Analysis of Measured, Predicted, and Estimated Hydraulic Conductivity Using the RETC Computer Program

S. R. Yates,* M. Th. van Genuchten, A. W. Warrick, and F. J. Leij

ABSTRACT

A nonlinear least-squares optimization program, RETC, which uses empirical relationships for describing the water-retention curve and predictive models for characterizing the unsaturated hydraulic conductivity relationship was used to analyze 36 unsaturated hydraulic conductivity distributions obtained from the literature for 23 different soils. By comparing the measured, predicted, and estimated relative conductivity for the group of data, the efficiency and accuracy of this approach for characterizing the soil hydraulic properties was determined. The analysis consisted of comparing measured, predicted, and estimated conductivities using three predictive methods and two simultaneous methods (which include known values of the conductivity). The results indicate that for this group of data, the best method for determining the model parameters that will accurately describe both the water retention and unsaturated hydraulic conductivity relationships is to use a simultaneous approach with either five or six parameters. It was also found that the predictive approach introduces a bias into the estimates of the unsaturated hydraulic conductivity and a predictive approach with scaling did not significantly improve the estimates of the unsaturated hydraulic conductivity.

Accurate numerical models are increasingly needed to solve groundwater-flow and contamination problems. To achieve this, better means for characterizing the soil hydraulic properties are needed. Presently, our ability to create complex numerical models far exceeds our capacity to describe the physical system on which the model is based. The basic soil hydraulic properties, in particular the unsaturated hydraulic conductivity, play an integral role in determining the accuracy of any numerical solution to flow and, therefore, transport problems. The inability to characterize the functional relationship between the unsaturated hydraulic conductivity and water content (or matric potential) will result in an inaccurate representation of the simulated flow process. Incorporating an inaccurate flow representation into a contaminant-transport model can seriously affect the accuracy of the transport simulation.

The problem of determining the unsaturated hydraulic conductivity is confounded by the expense of experimentally obtaining this relationship and the large number of observations required to adequately characterize the spatial distribution due to commonly occurring field-scale variability. This has led to the introduction of a number of techniques for reducing the data requirements necessary for determining the field hydraulic properties (Maulem, 1976a, 1986; van Genuchten, 1980; Arya and Paris, 1981; Saxton et al., 1985; Puckett et al., 1985; Haverkamp and Parlange, 1986; Kool and Parker, 1988; Tyler and Wheatcraft, 1989, 1990). One such method, described in detail by van Genuchten (1980) and van Genuchten and Nielsen (1985), provides a predictive technique for obtaining the unsaturated hydraulic conductivity from soil water-retention data, which, in general, are easier to obtain. The advantage of predictive methods is that, for a given dollar investment, more measurements of the water-retention relationship can be obtained compared with conductivity. Assuming that an estimation technique is available that provides an accurate prediction of the conductivity, a better spatial characterization of the conductivity can be achieved than with direct-measurement methods.

A number of examples using this approach can be found in the literature, including van Genuchten (1980), who introduced an empirical relationship for describing the water-retention curve that could be coupled to the model of Mualem (1976a) to provide predicted unsaturated hydraulic conductivities. It was found that the method worked well for a sandstone and two silt loams but not for a clay. Van Genuchten and Nielsen (1985) found that the comparison between the measured and predicted conductivity varied considerably for a silty clay loam, a sand, and a loam, even when a more general predictive model was used. Matching a conductivity data point in the near-saturated region improved the correspondence between the measured and predicted conductivity for the loam. Stephens and Rehfeldt (1985) compared a number of field values for unsaturated hydraulic conductivity to values generated by the predictive method. In general, they found agreement between the experimental and predicted conductivity.

In each of these studies, several comparisons between measured and predicted values of the unsaturated hydraulic conductivity are made, some of which provide a close match while others do not. Although a number of studies have been conducted on this subject, they do not address a number of important considerations concerning this methodology. For example, no known study has been conducted to determine whether the predictive methods introduce a systematic bias between the predicted and measured values. Also, little information exists on the effect of using known values of the unsaturated conductivity in a procedure for estimating the soil hydraulic parameters. For instance, it is unclear whether the correspondence between measured and estimated conductivity always improves as well as the effect on the moisture-retention relationship. Also of interest is information on other means for improving the predicted values of the conductivity that do not require a large increase in experimental measurements.

To begin obtaining some of this information, Yates et al. (1991) conducted a study to investigate the relationship between the measured, predicted, and estimated hydraulic conductivity when a predetermined procedure for determining the initial estimates for the soil hydraulic parameters was used. The initial param-

S.R. Yates, M.Th. van Genuchten, and F.J. Leij, U.S. Salinity Lab., 4500 Glenwood Dr., Riverside, CA 92501; and A.W. Warrick, Dep. of Soil and Water Science, Univ. of Arizona, Tucson, AZ 85721. Received 18 Sept. 1990. *Corresponding author.

