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Parameter estimation of unsaturated soil hydraulic properties from transient flow processes[1]

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Abstract

Three field methods recently proposed for estimating the soil hydraulic properties by numerical inversion of the Richards' equation are discussed. The first method involves the use of tension disc permeameter data, while the second method uses data collected with modified cone penetrometer. The third method involves the use of a multiple-step field extraction device. Experimental data for each of the above three methods were analyzed by using the HYDRUS-2D code coupled with the Levenberg–Marquardt parameter estimation algorithm. Advantages and disadvantages of the three methods are discussed.

Keywords: Parameter estimation; Soil hydraulic properties; Tension disc permeameter; Cone penetrometer

1. Introduction

Numerical models are increasingly used to study variably-saturated flow and chemical transport processes between the soil surface and the groundwater table. Effective use of these models depends to a large extent on the accuracy of available soil water retention and unsaturated conductivity data. Accurate measurement of the soil hydraulic properties is laborious because of the nonlinear nature of these properties, and the extreme spatial heterogeneity of the subsurface environment. While many laboratory and field methods exist to determine the soil water retention and unsaturated hydraulic conductivity curves (Klute and Dirksen, 1986; Green et al., 1986), most methods remain relatively expensive and too cumbersome for applications to larger areas of land. Hence, relatively cost-effective methods are needed for rapid determination of the hydraulic properties in the field.

In this paper, we discuss three field methods recently proposed for estimating the soil hydraulic properties by numerical inversion of the Richards' equation. One method currently being developed involves the use of tension disc permeameter data (Šimůnek and van Genuchten, 1996, 1997), while a second method uses data collected with a modified cone penetrometer (Gribb, 1996; Gribb et al., 1998). The third method involves the use of a field multiple extraction device (Inoue et al., 1998). Experimental data for each of the above three methods were ana-

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lyzed by coupling the HYDRUS-2D code (Šimůnek et al., 1996) with the Levenberg–Marquardt (Marquardt, 1963) parameter estimation algorithm.

2. Theory

Inverse methods are typically based upon the minimization of a suitable objective function which expresses the discrepancy between the observed values and the predicted system response. Soil hydraulic properties are assumed to be described by an analytical model with unknown parameter values, e.g. by Eqs. (2) and (3) given below. The system response is represented by a numerical solution of the flow equation augmented with the parameterized hydraulic functions and suitable initial and boundary conditions. Initial estimates of the optimized system parameters are then iteratively improved during the minimization process until a desired degree of precision is obtained.

2.1. Governing flow equation

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

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

where θ is the volumetric water content [L^3L^{-3}], h is the pressure head [L], K is the hydraulic conductivity [LT^{-1}], r is a radial coordinate [L], z is a vertical coordinate [L] positive upward, and t is time [T].

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

$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \frac{1}{(1 + |\alpha h|^n)^m} \qquad (2)$$

$$K(\theta) = K_s S_e^{0.5}[1 - (1 - S_e^{1/m})^m]^2 \qquad (3)$$

where S_e is the effective water content [-], K_s is the saturated hydraulic conductivity [LT^{-1}], θ_r and θ_s denote residual and saturated water contents [L^3L^{-3}], respectively, and α[L^{-1}], n[-], and $m(=1-1/n)$[-] are empirical parameters. The hydraulic characteristics defined by Eqs. (2) and (3) contain 5 unknown parameters: θ_r , θ_s, α, n, and K_s.

2.2. Inverse solution

The objective function Φ to be minimized during the parameter estimation process may be defined as

$$\begin{aligned}\Phi(b,q,p) = & \sum_{j=1}^{m_q} v_j \sum_{i=1}^{n_{qj}} w_{i,j}[q_j^*(x,t_i) - q_j(x,t_i,b)]^2 \\ & + \sum_{j=1}^{m_p} \bar{v}_j \sum_{i=1}^{n_{pj}} \bar{w}_{i,j}[p_j^*(\theta_i) - p_j(\theta_i,b)]^2 \\ & + \sum_{j=1}^{n_b} \hat{v}_j[b_j^* - b_j]^2 \end{aligned} \qquad (4)$$

