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Temporal and spatial (down profile) variability of unsaturated soil hydraulic properties determined from a combination of repeated field experiments and inverse modeling

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Abstract

An in situ method for estimating parameters necessary for characterizing unsaturated flow in porous media has been applied to 37 individual data sets from the same study site (a sand dune on the edge of a wetland). The measured field data include beginning and ending soil moisture profiles, and continuous records of net surface flux (infiltration/evaporation) and pressure head at the base of the profile. For each study period, the initial profile was used along with the upper and lower boundary conditions to simulate flow and storage changes in the profile from a form of the Richard's equation. Following each model run, the parameters in van Genuchten's characteristic equations were adjusted using the Levenberg–Marquardt procedure. Parameter adjustment and forward modeling continued until a minimum was reached in the difference between measured and simulated moisture profiles. An analysis of the resulting (optimized) parameter estimates indicated that repeated experiments, using the same method, resulted in a very consistent set of parameter values, particularly when parameters were estimated for individual soil layers rather than for the profile as a whole. Statistical analyses of the estimated parameter values indicated that most of the parameters have small coefficients of variability and the mean values are consistent with those generally considered to be valid for uniform sand. The optimization procedure also produced reasonable (and unique) values of saturated moisture content for a buried clayey layer within the otherwise homogeneous deposit of dune sand.

Keywords: Vadose zone; Hydrologic monitoring; Inverse methods; Parameter estimation

1. Introduction

Modeling groundwater flow in the vadose zone requires accurate information about the functional relationships between unsaturated hydraulic conductivity, soil moisture content and pressure head (the characteristic curves of Freeze and Cherry (1979, p. 43)). Over the years, various equations have been proposed for describing the characteristic curves (Burdine, 1953; Brooks and Corey, 1964; Campbell, 1974; Mualem, 1976; van Genuchten, 1980), the parameters of which are usually estimated by measuring the saturated hydraulic conductivity and

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assuming equality of the coefficients and exponents of moisture retention and hydraulic conductivity equations.

Parameterization traditionally was based on laboratory measurements using permeameters and moisture extractors. Recently, laboratory methods have become more sophisticated involving measurements of soil water tension and water movement in conjunction with inverse methods to derive the parameters of proposed characteristic equations (Eching et al., 1994; van Dam et al., 1994; Šimůnek et al., 1998; Young et al., 2002). Despite the elegance of these improved laboratory procedures, a major disadvantage of any laboratory-based analysis is that they can lead to inferred hydraulic properties that are non-representative of field conditions since the samples are small and the collection of soil cores invariably introduces some disturbance of the in situ soil matrix (Kool et al., 1987).

A desirable alternative is to determine characteristic curve parameters by combining field measurements of system variables such as moisture content, pressure head, and water flux with an inverse method that couples a numerical flow model with a parameter optimization algorithm. Dane and Hurska (1983) discussed a method for determining optimum characteristic curve parameters from a combination of field measurements and model calculations and applied their technique to a 'homogenous' clay loam. The initial moisture profile and profiles after 7 and 25 days of imposed gravity drainage were measured with a calibrated neutron probe. The soil surface was covered to impose a zero-flux surface boundary condition so that changes in moisture content could be attributed exclusively to gravity drainage from the initially saturated surface layer. Because there inversion method was not very sophisticated, Dane and Hurska could only estimate two of the five required parameters, and therefore used other 'experimental methods' to estimate the remaining parameters (Dane and Hurska, 1983, p. 623).

Since the initial work of Dane and Hurska, there have been many studies that have improved the inverse methods utilized to determine in situ hydraulic properties of soil materials, but most of those involved utilization of altered or artificial soils (Abbaspour et al., 1999; Jhorar et al., 2002). Abbaspour et al. (2000) applied inverse methods to determine the characteristic curve parameters of a 'layered field soil'. While the latter study involved a more realistic approach to in situ determination of soil hydraulic properties, including determination of characteristic curve parameters for each of the four identified soil layers, it still utilized artificial controls such as prescribed constant irrigation and the application of a gravel layer on top of the soil surface to reduce evaporation and to prevent the soil surface from sealing. Although this approach is potentially very useful in a variety of field situations, there are many instances when imposing controlled boundary conditions is not feasible. In addition, it is important to know whether different rates and types of boundary fluxes result in different optimal parameter values.

In this study, a less restrictive approach to in situ determination of characteristic curve parameters is evaluated. Rather than imposing artificial boundary conditions on the soil profile, field measurements of pressure head at the base of the profile and net surface flux (infiltration/evaporation) are combined with measured moisture profiles to constrain an inverse model. The methodology was applied to a profile of uniform dune sand where multiple sets of necessary input data were collected. A subsequent analysis of the best-fit parameters was undertaken to evaluate any spatial (down profile) and temporal trends in the parameter estimates. The results of the repeated experiments indicate that a remarkably consistent set of parameter values can be achieved from a relatively cost-effective approach despite the probable existence of error in some of the field measurements.

2. Optimization procedure

Since the initial review by Kool et al. (1987), there have been several papers published that describe and compare different methods for determining optimum parameters for unsaturated characteristic equations and their sensitivities to initial parameter estimates and experimental procedures (Šimůnek and van Genuchten, 1996; Abbaspour et al., 1997; Finsterle and Faybishenko, 1999; Vrugt et al., 2001). Regardless of which optimization procedure is used, estimation for unsaturated zone hydraulic properties includes the following steps.

