometer data set at a time was used for the second scenario. Readings from tensiometers located closest to the upper and lower boundaries (Tensiometers 1 and 5) were included in the objective function for the third scenario. In this way we hoped to find the minimum information needed for successful numerical inversion. The resulting optimized soil hydraulic parameters are listed in Tables 3 and 4 for both experiments, together with the final values of the objective function Φ and the R^2 for regression of predicted vs. measured values. Soil hydraulic character-

Table 3. Results of parameter estimation and Wind's method for Experiment I.

Scenario	Run	Φ	θ_r	θ_s	α	n	K_s	R^2
					cm^{-1}		cm d^{-1}	
1	All tensiometers	0.00318	0.0055	0.321	0.0274	1.22	93.1	0.9987
2	Tensiometer 1	0.00250	0.0001	0.321	0.0284	1.20	181.	0.9989
	Tensiometer 2	0.00127	0.0228	0.322	0.0317	1.22	45.1	0.9995
	Tensiometer 3	0.00150	0.1365	0.307	0.0210	1.55	24.8	0.9994
	Tensiometer 4	0.00154	0.1317	0.309	0.0229	1.49	33.1	0.9994
	Tensiometer 5	0.00250	0.0210	0.321	0.0279	1.23	131.	0.9990
3	Tensiometers 1 and 5	0.00288	0.0000	0.321	0.0277	1.21	105.	0.9988
Wind's method		–	0.0045	0.321	0.0249	1.23	73.3	0.992

Table 4. Results of parameter estimation and Wind's method for Experiment II.

Scenario	Run	Φ	θ_r	θ_s	α	n	K_s	R^2
					cm^{-1}		cm d^{-1}	
1	All tensiometers	0.00437	0.136	0.399	0.00429	2.90	9.69	0.9993
2	Tensiometer 1	0.00412	0.134	0.399	0.00432	2.84	13.2	0.9993
	Tensiometer 2	0.00341	0.142	0.393	0.00435	3.07	2.99	0.9995
	Tensiometer 3	0.00343	0.150	0.391	0.00447	3.15	4.09	0.9995
	Tensiometer 4	0.00304	0.154	0.389	0.00451	3.21	5.00	0.9995
	Tensiometer 5	0.00313	0.157	0.388	0.00453	3.27	5.55	0.9995
3	Tensiometers 1 and 5	0.00445	0.133	0.399	0.00429	2.85	8.76	0.9993
Wind's method		–	0.0796	0.395	0.00380	2.52	2.03	0.963

istics obtained by numerical inversion and by Wind's method are shown in Fig. 5 and 7 for both experimental runs.