where the first term on the right-hand side represents the deviations between the measured and calculated space-time variables (e.g. observed pressure heads or water contents at different locations and/or time, or the actual or cumulative infiltration or extraction rate versus time). In this term, m_q is the number of different sets of measurements, and n_{qj} is the number of measurements in a particular measurement set. $q_j^*(x,t_i)$ represents specific measurements at time t_i for the jth measurement set at location $x(r,z)$, $q_j(x,t_i,b)$ are the corresponding model predictions for the vector of optimized parameters 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. The second term of Eq. (4) represents differences between independently measured and predicted soil hydraulic properties (e.g. retention, $\theta(h)$, hydraulic conductivity, $K(\theta)$ or $K(h)$, and/or diffusivity, $D(\theta)$ or $D(h)$, data), while the terms m_p, n_{pj}, $p_j^*(\theta_i)$, $p_j(\theta_i,b)$, $\bar{v}_j$ and $\bar{w}_{i,j}$ have similar meanings as for the first term but now for the soil hydraulic properties. The last term of Eq. (4) represents a penalty function for deviations between prior knowledge of the soil hydraulic parameters, b_j^*, and their final estimates, b_j, with n_b being the number of parameters with prior knowledge and $\hat{v}_j$ representing pre-assigned weights. Estimates which make use of prior information (such as those used in the third term of Eq. (4)) are known as Bayesian estimates. We note that the covariance (weighting) matrices which provide information about the measurement accuracy, as well as any possible correlation between measurement errors and/or parameters, are assumed to be diagonal in this study.

Minimization of the objective function Φ is accomplished by using the Levenberg–Marquardt nonlinear minimization method (Marquardt, 1963), which combines the Newton and steepest descend methods, and generates confidence intervals for the optimized parameters.

3. Tension disc infiltrometer

Tension infiltration data have, thus, far been used primarily for evaluating saturated and unsaturated hydraulic conductivities, and for quantifying the effects of macropores and preferential flow paths on infiltration (Perroux and White, 1988; Ankeny et al., 1991; among many others). A relatively standard way for estimating unsaturated hydraulic conductivities from tension infiltrometer data has been to invoke Wooding's, 1968 analytical solution. This approach requires steady-state infiltration rates for two different supply pressure heads, and assumes applicability of Gardner's, 1958 exponential function for $K(h)$. Šimůnek and van Genuchten, 1996 suggested the combined use of transient infiltration data obtained during a single tension infiltration experiment, and tensiometer or TDR data measured in the soil below the disc to estimate the unknown soil hydraulic parameters in Eqs. (2) and (3) via parameter estimation. Šimůnek and van Genuchten, 1997 later revised this method by using multiple tension infiltration experiments in combination with knowledge of the initial and final water contents. This modification avoided the cumbersome use of tensiometers and TDRs. Evaluation of the numerical stability and parameter uniqueness using numerically generated data with superimposed stochastic and deterministic errors showed, that a combination of the 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 and van Genuchten, 1997).

The numerical inversion method was applied to tension disc infiltrometer data obtained in two field studies. In the first study (Šimůnek et al., 1998a), two tension disc experiments were carried out on a fine sandy loam in Riverside, California. The tension disc had a diameter of 20 cm, and the experiment was executed with three consecutive tensions of 20, 10, and 3 cm. Each tension was maintained for about 1 h. Pressure transducers were used to record transient infiltration rates in a setup similar to that described by Ankeny et al., 1988. The soil hydraulic properties were also independently measured with standard laboratory methods on five soil samples. Fig. 1 shows the experimental and fitted cumulative infiltration curves versus time for the two runs, including deviations between the best-fit and measured values. The soil hydraulic parameters determined by parameter estimation and by Wooding's analysis are given in Table 1.

Excellent agreement between the measured and fitted cumulative field infiltration curves was obtained when the five major soil hydraulic parameters in van Genuchten's model were optimized (Fig. 1). Hydraulic conductivities (both saturated and unsaturated) as determined by the numerical inversion compared well with those obtained using Wooding's analytical solution (Table 1). Agreement between retention curves obtained by numerical inversion of the field infiltration experiment and by direct laboratory measurement, however, was relatively poor. The entire laboratory retention curve shifted by about 0.10 units towards higher water contents, while also the parameter n had different values (α-values were much closer for both analyses). The infiltration experiment could not be closely reproduced when the mean laboratory soil hydraulic parameters were used and validity of the closed-form van Genuchten–Mualem model was assumed (Šimůnek et al., 1998a).