Published in Soil Sci. Soc. Am. J. 56:347–354 (1992).

eters were modified only if the minimization process failed to converge. The term *predicted method* is used here to describe procedures that do not require known values of the conductivity and, hence, enable conductivity predictions. The term *estimated method* is used for procedures that use known conductivity values to improve estimates of the conductivity compared with the predicted methods. The purpose of this study was to investigate the sensitivity of the nonlinear estimation method to the initial parameter values as well as to determine which of a number of approaches would provide the best soil hydraulic parameters, given the stringent conditions imposed. Although the study provides some information concerning difficulties with convergence and uniqueness, in a general sense the results are not realistic since most scientists would attempt to develop optimal parameters for a given soil by using many different initial conditions for the model parameters.

The approach used in this study was to analyze a group of soils as a whole, assuming that the measured values are error free, and to compare the measured, predicted, and estimated relative hydraulic conductivities to judge the accuracy of the technique. This should also give indications of whether the predicted hydraulic conductivity is systematically biased and whether measured values of the unsaturated hydraulic conductivity are necessary to obtain an accurate representation of the soil hydraulic properties and the sensitivity of the model parameters. The computer program RETC was developed to carry out the lengthy numerical computations required to estimate the model parameters.

METHODS

A data set consisting of 23 different soil types and 36 distributions for the water-retention relationship and unsaturated hydraulic conductivity were obtained from the literature. This data set is reported in Table 1 and includes the Mualem (1976b) soil index number (if applicable) and the soil name. Also reported in Table 1 are the model parameters that can be used to describe the soil hydraulic properties for several test cases, which will be described more fully below. Since the program RETC has been described in detail by Leij et al. (1991), only a brief description of the approach follows.

The Nonlinear Least-Squares Optimization Program

The program, RETC, was developed to provide a means for obtaining optimal model parameters for nonlinear equations with multiple parameters. The parameters are deemed optimal in the sense that they provide the minimum least-square error between the estimated and measured values. To use the optimization procedure in RETC, descriptions for the soil hydraulic properties are required.

The soil water-retention relationship can be described using any of a number of empirical equations that have the proper shape. The program allows use of two of these, the Brooks and Corey (1964) equation:

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

and the van Genuchten (1980) equation:

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

where h is the suction head form of the matric potential (L) having positive values, θ is the volumetric water content (L^3/L^3), θ_r and θ_s are the residual and saturated water contents, respectively, and α (L^{-1}), m, and n are empirical constants that enable the model (i.e., Eq. [1] or [2]) to characterize the retention relationship.

Since the Brooks and Corey (1964) relationship is a special case of Eq. [2] as $n \rightarrow \infty$ (with $n\ m$ finite), we will discuss only Eq. [2]. The general case, where n and m are not related, has been described in detail by van Genuchten and Nielsen (1985). A simplified case, which appears to be valid for many soils, can be obtained by adopting the relationship $m = 1 - 1/n$. Using this relationship simplifies the mathematics, as shown by van Genuchten (1980) and van Genuchten and Nielsen (1985).

Predictions of the unsaturated hydraulic conductivity can be obtained provided a relationship between the hydraulic conductivity and moisture-retention relationship is available. The RETC program uses the approach of either Burdine (1953) or Mualem (1976a). For either approach, the relative conductivity, K_r, can be written as

$$K_r\,(S_e) = (S_e)^{\ell}\,\frac{\eta\,(S_e)}{\eta\,(1)} \qquad [3]$$

where S_e is the effective saturation: $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$, ℓ is an empirical constant, and the mathematical form for the arbitrary function $\eta\,(S_e)$ depends on which model is used. Using the Mualem (1976a) model:

$$\eta\,(S_e) = \left[\int_0^{S_e} \frac{1}{h(x)}\,dx\right]^2 \qquad [4]$$

Combining Eq. [2] and [4] and the condition $m = 1 - 1/n$ allows the hydraulic conductivity, $K(S_e)$, to be expressed as

$$K(S_e) = K_s\,S_e^{\ell}\,[1 - (1 - S_e^{1/m})^m]^2 \qquad [5]$$

where K_s is the saturated hydraulic conductivity. An expression similar to Eq. [5] can be developed for the Burdine (1953) approach (i.e., where $\eta\,(S_e) = \int_0^{S_e} [1/h\,(x)^2]\,dx$). Since this method was not used here, it is not included in this discussion.

Predictions for the conductivity can be obtained once the model parameters (θ_r, θ_s, α, m, n, ℓ, K_s) in Eq. [2] are determined. Assuming the Mualem model, $\ell = 0.5$ and K_s is known, Eq. [5] can be used to obtain predicted unsaturated hydraulic conductivity. Alternatively, given known values of the conductivity, the model parameters ℓ and m can be obtained. If the parameters are obtained using the relative conductivity in Eq. [5], then Eq. [5] can be written as

$$K_r\,(S_e) = K_o\,S_e^{\ell}\,[1 - (1 - S_e^{1/m})^m]^2 \qquad [6]$$

where the dimensionless parameter K_o is analogous to the dimensional parameter K_s in Eq. [5], allowing a linear translation of the relative-conductivity curve. Using Eq. [5] or [6] will produce essentially identical results since during the minimization process, any constant value (e.g., the measured saturated hydraulic conductivity [K_{sat}] will cancel out. This can be shown by incorporating the definitions for W_1 (see Eq. [8] below) and $K_s = K_{sat}K_o$ into Eq. [7], below, and simplifying. Equation [6] was used to obtain the model parameters described below.