Step 1. Evoke parametric equations that adequately describe the functional relationships among soil water tension, moisture content, and unsaturated hydraulic conductivity. As in most other recent work on the subject, the equations of van Genuchten (1980) were used. The soil moisture retention curve is described by:

$$\theta(\psi) = \theta_r + (\theta_s - \theta_r)\mathrm{Se} \qquad \psi < 0 \tag{1a}$$

$$\theta(\psi) = \theta_s \qquad \psi \geq 0 \tag{1b}$$

and the unsaturated hydraulic conductivity function is:

$$K(\mathrm{Se}) = K_s \mathrm{Se}^{1/2}[1 - (1 - \mathrm{Se}^{1/m})^m]^2 \tag{2}$$

θ_s is the field saturated moisture content, θ_r is the residual moisture content, K_s is the saturated hydraulic conductivity, and Se is the effective saturation which is related to the pressure head (ψ) as follows:

$$\mathrm{Se} = [1 + (\alpha|\psi|)^n]^{-m} \qquad \psi < 0 \tag{3a}$$

$$\mathrm{Se} = 1 \qquad \psi \geq 0 \tag{3b}$$

α, n, and m $(= 1 - 1/n)$ are parameters that modulate the steepness and curvature of van Genuchten's sigmoidal functions.

Step 2. Solve the one-dimensional unsaturated flow equation subject to the initial and boundary conditions measured during a given interval of time. The equation for vertical flow in unsaturated porous media is (Freeze and Cherry, 1979, p. 212):

$$\frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial \psi}{\partial z} + 1\right)\right] = C(\psi)\frac{\partial \psi}{\partial t} \tag{4}$$

where z is a vertical coordinate (positive upward), t is time, and $C(\psi) = \partial\theta/\partial\psi$ is the specific moisture capacity of the porous medium. In this study Eq. (4) was solved numerically using an implicit finite-difference procedure based on that of Freeze (1971). The initial condition was a measured soil moisture profile at the beginning of a period between moisture-profile measurements. The boundary conditions were measured time-dependent surface flux's (net infiltration or evaporation), and pressure heads at the base of the profile during the period between moisture-profile measurements. Using a time-step of 1 h, the successive approximations of pressure head values consistently converged to a tolerance of <1 cm when under-relaxation was employed.

Step 3. Compare simulated values of $\theta_{z,t}$, $\psi_{z,t}$, or both, with those measured at the end of the same time period and keep adjusting the characteristic equation parameters until the difference between measured and predicted values of $\theta_{z,t}$ and/or $\psi_{z,t}$ are minimized. In this study, values of $\theta_{z,t}$ obtained from a neutron moisture gauge were utilized in the comparison. The simulated moisture content values were deduced from the ψ values that were determined by the solution of Eq. (4) and the assumed $\theta(\psi)$ relationship (Eqs. (1) and (3)). The objective function:

$$\mathbf{O}_i(\mathbf{p}) = \sum_{i=1}^{k}[\theta_i' - \theta_i]^2 = \mathbf{r}^{\mathrm{T}}\mathbf{r} \tag{5}$$

was minimized with respect to the parameters in vector $\mathbf{p}$ which consists of θ_s, θ_r, α, K_s, and m. In the objective function, the index $i = 1, \ldots, k$ refers to points within the target soil moisture profile at the end of the measurement interval. θ_i' is the calculated moisture content at depth interval i, and θ_i is the measured moisture content at the same depth interval.

The Levenberg–Marquardt method (Nash, 1978) for iteratively seeking an optimum set of parameter values is the most frequently used method for determining unsaturated zone hydraulic properties by inverse methods. The fundamental equation governing the iterative procedure is:

$$\Delta\mathbf{p} = (\mathbf{J}^{\mathrm{T}}\mathbf{J} + \lambda\mathbf{D})^{-1}\mathbf{J}^{\mathrm{T}}\mathbf{r} = \mathbf{M}^{-1}\mathbf{J}^{\mathrm{T}}\mathbf{r} \tag{6}$$

where $\Delta\mathbf{p}$ is a parameter update vector (with elements $\Delta\theta_s$, $\Delta\theta_r$, $\Delta\alpha$, ΔK_s, and Δm), and $\mathbf{J}$ is the Jacobian matrix containing the partial derivatives of θ_i with respect to the five van Genuchten parameters:

$$\mathbf{J} = \begin{bmatrix} \frac{\partial\theta_1}{\partial\theta_s} & \cdots & \cdots & \cdots & \frac{\partial\theta_1}{\partial m} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \frac{\partial\theta_k}{\partial\theta_s} & \cdots & \cdots & \cdots & \frac{\partial\theta_k}{\partial m} \end{bmatrix}. \tag{7}$$

Analytical expressions for the various partial derivatives, as well as for $C(\psi)$, are presented in Ebraheem (1993). **D** is a diagonal scaling matrix, the elements of which are set equal to the norms of the corresponding columns of **J** (Kool et al., 1987, p. 264), and λ is a positive scalar (Marquardt parameter) that was initially set to a large value (500 or 1000) then reduced by a factor of 2 in successive iterations as the solution approached the minimum.

The resolution matrix (**R**) for the solution is given by:

$$\mathbf{R} = \mathbf{M}^{-1}\mathbf{J}^{\mathrm{T}}\mathbf{J} \tag{8}$$

and the variance–covarience matrix (**C**) is:

$$\mathbf{C} = \sigma^2\mathbf{M}^{-1}\mathbf{R} \tag{9}$$

where σ^2 is the error variance of the soil moisture calculations:

$$\sigma^2 = \frac{\sum[\theta_i' - \theta_i]^2}{k-5} \tag{10}$$

k is the number of target points in the entire soil profile (or sub-layer) and 5 represents the number of parameters to be estimated. A resolution matrix, which has diagonal elements close to unity and off-diagonal elements close to zero, is desirable for a stable and accurate solution. The standard errors of the hydraulic parameters are given by the square roots of the diagonal elements in **C**.