The second experiment was used to estimate the soil hydraulic characteristics of a two-layered soil system involving a crusted soil in a Sahel region (Šimůnek et al., 1998b). Here, we will report only results for the sandy subsoil obtained with a tension disc diameter of 25 cm and with supply tensions of 11.5, 9, 6, 3, 1, and 0.1 cm. Fig. 2 shows measured and optimized cumulative infiltration curves and their differences. The small breaks in the cumulative infiltration curve (Fig. 2(a)) were caused by brief removal of the infiltrometer from the soil surface to resupply it with water and to adjust the tension for a new time interval. Very close agreement between the measured and optimized

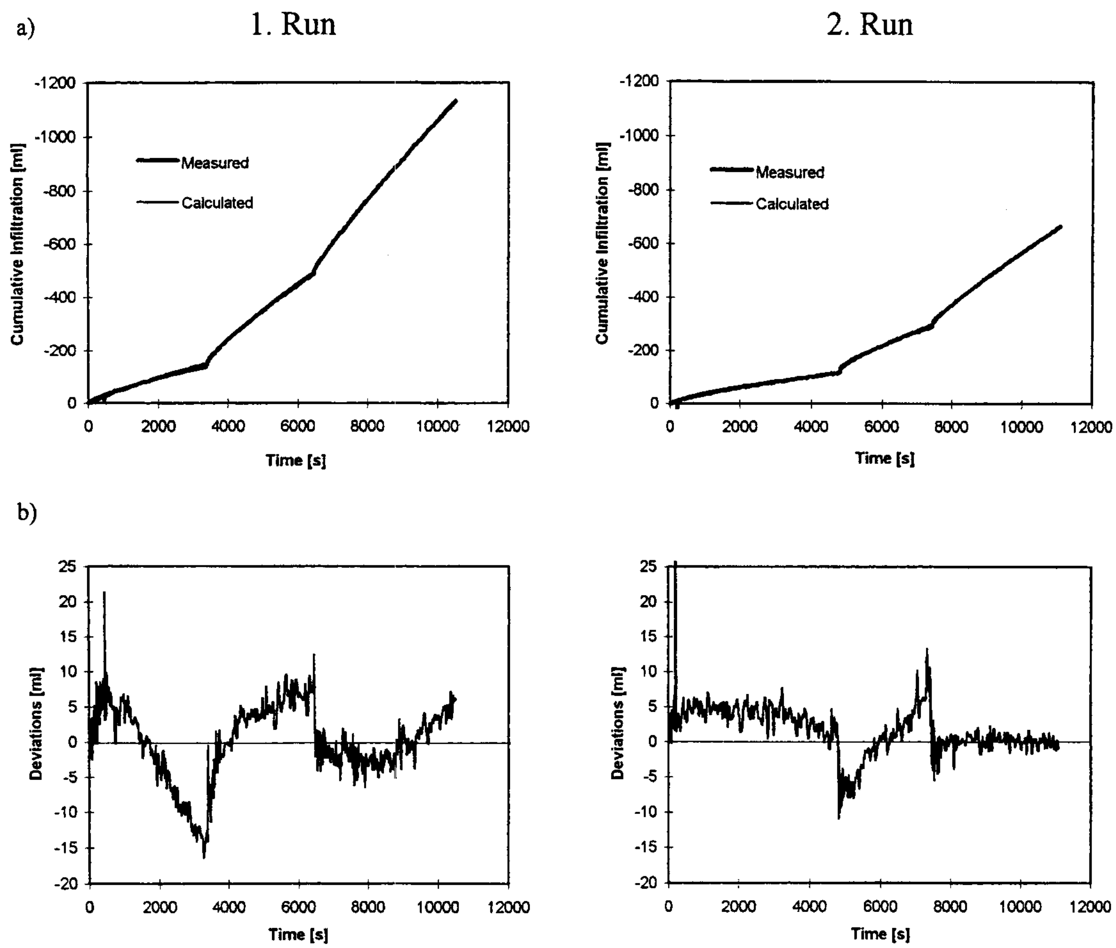

Fig. 1. Measured and fitted cumulative infiltration curves (a) and their differences (b) for two tension disc infiltrometer experiments carried out in Riverside, California.