Notice a very good correspondence between retention curves obtained by all optimization scenarios and the $\theta(h)$ data points determined using Wind's method or their analytical fit for Experiment I (Fig. 5a). The soil water retention parameters obtained with Wind's method and by optimization of the pressure head readings at all tensiometers, Tensiometer 1 or 5, and both Tensiometers 1 and 5 are almost identical and indistinguishable from each other in Fig. 5a. A close match of all retention curves for Experiment I was obtained even though different hydraulic parameters were obtained for numerical inversions using pressure head readings from Tensiometers 3 or 4. Optimizations using these two tensiometers resulted in substantially higher predicted values of both n and θ_r, and slightly lower values of θ_s. This result illustrates that a close match or prediction of the soil hydraulic properties within the experimental range (-20 to -700 cm) does not guarantee accurate estimation outside the range of measurements, especially toward the higher tensions. This is due to a low sensitivity of the parameter optimization technique to θ_r. If, however, an independent estimate of θ_r is available, the estimated retention curve can be extrapolated with much more certainty beyond the experimental range (Parker et al., 1985). As an estimate for θ_r one could either use the true value of the residual water content directly (in which case θ_r is no longer an optimized parameter) or could include θ_r into the objective function in a Bayesian sense as explained above. Although this approach can only worsen the model fit, incorporation of prior information into the inverse problem will reduce parameter uncertainty (Yeh, 1986). The final fit cannot be improved by using prior information since this knowledge represents an additional constraint on the inverse solution. This lack of improvement is, however, balanced by more stable and reliable parameter estimates. By comparison, the value of θ_s can be predicted better due to knowledge of the final average
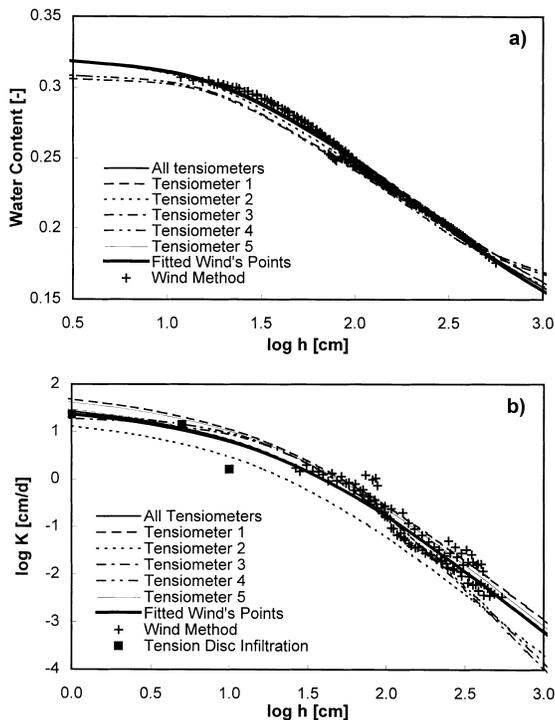
Fig. 5. (a) Water retention curves and (b) hydraulic conductivity functions determined with inverse parameter estimation and Wind's method for Experiment I.
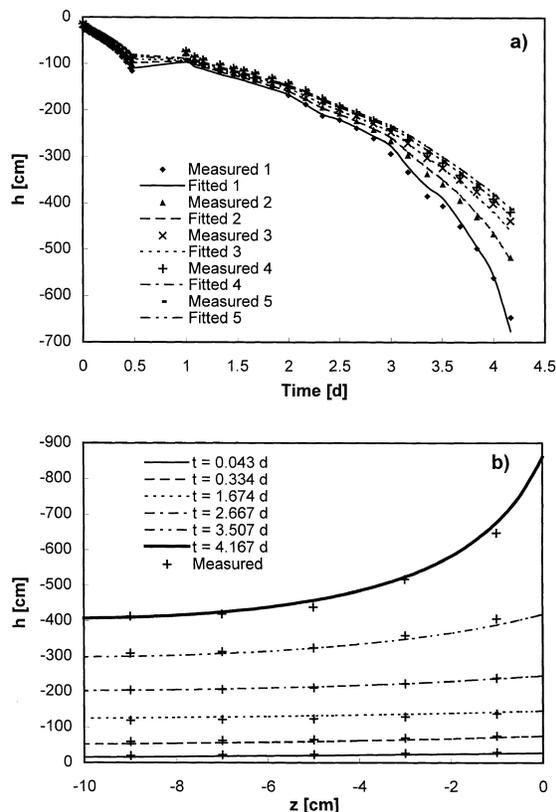
Fig. 6. Measured and fitted tensiometer readings for Experiment I as a function of (a) time and (b) depth.

water content and the evaporation loss during the entire experiment.

We obtained relatively large differences in terms of the unsaturated hydraulic conductivity (Fig. 5b). The estimated unsaturated hydraulic conductivity functions are, again, almost identical for optimizations using all tensiometer readings and for Wind's method. Also, the hydraulic conductivity function resulting from fitting the pressure heads from Tensiometers 1, 3, 4, and 5 follows the same pattern of data points obtained by Wind's method. However, there is now more scatter in the $K(h)$ data points determined by Wind's method; differences are about a half order of magnitude. Unsaturated hydraulic conductivities obtained with the tension infiltrometer disk on the same sample for pressure heads of -1, -5, and -10 cm are displayed as black squares in Fig. 5b. These values were not used in the parameter optimization, although they could have been easily included in the objective function, thus forcing the unsaturated hydraulic conductivity function to be located close to these points.

Measured and fitted tensiometer readings for Experiment I are shown in Fig. 6. The highest deviations were about 5 and 20 cm for the first and second evaporation rates, respectively, with the majority of values being much lower. The model was unable to accurately predict redistribution during the interruption between the first and second evaporation rates (Fig. 6a). This could have been caused in part by hysteresis effects since, during redistribution, the upper part of the soil profile is getting wetter. Hysteresis was not considered in our direct simulations.