A computer algorithm was developed to utilize the above procedure of parameter estimation to determine the van Genuchten parameters for an entire soil profile or for individual soil layers. In this study, both approaches were used to evaluate the hydraulic properties of a profile consisting primarily of aeolian sand. The numerical experiments were replicated using 37 individual data sets from the same study site. Initial estimates of the van Genuchten parameters θ_s, θ_r, K_s, α, and m were based on: (a) typical values for uniform sand that are reported in the literature (van Genuchten and Nielsen, 1985; Schaap et al., 2000), (b) field measurements at the study site and (c) a sensitivity analysis that identified what values, within a reasonable range for sand, would produce final estimates that had the lowest root mean square errors. The value of the exponent n was set equal to $1/(1-m)$ in order to reduce the number of parameters to be estimated and thereby increase the degrees of freedom associated with the estimation procedure. Soil water hysteresis was not explicitly incorporated into the model because it was felt that if hysteresis was important, that would be reflected in the optimum parameter values obtained for wetting versus drying periods.

3. Field site and data collection

The field data were collected on the crest of a low sand dune adjacent to the Great Marsh in the Indiana Dunes National Lakeshore, northwest Indiana. The dune is stable and contains a sparse cover of marram grass and trees. Borings indicated that the dune material was mostly massive, fine-grained sand, but a layer of soil-like material occurred at a depth of about 2 m. The buried soil is about a half-meter thick and contains some organic matter and clay within the sand matrix.

Soil moisture-profile measurements were facilitated by installing a watertight aluminum access tube into the dune sand to a depth of 4.25 m. The lower part of the access tube penetrated into the shallow water table aquifer so continuous moisture profiles through the entire vadose zone could be measured using a neutron moisture gauge. A continuous (intact) core of the dune sand was never obtained. Consequently, calibration had to be accomplished by comparing laboratory-determined moisture contents of shallow cores with the neutron gauge measurements of moisture content near the surface. The resulting calibration of the neutron gauge differed only slightly from the original factory calibration (the actual moisture contents were higher than the factory calibration indicated). The calibration was rechecked approximately every 3 months and did not change appreciably over the course of the study.

Neutron gauge measurements of soil moisture may be adversely influenced by a variety of sources (Kramer et al., 1992). Over time, instrument drift occurs; this is why measurements are typically expressed as count ratios wherein the actual slow neutron counts are divided by a standard count taken in a stable standard material (commonly paraffin). However, standard counts are also subject to error, so they are made immediately before and after the soil moisture measurements and averaged in an effort to minimize the error. Neutron measurements are subject to random errors in the counting apparatus and, therefore, a longer counting period is likely to increase the precision of the measurements. Kramer et al. (1992) show that a 16-s counting time should provide good precision and this counting time was used in the present study. Neutron gauge measurements are not as accurate near the ground surface because some neutrons are lost to the atmosphere resulting in a neutron count rate below that expected for the existing moisture content (Hauser, 1984). In this study, the uppermost moisture reading was made at a depth of 30 cm to reduce the effect of neutron losses while still achieving a meaningful measurement of the near-surface moisture content.

During each site visit, moisture content measurements were made at 0.3-m intervals and continuous profiles were calculated from the neutron moisture gauge measurements using Gregory–Newton interpolation formulas. The interpolation procedure utilized a step size of 5 cm (this was also the value of Δz used in the numerical solution of Eq. (4)), therefore, the interpolated profiles consisted of 84 individual moisture content values. A total of 40 moisture-profile measurements were made at 2- to 4-week intervals during a 26-month period of monitoring that commenced in June 1993 and ended in September 1995.

A small weighing lysimeter was deployed in an attempt to quantify surface fluxes at the crest of the dune. The weighing lysimeter consisted of a cylindrical column of vegetated (marram grass) soil, contained within a bucket that was 27 cm in diameter and 18 cm deep. The bucket had a perforated base to allow infiltrated water to freely drain into an underlying collection bucket and a spillway to allow for surface runoff. The runoff and gravity drainage were trapped in containers so that a water balance could be established for the lysimeter. The vegetated soil monolith and collection bucket rested on a sensitive load cell that registered weight changes due to additions (infiltration, I) and losses (evapotranspiration, E) of water. The weight gains or losses then were related to actual volumetric changes per unit area and recorded in centimeters of water. Small lysimeters, such as the one used in this study, are error prone for the following reasons: (1) Excess water can drain down the edges of the container and increase infiltration relative to a natural soil. (2) The edges of the lysimeter can influence the wind stress and thereby alter the evapotranspiration rate relative to a natural soil surface. (3) Small lysimeters cannot be used to estimate transpiration from large and deep-rooted plants such as trees. (4) The lack of an intimate connection between the base of the soil monolith and underlying undisturbed soil can alter the moisture balance relative to that of the surrounding soil. As a result, evapotranspiration rates estimated by the lysimeter apparatus may be different from those of the real field soil. These limitations were taken into consideration when designing the field experiment. The study site was located on an open area of the dune away from the tree cover. The soil monolith placed in the lysimeter included the marram grass cover from the point of measurement. The rim of the lysimeter was covered by a 2-cm-wide flexible polyvinyl flap that prevented water from draining down the edges of the container and created a smooth transition from the surrounding sand to the soil monolith. In an effort to evaluate the ability of the lysimeter to measure surface fluxes, daily infiltration rates were compared to rainfall rates measured at the field site using a tipping bucket rain gauge, and daily evapotranspiration rates were compared to estimates of potential evaporation using the method of Penman (1948). Data for the Penman calculations were obtained from a micrometeorological station located about 2 km away in the Great Marsh. As expected, the correspondence between rainfall and lysimeter infiltration was much closer than that between lysimeter evapotranspiration and Penman potential evaporation (see Dintaman (1997, p. 68) for plots of the data). In both comparisons, however, the data pairs straddled a line of one-to-one correspondence indicating that the lysimeter measurements were not persistently over- or underestimating the net surface fluxes.