Table 1

Comparison of results obtained with Wooding's analysis and using parameter estimation for two multiple tension infiltration experiments

Parameter	Run 1			Run 2			Mean lab. curve
	Wooding's analysis		Parameter estimation	Wooding's analysis		Parameter estimation	
α (cm^{-1})			0.0412			0.0406	0.0401
n			3.61			2.76	1.55
θ_r			0.0			0.0	0.107
θ_s			0.274			0.238	0.347
K_s (cm d^{-1})	32.0	14.0	9.24 (−34%) [a]	20.4	12.3	6.57 (−47%)	272
K(−6.5 cm) (cm d^{-1})		9.65	8.80 (−8.8%)		7.26	5.34 (−26%)	
K(-15 cm) (cm d^{-1})	6.81		4.95 (−27%)	3.74		2.49 (−33%)	

[a] The number in parentheses shows by how many percent the hydraulic conductivity obtained by parameter estimation differs from corresponding values obtained using Wooding's analysis.

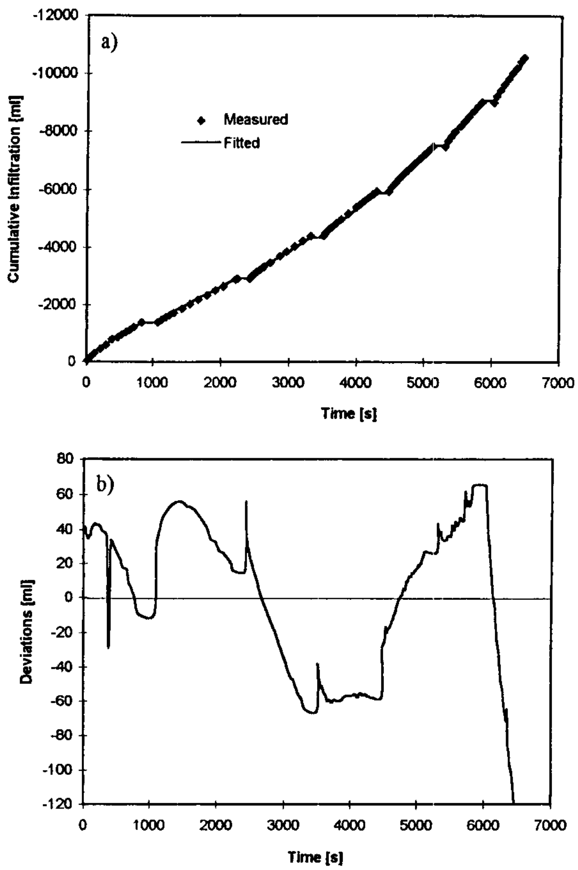

Fig. 2. Measured and optimized cumulative infiltration curves (a) and their differences (b) for a tension disc infiltrometer experiment carried out in the Sahel region.

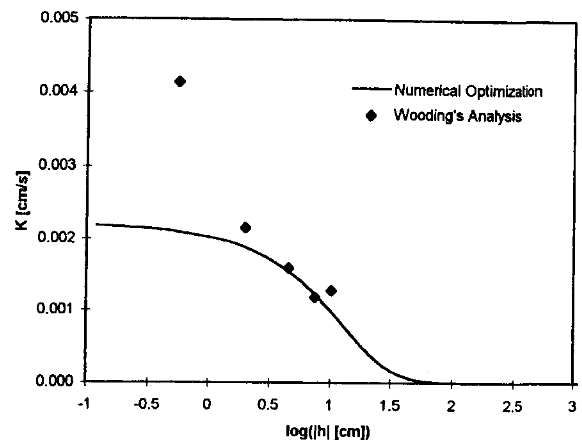

Fig. 3. Unsaturated hydraulic conductivities calculated using Wooding's analytical solution for particular pressure heads, and the complete function obtained with numerical inversion.