The resulting soil hydraulic characteristics for Experi-

ment II are shown in Fig. 7, and their hydraulic parameters are given in Table 4. As for Experiment I, a close match was obtained for all estimated retention functions and data points derived with Wind's method. All inversion scenarios resulted in very similar soil hydraulic parameters. Although the retention curves did have similar shapes within the experimental range, the soil hydraulic parameters differed slightly from those obtained by fitting $\theta(h)$ data points determined by Wind's method. The values of θ_r and n were overestimated by about 0.05 and 0.4, respectively. These differences lead to different retention values at the higher tensions beyond the experimental pressure head range (greater than -700 cm). The differences in unsaturated hydraulic conductivities as determined by different optimization scenarios or methods differed again by about half an order of magnitude, which appear acceptable for most practical applications. Figure 7b displays unsaturated hydraulic conductivities obtained with a tension disk infiltrometer as black squares. These three values lie well within the range of values covered by the optimized hydraulic conductivity functions and the fitted Wind conductivity data. The three infiltrometer data points were not considered in inverse solution, but used together with the Wind data points to calculate the fitted unsaturated hydraulic conductivity function. The three values are actually somewhat lower than the Wind data for pressure heads up to -75 cm. Hence, excluding the tension infiltrometer data would have resulted in an unsaturated hydraulic function that would have corre-

Fig. 7. (a) Water retention curves and (b) hydraulic conductivity functions determined with inverse parameter estimation and Wind's method for Experiment II.
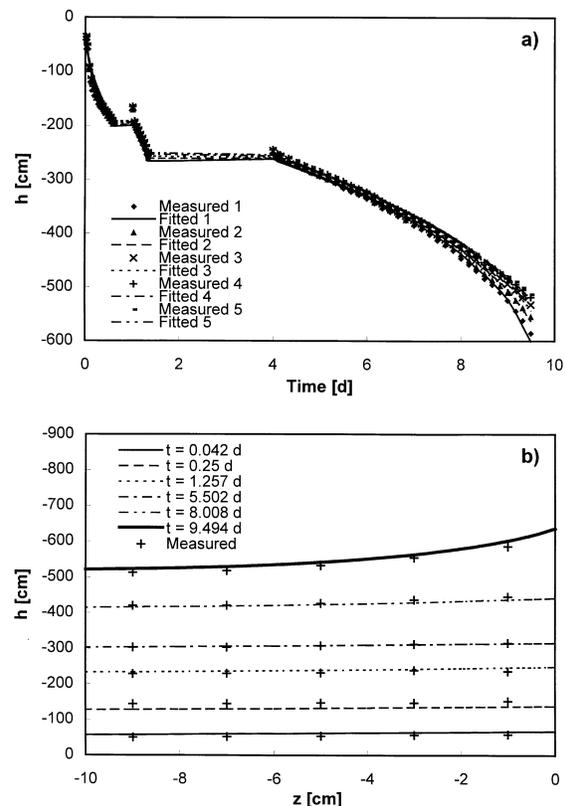
Fig. 8. Measured and fitted tensiometer readings for Experiment II as a function of (a) time and (b) depth.

sponded more closely with the inverse solution. Finally, in Fig. 8 we show an excellent match of the inverse solution with the tensiometer readings as a function of time and depth.

Analysis of both experiments showed that the retention curves within the measurement range can be obtained with far less information required than that needed for Wind's method. Moreover, retention curves obtained using pressure head readings from only one tensiometer were always very similar to those determined when all information was used, or when Wind's method was employed. Although the unsaturated hydraulic conductivity estimates showed much more uncertainty, this uncertainty was of the same order of magnitude as the scatter in $K(h)$ data points determined with Wind's method, which in turn is probably caused by small-scale soil heterogeneities between the different compartments, and perhaps some variability in the tensiometer readings.