A calibrated pressure transducer for measuring water table fluctuations was placed in a monitoring well that was installed adjacent to the weighing lysimeter and neutron gauge access tube. The transducer contained a breather tube and was designed to compensate for variations in atmospheric pressure. The accuracy of the instrument calibration was checked during each site visit by measuring depth to water from the ground surface using a commercial depth indicator.

The lysimeter load cell, raingauge, and pressure transducer were connected to a digital data logger that sampled the instruments every 15 s and stored the data as hourly averages and totals for subsequent analysis. Some data were lost due to equipment problems, especially during winter. Over the entire period of monitoring, 37 complete data sets consisting of (1) initial and final soil moisture profiles, and (2) continuous records of net surface flux and pressure head at the base of the profile, were obtained. One example of the data used as input to the parameter optimization procedure is presented in Fig. 1.

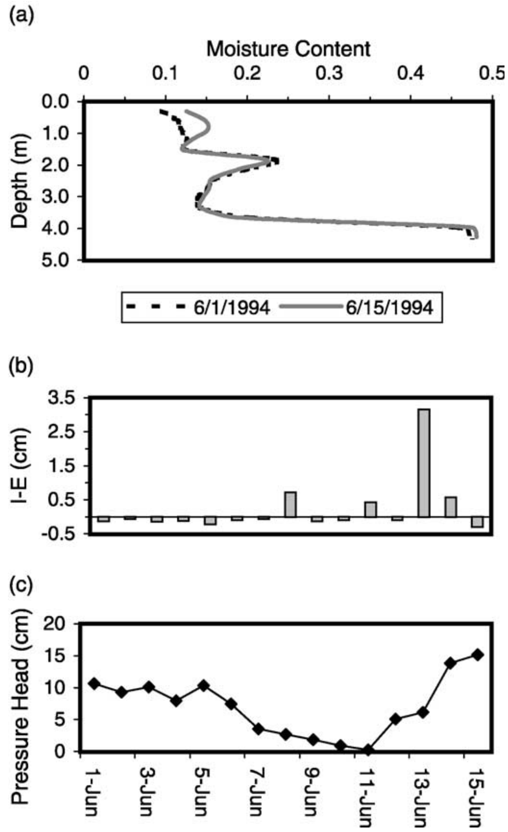

Fig. 1. Example of data used as input to the parameter optimization procedure. The period between moisture-profile measurements started out dry, but rainfall at the end of the period produced a bulge of moisture near the surface (a) and a water table rise (b).

The iterative procedure was used to calculate van Genuchten parameter values that satisfy each of the 37 data sets. The algorithm was first used to estimate a set of parameters that would be representative of the soil profile as a whole. Then the algorithm was run a second time, this time with the soil profile subdivided into seven sub-layers, each having a thickness of 61 cm.

4. Results

4.1. Background data

Data on the daily variation of net surface flux ($I - E$) and water table elevation are displayed graphically in Fig. 2. Over the entire period of monitoring, the weighing lysimeter registered 153 cm of net (daily integrated) infiltration and 77 cm of net evapotranspiration. The maximum range of water table variation was slightly less than 1 m. This range of variation was realized in both 1994 and 1995, but the water table remained at a fairly high level throughout the late summer and autumn of 1993.

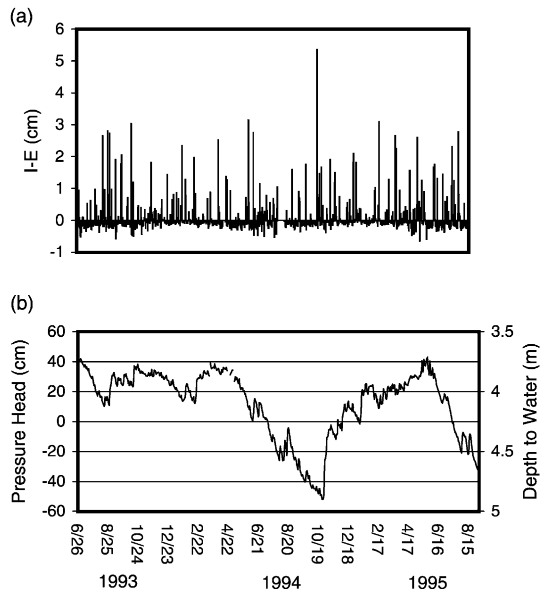

Fig. 2. Net surface flux (a) and water table variation (b) during the period of monitoring. Note that the water table was above the bottom of the neutron gauge access tube (4.25-m depth) during most of the study period.

Field tests of in situ hydraulic conductivity indicated that the dune sand was highly permeable. A Guelph permeameter was used to estimate the saturated hydraulic conductivity of the uppermost 30 cm. This test produced a value of $K_s = 1.8 \times 10^{-2}$ cm/s. A pump test was also conducted to determine the hydraulic conductivity of the saturated zone. For this test a second well was installed into the saturated zone 1.5 m away from the monitoring well and pumped at a constant rate of 3 l/min. Equilibrium of the drawdown in the observation well was achieved in approximately 2 h. The measured time-drawdown curve was compared to the theoretical curves of Neuman (1975). The curve matching indicated that the water table aquifer has a hydraulic conductivity of 1.5×10^{-2} cm/s and a specific yield of 0.13 (Dintaman, 1997).

Each of the 40 measured moisture profiles were integrated with respect to depth; the temporal variation of the integrated storage values is presented in Fig. 3(a). Maximum storage, exceeding 100 cm of water, occurred in the early spring of 1995 and the minimum storage of about 65 cm of water occurred in late summer of 1994. Continuous profiles showing the average, maximum, and minimum moisture contents observed over the period of monitoring are presented in Fig. 3(b). The largest range of moisture contents occurred in the lowermost meter of the profile where the water table fluctuation occurred; the smallest range occurred near the ground surface where the sand was loosest and subject to both evaporative losses and gravity drainage. Note that there is a consistent moisture bulge at a depth of 2 m. This is where the buried soil occurs and presumably is a reflection of the higher clay content that tends to hold more water than pure sand. In general, the range of moisture contents is higher below the buried soil and lower above (Fig. 3(b)). The excessively high moisture contents at the bottom of the profile suggest that the calibration determined for the upper part of the unsaturated zone may not have been representative of the underlying saturated zone.