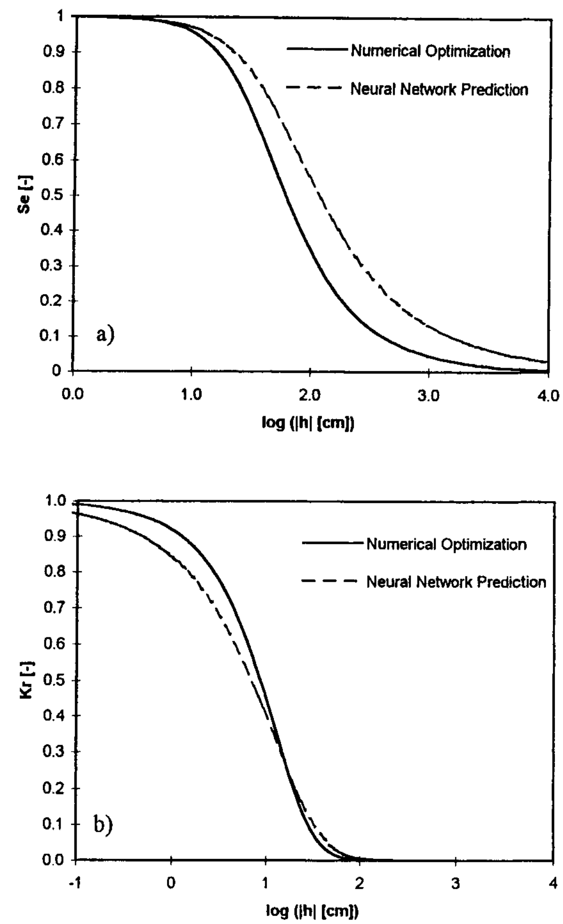

Fig. 4. Soil hydraulic functions obtained with numerical inversion and using neural network predictions.

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. Fig. 3 shows a comparison of parameter estimation results against results obtained with Wooding's analysis. Both methods give almost identical unsaturated hydraulic conductivities for pressure heads in the interval between −2 and −10.25 cm. However, the hydraulic conductivity at the highest pressure head interval was overestimated by a factor of two using Wooding's analysis. In Fig. 4, we further compare the numerical inversion results with hydraulic properties estimated from available soil textural information using a neural-network-based pedotransfer function approach (Schaap et al., 1998). Relatively good agreement between the inverse and neural network predictions was obtained.

4. Cone penetrometer

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) can be used at depth. Cone penetrometers were originally used to obtain soil strength characteristics by measuring the tip resistance and sleeve friction during penetration at a constant rate. To obtain the hydraulic properties, a modified cone penetrometer, instrumented with a porous filter close to the penetrometer tip and two tensiometer rings 5 and 9 cm above the filter, is used (Fig. 5). The device is pushed into a soil to the desired depth, and a constant 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 for a short period of time (300–500 s).

Gribb, 1996 gave a detailed numerical analysis of this experiment, including a study of the identifiability of the soil hydraulic parameters. She showed that the inverse solution was least sensitive to n and θ_s, and

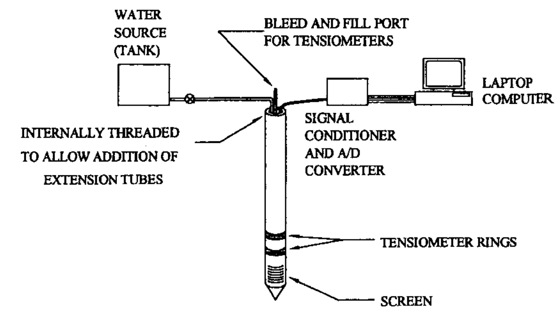

Fig. 5. Schematic of the modified cone penetrometer (Gribb, 1996).

most sensitive to K_s and α. The method was recently used to estimate the hydraulic parameters of a sandy soil in a laboratory aquifer system measuring $5\times5\times3$ m (Gribb et al., 1998; Kodešová et al., 1998).

Fig. 6 shows observed flow data, as well as results of the numerical inversion. Excellent agreement between measured and optimized values was obtained for the inverse solution with four optimized parameters. Fig. 7 presents the retention curves obtained with selected laboratory methods and the parameter estimation technique. Optimized curve is close to the wetting curves determined in the laboratory. The overprediction of θ_s for the inverse solution could be caused by anisotropy of the soil. Gribb et al., 1998 showed that the estimated saturated hydraulic conductivities were similar to those obtained with

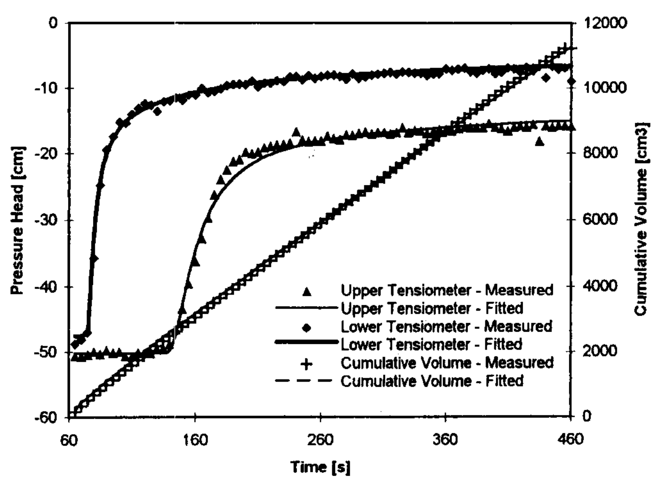

Fig. 6. Comparison of observed and optimized cumulative infiltration curves and tensiometer readings for the modified cone penetrometer test (α, n, θ_s, and K_s are optimized, θ_r is fixed).