SUMMARY AND CONCLUSIONS

The evaporation experiment is a widely used experimental technique for simultaneous estimation of soil hydraulic functions, especially in European laboratories (Halbertsma and Veerman, 1994; Halbertsma, 1996; Wendroth et al., 1993; Ciollaro and Romano, 1995; Santini et al., 1995). The experiment is usually analyzed by means of a modified Wind (1968) method; the perception exists that parameter estimation techniques, in spite of their successful application in several studies (Ciollaro and Romano, 1995; Santini et al., 1995), are unsuitable for its analysis (Halbertsma, 1996).

In this study we showed that the parameter estimation technique can be successfully used to analyze an evaporation experiment. Although our study was carried out on three specific examples (one numerical and two experimental), we discussed a relatively wide range of soils with n values ranging from 1.23 to 2.52 and α values from 0.0038 to 0.0249 cm^{-1}. Although some uncertainty exists in the soil hydraulic parameters caused by high correlation between θ_r and n, both the retention curve and the unsaturated hydraulic conductivity function were predicted well within the range of the Wind-type measurements. Extrapolation beyond the range of measurement is associated with a high level of uncertainty. Inclusion of independently measured information beyond the measurement range, i.e., water contents at some high suction, or directly the residual water content, could greatly decrease this uncertainty.

Evaporation experiments are usually carried out with four to five tensiometers (Halbertsma and Veerman, 1994). Methods have been proposed to decrease the number of tensiometers to two (Becher, 1971; Schindler, 1980; Wendroth et al., 1993). Using our parameter estimation technique on both numerically generated and laboratory data, we showed that for the existing experimental setup (five tensiometers in a 10-cm-long sample) one tensiometer reading is already sufficient to guarantee precise estimation of the soil hydraulic characteristics within the range of measurements. We also showed

that measurements taken closer to the soil surface exhibit a higher sensitivity to the optimized parameters than measurements from deeper locations, at least for the relatively short measurement time scale of our study.

While a two-rate evaporation experiment has important advantages over a one-rate experiment in terms of determining the unsaturated hydraulic conductivity using the modified Wind method, its use in combination with the parameter estimation technique did not show any benefits compared with the traditional one-rate approach, except for accelerating the experiment by several days.

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ERRATUM

Rapid Laboratory Callibration of Time-Domain Reflectometry Probes Using Upward Infiltration

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An error was found in the third coefficient of Eq. [1] for each of the three soil types.

$$\theta_v = A + B\epsilon_a^2 + C\epsilon_a^2 + D\epsilon_a^3$$

The coefficients, in scientific notation, should have been E raised to the power -3, instead of -4. The correct coefficients are listed in the revised Table 2, found below. All other coefficients are correct.

Table 2. Results of fitting Eq. [1] and [2] to observed data.

Soil	Coefficients for Eq. [1] ± Std. Dev.				RMSE of θ_v estimate†	r^2
	A	*B*	*C*	*D*		
Vinton	−0.075 ± 0.002	0.041 ± 6.4E-4	−1.6E-3 ± 6.1E-5	3.1E-5 ± 1.8E-6	0.0051	0.997
Casa Grande	−0.140 ± 0.006	0.050 ± 0.002	−2.0E-3 ± 1.3E-4	3.3E-5 ± 3.5E-6	0.0071	0.995
Pima	−0.117 ± 0.004	0.048 ± 0.001	−1.8E-3 ± 7.7E-5	2.7E-5 ± 1.8E-6	0.0070	0.996
	Fitted parameters in Eq. [2] ± Std. Dev.‡				RMSE of θ_v estimate	r^2
	α	ϵ_s	ϵ_{bw}	θ_{bw}		
Vinton	0.651 ± 0.004	3.21 ± 0.07	2.78 ± 1.68	0.023 ± 0.001	0.0068	0.993
Casa Grande	0.530 ± 0.012	6.74 ± 0.21	5.15 ± 2.78	0.0381§	0.0064	0.985
Pima	0.527 ± 0.012	5.72 ± 0.22	4.91 ± 2.71	0.042 ± 0.013	0.0074	0.987

† RMSE = root mean squared error; θ_v = volumetric water content.
‡ α = curve-fitting factor related to applied electric field; ϵ_s = soil dielectric constant; ϵ_{bw} = bound water dielectric constant; θ_{bw} = bound water content.
§ Taken as average air-dried θ_v for three experiments.