4.2. Optimized parameters: algorithm performance

In the initial set of runs, one set of optimum parameters was calculated to be representative of the profile as a whole. A total of $37 \times 5 = 185$ parameters were estimated in the initial set of runs. Statistical tests, employing Student's t-distribution, indicated that 84% of the parameter estimates were statistically different from zero at the 95% confidence level. Of the 30 parameter estimates that were not significant, 2 were estimates of θ_r, one was an estimate of α, and the remaining 27 were estimates of K_s. Indeed only 27% of the estimated K_s values were statistically significant at the 95% confidence level.

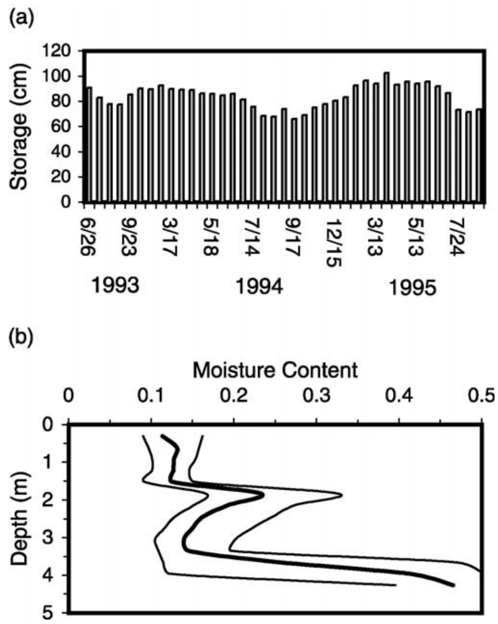

Fig. 3. Temporal variation in soil moisture storage (a), and range of soil moisture content (by depth) during the period of monitoring (b). Storage pertains to the entire 4.25 m thickness of porous medium penetrated by the neutron gauge access tube. The thick line in the plot of moisture profiles represents the average of all measurements made during the period of monitoring and the thin lines indicate the maximum and minimum measured values.

When the optimization algorithm was run in layer mode, seven separate sets of parameters were estimated for each data set. The algorithm was modified to minimize the objective function for each of the individual soil layers, which contained 12 data points. Table 1 provides a summary of how the algorithm performed in layer mode. The algorithm performed well except at the bottom of the profile where saturation conditions prevailed most of

Table 1
Algorithm performance by layer

Layer	Depth (m)	nNSP[a]	nK_s[b]	$n\alpha$[c]	$n\theta_r$[d]
7	0–0.61	1 (0.5%)	1	0	0
6	0.61–1.22	3 (1.6%)	2	1	0
5	1.22–1.83	5 (2.7%)	2	0	3
4	1.83–2.44	2 (1.1%)	1	0	1
3	2.44–3.05	3 (1.6%)	1	0	2
2	3.05–3.66	8 (4.3%)	5	1	2
1	3.66–4.27	22 (11.9%)	10	6	6

[a] Number of non-significant parameter estimates out of 185 total parameters estimated.
[b] Number of non-significant K_s estimates out of the total of 37.
[c] Number of non-significant α estimates out of the total of 37.
[d] Number of non-significant θ_r estimates out of the total of 37.

the time. Of the 37 sets of parameters that were estimated for the bottom layer, there were 10 that produced K_s values that were not significantly different from zero at the 95% confidence level and an additional 6 each that produced non-significant values of α and θ_r. However, even at the bottom of the profile, all of the estimates of θ_s and m were statistically significant at the 95% confidence level. As shown in Table 1, the number of insignificant parameter estimates associated with individual soil layers was typically less than 2%. A total of 1295 individual parameters were estimated for the layered profile and only 44 (3.4% of total) were insignificant according to the Student's t-test criterion. Seventeen of those (39%) were derived from three data sets. An inspection of those data sets revealed that their common feature was a major discrepancy between the integrated net surface flux (weighing lysimeter data) and the observed change in storage indicated by the neutron moisture gauge measurements.

4.3. Optimized parameters: whole profile

A statistical summary of the parameter estimates representative of the soil profile as a whole is provided in Table 2. All of the average estimated parameter values are larger than the seed values except for the saturated hydraulic conductivity. The average estimated value of θ_s exhibits the greatest deviation from its seed value, yet the coefficient of variation of θ_s values is the smallest of the estimated parameters.

Table 2
Summary of parameter estimates: whole profile

Parameter	θ_s	θ_r	α	$\log K_s$	m
Mean	0.478	0.058	0.068	−2.200	0.390
St. Dev.	0.035	0.021	0.020	0.435	0.085
Coef. Var.	7.29	35.69	29.82	19.76	21.75
Seed	0.400	0.050	0.040	−2.000	0.350

This indicates that the parameter estimation procedure consistently was producing high θ_s values. The estimated values of θ_s and θ_r are plotted as a function of time in Fig. 4. Although there is some variability in the trends of these two parameters, neither shows any tendency to increase, decrease, or cycle over the duration of the study. Although not shown here, plots of the parameters α and m exhibit the same quasi-steady trend. In contrast, a plot of the estimated K_s values reveals a cyclic trend over time (Fig. 5). Although the trend is not perfect, the estimated K_s values tend to increase in the warm seasons and decrease in the cool seasons.