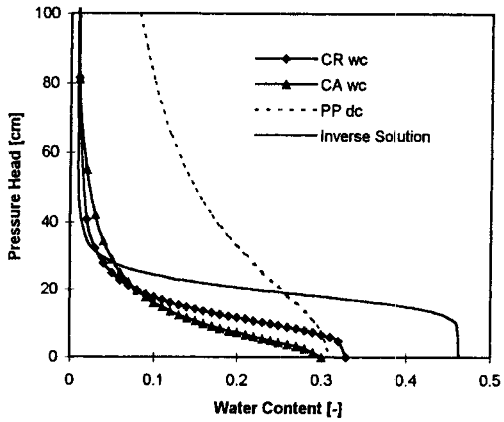

Fig. 7. Comparison of soil-water characteristic curves obtained by direct methods and that obtained by inversion of cone penetrometer data (CR – capillary rise test, CA – computer automated wetting curve test, PP – pressure plate test, wc – wetting curve, dc – drying curve).

other test methods, such as Guelph permeameter, slug tests, and laboratory constant head tests. Issues related to soil disturbance due to cone penetration are under investigation (Gribb et al., 1998).

5. Multiple step extraction

While the tension infiltrometer and cone penetrometer methods provide information about wetting branches of the soil hydraulic properties, a multiple step extraction device can be used to obtain draining branches. The device consists of a ceramic soil solution sampler (Fig. 8) which is inserted into an initially wet soil profile and subjected to a series of vacuum extraction pressures. The cumulative amount of soil solution extracted during an experiment, as well as pressure heads at various locations near the extraction device, are monitored during the experiment and subsequently used in an objective function for the nonlinear minimization problem. Inoue et al., 1998 first evaluated the feasibility of the vacuum extraction technique using numerically generated data, and concluded that the method is well suited for loamy-textured soils, but not necessarily for sandy soils. They tested the method in the laboratory and in the field. Here we briefly discuss one field application.

The experiment (Inoue et al., 1998) was carried out on a Yolo silt loam with a clay content of about 22%.

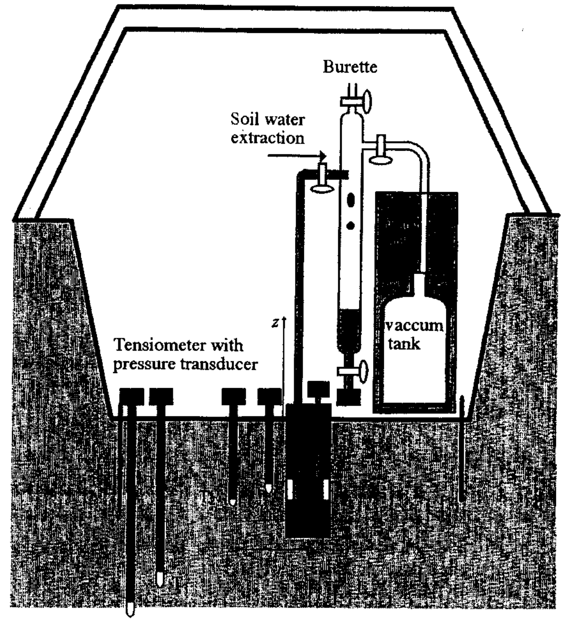

Fig. 8. Schematic of the in situ multistep extraction experiment (Inoue et al., 1998).