4.4. Optimized parameters: layered profile

Because so many of the parameters estimated for the bottom layer were not statistically significant, data from that layer are not included in the subsequent analyses. A lumped statistical summary of the remaining set of 1100 parameter estimates is provided in Table 3. The sample size for each parameter summary statistic is $N = 222$ because six separate

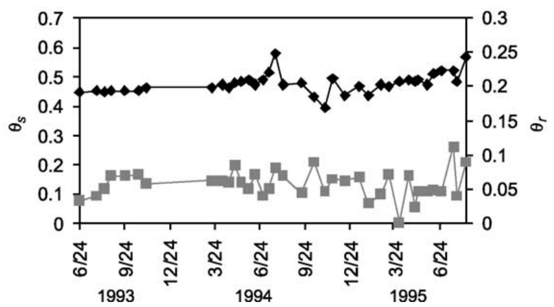

Fig. 4. Temporal trends of saturated (black diamonds) and residual (gray squares) moisture content derived from parameter estimation of the profile as a whole. Note that these trends are basically steady with a few minor fluctuations.

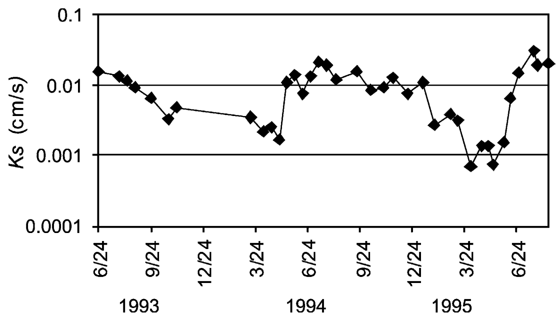

Fig. 5. Temporal trend of saturated hydraulic conductivity derived from parameter estimation of the profile as a whole. Note that the *y*-axis has a logarithmic scale. The trend is quasi-cyclic with highest values in early summer.

values of the van Genuchten parameters were estimated using each of the 37 data sets. Note that the average parameter values associated with the combined set of layers are closer to the seed values than the mean values estimated for the whole profile. Indeed, the mean value of θ_s, which deviated the most from its seed value in whole profile mode, practically equaled the seed value when the individual layer estimates were combined. Also, the standard deviation and coefficient of variation of θ_s became smaller when estimates were made in layer mode. This pattern was the same for three of the other parameter estimates. Only the estimates of θ_r departed from this trend, yet its mean value still was less than 0.02 units smaller than the seed value. The substantially smaller coefficients of variability in Table 3 (as compared to those in Table 2) seem to indicate that estimating parameters by layer provides more consistent estimates than estimating one set of parameters for the whole profile. This does not mean, however, that the average parameter values of the individual soil layers are the same. For example, a statistical plot showing how the mean $\pm$ 2 standard deviations of θ_s varies down profile reveals a degree

Table 3
Summary of parameter estimates: combined layers

Parameter	θ_s	θ_r	α	log K_s	m
Mean	0.396	0.031	0.042	−2.108	0.368
St. Dev.	0.018	0.014	0.006	0.218	0.021
Coef. Var.	4.54	45.16	14.93	10.35	5.67
Seed	0.400	0.050	0.040	−2.000	0.350

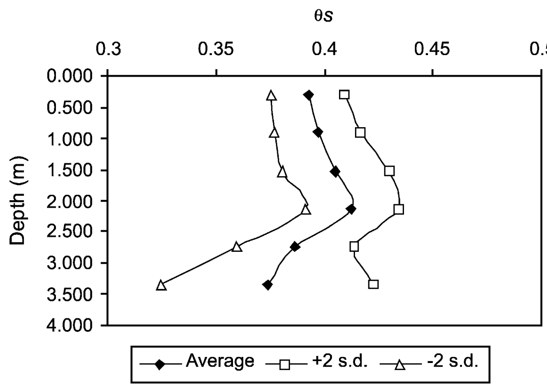

Fig. 6. Profiles of saturated moisture content derived from parameter estimation by layers. Maximum values occur at the depth of the buried soil and the variance of estimates is greatest at the bottom of the profile.

of systematic heterogeneity (Fig. 6). The values of θ_s are relatively low near the ground surface and then increase in the vicinity of the buried soil. The values of θ_s decrease immediately below the buried soil layer but then they increase again at the bottom of the profile. Note that the variance of the parameter estimates increases with depth. The widest spread of θ_s estimates occurs at the bottom of the profile (layer 2) where saturation conditions prevailed during part of the study period. The variation of K_s estimates with depth does not reveal an equivalent systematic trend. A mean value of 10^{-2} cm/s is prevalent through most of the profile (Fig. 7). A slightly higher average value occurs in layer 6 near the surface, but the variance of K_s is greatest in this layer as well.

Statistical comparisons of the average parameter values (using Student's *t*-test) indicated that every layer has a statistically unique mean value of θ_s. In contrast, none of the other four parameters exhibited any statistically significant differences between layers at the 95% confidence level. Temporal trends of the parameter estimates for three of the layers are presented in Fig. 8. Layer 7 is the uppermost layer, layer 4 contains the buried soil, and layer 2 is near the water table. The estimates of θ_s remained mostly steady over the course of the study with consistent separation between the layers (Fig. 8(a)). Note that there is a weak tendency for an inverse relationship to exist between the parameter estimates of layers 2 and 4. Also, two anomalously low values of θ_s were estimated from the final two data sets. These estimates

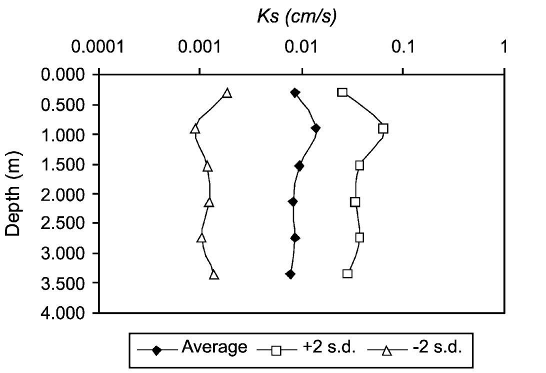

Fig. 7. Profiles of saturated hydraulic conductivity derived from parameter estimation by layers. Note the logarithmic scale of hydraulic conductivity. There is little variation in the average values and the wide variance throughout the profile precludes identification of any statistically significant differences between layers.

were checked for significance and both were statistically different from zero at the 95% confidence level (t-test criterion). As shown in Fig. 8(b), there is more fluctuation of the θ_r estimates over time. Higher estimated values occur in midsummer (dry season) and lower estimated values occur in late spring (wet season), however, the trend is not perfect. The trend of the estimated exponent values (Fig. 8(c)) is very steady at first, but a pattern of fluctuation developed in the estimates derived from data collected during the final year of the study. Note that even during the period of fluctuation, the estimated values of m did not differ by layer; indicating spatial stationarity of this parameter. The temporal trend of K_s mostly is steady over time and there is strong overlap between layers (Fig. 8(d)). Anomalous values were produced by data sets

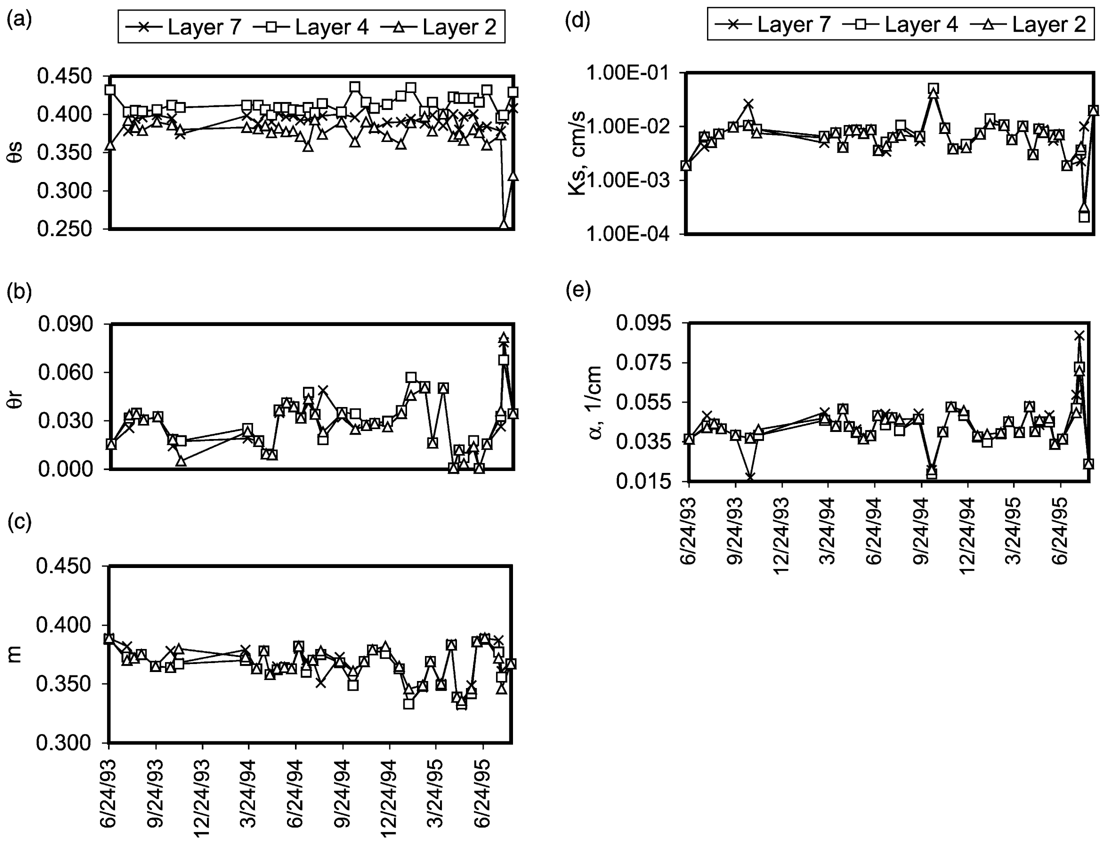

Fig. 8. Temporal trends of estimated van Gunuchten parameters for selected model layers. Most of the parameters exhibit a quasi-steady trend over time, but anomalous values occurred near the end of the period of monitoring. Note that little separation occurs between layer trends except in the case of saturated moisture content, which appears to be the parameter that best distinguishes the individual model layers.

Table 4
Statistical comparison of parameters derived for net wetting and drying periods

	Wetting periods $N = 84$				Drying periods $N = 138$			
Parameter	θ_s	θ_r	α	m	θ_s	θ_r	α	m
Maximum	0.472	0.063	0.052	0.471	0.467	0.061	0.056	0.448
Minimum	0.320	0.000	0.016	0.334	0.313	0.000	0.025	0.334
Mean	0.398	0.034	0.039	0.366	0.394	0.028	0.044	0.369
St. Dev.	0.021	0.014	0.007	0.026	0.016	0.013	0.005	0.017
t-ratio	1.51	3.51[a]	−5.11[a]	−1.03	–	–	–	–

[a] Difference in average parameter values (wetting versus drying periods) is statistically different from zero at the 95% confidence level.

collected on 10/13/94 and 7/30/95, but all of these estimates are statistically significant according to the t-test criterion. The temporal trend of estimated values of α (Fig. 8(e)) is very similar to that of the K_s estimates, except that they change in the opposite direction. A statistical correlation analysis indicated that there is indeed a strong negative correlation between these two sets of parameter estimates ($r = -0.688$). The next highest correlation between parameter estimates is -0.369 (relating estimates of θ_r and m), and the rest of the correlation coefficients are less than ± 0.3.