The center of the ceramic ring (with a radius of 3 cm, and a length of 3 cm) was located 10 cm below the soil surface. The tensiometers were installed at the following positions: $T_1(r,z)=(4,\ -10\ \text{cm})$, $T_2=(6,\ -15)$, $T_3=(20,\ -40)$, and $T_4=(20,\ -55)$. Readings of the forth tensiometer (T_4) were used as the bottom boundary condition. The initially saturated soil was allowed to drain for a period of 46.5 h, after which three vacuum extraction steps were applied: $h_{ex}=-195$ cm h for $46.5<t<71.2$ h, $h_{ex}=-415$ cm for $71.2<t<93.0$ h, and $h_{ex}=-685$ cm for $93.0<t<120$ h. Experimental data, as well as the final results of two numerical inversions are presented in Fig. 9. The saturated hydraulic conductivity of the ceramic ring was optimized simultaneously with van Genuchten's hydraulic parameters. Only the cumulative extraction volume versus time and transient tensiometer measurements were included in the objective function for the first optimization. Three additionally measured $\theta(h)$ data points were used for the second optimization. Agreement between measured and calculated values in Fig. 9 was relatively good. Fig. 10 compares the optimized soil hydraulic functions with independently measured data obtained with the instantaneous profile method. While correspondence between the measured

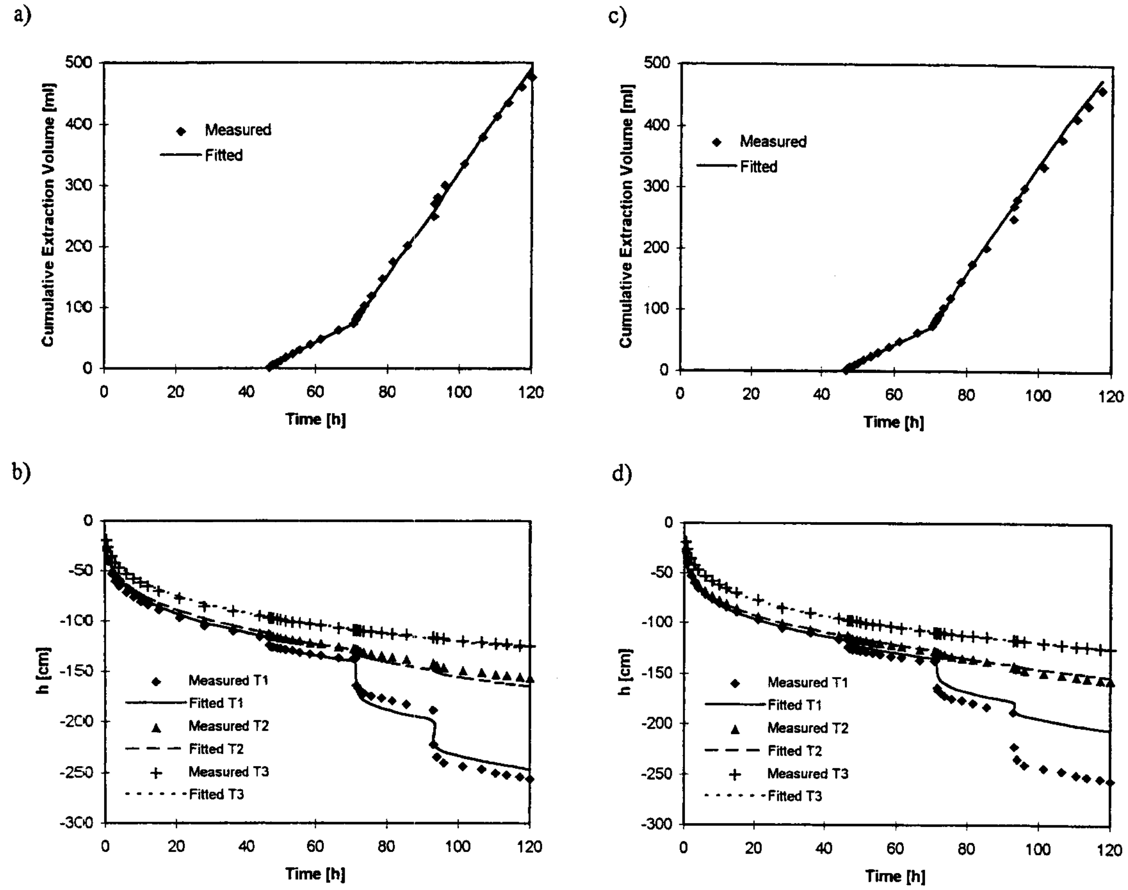

Fig. 9. Comparison of measured and optimized cumulative extraction and pressure head values. The objective function included cumulative extraction volumes, tensiometer measurements (a and b), and additionally 3 measured $\theta(h)$ data points (c and d).

and estimated hydraulic conductivities seems good for both optimizations, only the second optimization gave acceptable results for the retention curve (Inoue et al., 1998).