In an effort to evaluate the possible presence of hysteresis in the soil moisture retention characteristics at the study site, optimum parameters derived for the periods of net wetting (as indicated by the change in storage determined from neutron gauge measurements) were compared to those derived for the periods of net drying. A statistical summary of the wetting/drying comparison is provided in Table 4. As shown in the table, the only parameters that are statistically different (on average) between net wetting and drying periods are θ_r and α and these average parameter values only differ by 16 and 12%, respectively.

5. Discussion and conclusion

As the importance of vadose zone hydrology to critical environmental issues continues to grow (Looney and Falta, 2000), more emphasis is likely to be placed on accurate characterization of soil hydraulic properties and their heterogeneity. Despite several potential sources of error in the weighing lysimeter and neutron moisture gauge data, this study has demonstrated the great potential for coupling an unsaturated flow model with a parameter optimization method to estimate critical flow model parameters from field measurements of soil moisture profiles, surface fluxes, and pressure head. Previous studies had already shown that the methodology was promising, but this study is the first to demonstrate that a consistent set of parameter values can be achieved from repeated experiments at the same location and under real (uncontrolled) field conditions. A relatively simple hydrogeological situation was purposely selected to undertake the demonstration study because a reasonably accurate outcome could be anticipated. The uniform dune sand at the study site was expected to have a high degree of homogeneity of hydraulic properties, but the existence of weakly developed soil part way down the profile provided a basis for evaluating the ability of the parameter estimation methodology to ‘fingerprint’ the anomalous layer. Thirty-seven separate parameter estimation experiments were undertaken and the results were remarkably consistent given the wide range of conditions that were encountered over the course of the investigation. Indeed, there appeared to be only three or four data sets that produced parameter values that were inconsistent with the norms. The fact that these anomalous data sets occurred, and that the parameter values appeared to be statistically significant, is strong evidence for the need to undertake repeated experiments prior to concluding that a truly representative set of unsaturated zone hydraulic properties have been determined.

One potentially important outcome of the study was that even though the study profile was fairly uniform, estimating parameters by layer rather than for the profile as a whole, yielded more significant and seemingly more accurate parameter values. When the parameter estimation algorithm was run in whole profile mode, the 'best-fit' values of saturated conductivity were rarely significant (95% confidence level) and the average value of saturated moisture content was seemingly too high for a deposit of fine-grained dune sand. In contrast, when the algorithm was run in layer mode, a very reasonable set of parameter values was achieved for most of the profile. Problems of parameter uncertainty beset the bottom layer of the profile; that layer was almost always saturated during the study period and probably should not have been included in the first place. When the parameter estimates of the remaining six layers were pooled, they produced a set of average parameters that were very consistent and seemingly realistic for a deposit of fine sand. Fig. 9 shows the soil moisture characteristic curve produced by the parameters estimated in this study. The dashed lines are curves generated by the average ± 2 standard deviations of each parameter value. The resulting range of the function is remarkably narrow, again emphasizing the consistently similar parameter values that were derived from the 37 data sets.

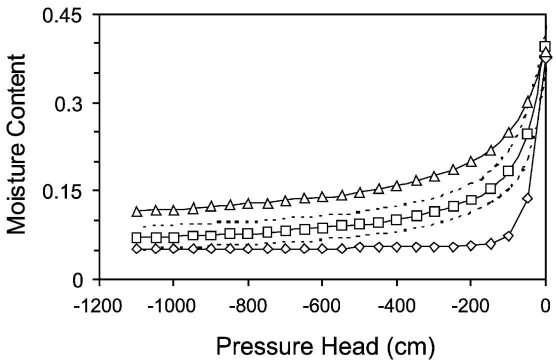

Fig. 9. Plot of moisture retention curve based on average estimated parameters (layer mode, Table 3) for the study site. Curve with open squares is the average curve, dashed lines are curves based on mean $\pm$ 2 standard deviation parameter values. Bounding curves are based on average parameter values for loamy sand (triangles) and sand (diamonds) reported by Schaap et al. (2000).

The seven soil layers were distinguished by their average values of saturated moisture content. A higher θ_s value was expected in the vicinity of the buried soil, but the significant differences between other layers came as somewhat of a surprise. Apparently subtle differences in the dominant grain sizes of individual soil layers and perhaps their degree of compaction can influence their best-fit hydraulic properties. On the other hand, a lower than average K_s value was expected for the soil layer, but that did not turn out to be the case. The amount of clay in the interstices of the pedogenic soil may not be sufficient to influence the conductivity of that layer. Another possibility is that the large variance of K_s estimates precluded the generation of statistically significant differences between layers.

A statistical comparison of the average parameter values derived for net wetting and drying periods indicated that there is little difference in the shape of the associated moisture retention curves. The statistically significant differences were a larger value of θ_r for the net wetting periods and a larger value of α for the net drying periods. These findings are somewhat troublesome in that the upper and lower bounds of hysteretic moisture retention curves should be equal and the slope of the wetting curve should be steeper than that of the drying curve. However, it should be realized that periods of both wetting and drying (driven by changes in both the surface flux and water table elevation) occurred during each of the study periods so the optimum parameter values are theoretically integrating the effects of scanning between wetting and drying curves. Regardless of the cause of the statistically different average parameter values, the actual differences are quite small and may be within the uncertainty resulting from measurement error.

The soil moisture characteristics implied by average parameter values for sand and loamy sand reported by Schaap et al. (2000) are also plotted in Fig. 9. Note that these curves neatly bracket the curve developed from the in situ parameter-estimation procedure utilized in this study. This result seems reasonable since the dune material at the study site, which has experienced some pedogenic soil development, should not behave like a pure sand, yet the degree of soil development is insufficient to cause the material to behave like a typical loamy sand.

Of course, the differences in these curves simply could be a result of different measurement techniques. Many more comparisons between in situ and laboratory-derived hydraulic properties of similar materials must be made before the effects of different parameter estimation methods are fully understood. Unfortunately, until that happens, a great amount of uncertainty will persist in our efforts to model the flow of water in real variably saturated sediments.

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