6. Conclusions

We briefly reviewed three field methods which may be used for estimating the soil hydraulic properties by parameter estimation. A common feature of all three methods is the coupling of a numerical solution of the Richards equation with the Levenberg–Marquardt parameter estimation algorithm. Of the three methods, the tension disc infiltrometer and cone penetrometer experiments provide information of the wetting branches of the soil hydraulic properties, while the multiple extraction device leads to draining branches. Use of the tension disc infiltrometer and multiple extraction device is limited to the soil surface or the near surface. Although tested up to now only in the laboratory, cone permeameter can potentially be used to depths of 30 m or more in accordance with established cone penetration technology. All three methods, except perhaps the tension infiltrometer approach, are still being perfected and require further research to test their applicability in the field.

Parameter estimation approaches as discussed here provide unique tools for evaluating the design and performance of these and related experimental approaches, and for optimally analyzing data collected with the different field instruments.

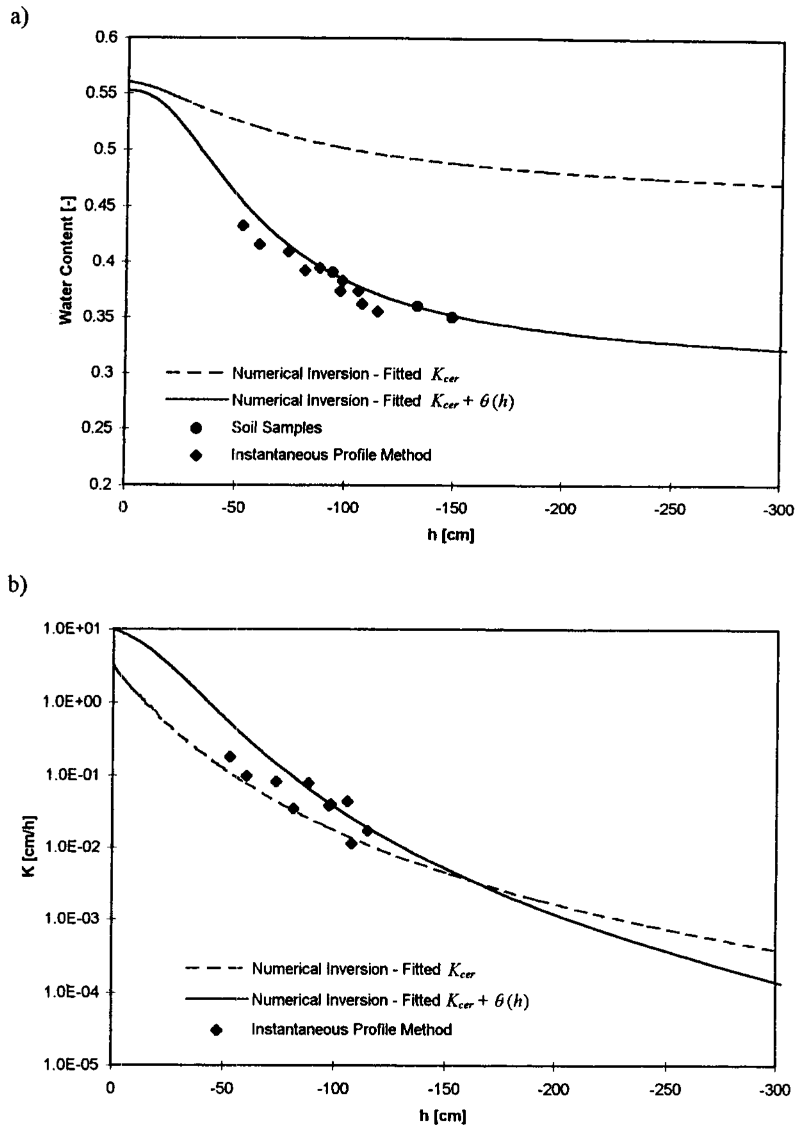

Fig. 10. Estimated soil water retention (a) and hydraulic conductivity (b) functions for the two optimizations of multi-step extraction data compared with independently determined retention and unsaturated hydraulic conductivity data.

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