Nonlinear Optimization Technique

The RETC program uses a nonlinear least-squares optimization technique to minimize an objective function. The

Table 1. Data set and model parameters (residual volumetric water content [θ_r], saturated water contents [θ_s], empirical constants α, n, and ℓ, and dimensionless saturated hydraulic conductivity [K_o], obtained using a nonlinear least-squares procedure.

Soil index	Soil name	Predictive† method θ_r	θ_s	α	n	Simultaneous method,‡ 5 parameters θ_r	θ_s	α	n	ℓ	Simultaneous method, 6 parameters θ_r	θ_s	α	n	ℓ	K_o
				cm^{-1}				cm^{-1}					cm^{-1}			
—§	Yolo light clay K(WC)	0.205	0.499	0.02793	1.71	0.212	0.496	0.0268	1.76	−2.35	0.199	0.499	0.0284	1.67	−2.00	1.67
—	Yolo light clay K(H)	0.205	0.499	0.02793	1.71	0.097	0.472	0.0102	1.66	0.072	0.214	0.496	0.0264	1.77	−2.03	1.30
1003	Lamberg clay	0.000	0.502	0.140	1.93	0.000	0.498	0.135	1.96	2.56	0.000	0.501	0.138	1.94	2.53	1.13
1006	Beit Netofa clay soil	0.000	0.447	0.00156	1.17	0.090	0.435	0.00095	1.26	17.7	0.007	0.428	0.00073	1.21	32.1	1.22
1101	Shlohot silty clay	0.000	0.456	18.3	1.17	0.000	0.272	0.0764	2.55	−2.53	0.100	0.422	7.12	1.31	−5.09	513
2001	Silt Columbia	0.146	0.397	0.0145	1.85	0.158	0.385	0.00994	2.38	0.192	0.162	0.403	0.0142	2.02	0.002	1.70
2002	Silt Mont Cenis	0.000	0.425	0.0103	1.34	0.055	0.388	0.00290	1.97	1.52	0.049	0.386	0.00327	1.82	1.07	1.04
2004	Slate dust	0.000	0.498	0.00981	6.75	0.058	0.523	0.0159	2.34	−0.080	0.003	0.518	0.0120	2.87	1.96	0.817
3001	Weld silty clay loam	0.159	0.496	0.0136	5.45	0.120	0.469	0.0124	4.52	0.954	0.115	0.505	0.0133	4.07	1.17	2.23
3101a	Rideau clay loam, wetting	0.279	0.419	0.0661	1.89	0.191	0.445	0.104	1.33	0.000	0.218	0.443	0.102	1.40	0.000	0.670
3101b	Rideau clay loam, drying	0.290	0.419	0.0177	3.18	0.135	0.433	0.0312	1.29	2.92	0.234	0.435	0.0261	1.65	0.911	0.244
3301a	Caribou silt loam, drying	0.000	0.451	0.00845	1.29	0.167	0.441	0.00688	1.63	0.029	0.163	0.441	0.00654	1.66	0.239	0.905
3310b	Caribou silt loam, wetting	0.000	0.450	0.140	1.09	0.294	0.442	0.0496	1.67	−3.31	0.182	0.443	0.00978	1.64	0.025	1.10
3302a	Grenville silt loam, wetting	0.013	0.523	0.0630	1.24	0.084	0.444	0.0102	1.61	3.64	0.017	0.532	0.0681	1.25	2.14	72.7
3302c	Grenville silt loam, drying	0.000	0.488	0.0112	1.23	0.051	0.453	0.00433	1.36	6.08	0.002	0.0482	0.00966	1.24	5.69	6.72
3304	Touchet silt loam	0.183	0.498	0.0104	5.78	0.157	0.521	0.0106	4.62	0.007	0.157	0.503	0.0103	4.87	0.001	0.790
3310	Silt loam	0.139	0.394	0.00414	2.15	0.154	0.393	0.00414	2.28	3.00	0.154	0.393	0.00415	2.25	3.08	0.973
3402a	Gilat loam	0.000	0.454	0.0291	1.47	0.007	0.438	0.0172	1.80	1.96	0.014	0.440	0.0189	1.78	0.490	0.604
3403	Pachapa loam	0.000	0.472	0.00829	1.62	0.013	0.455	0.00644	1.79	1.61	0.006	0.469	0.00780	1.66	2.05	3.44
3404	Adelanto loam	0.000	0.444	0.00710	1.26	0.029	0.401	0.00261	1.43	0.643	0.050	0.446	0.00597	1.43	0.022	2.05
3405a	Indio loam	0.000	0.507	0.00847	1.60	0.000	0.558	0.0118	1.56	0.000	0.002	0.536	0.0105	1.56	0.670	1.23
3407a	Guelph loam	0.000	0.563	0.0275	1.27	0.208	0.493	0.0098	2.00	0.321	0.210	0.503	0.0106	1.99	0.072	1.09
3407b	Guelph loam	0.236	0.435	0.0271	2.62	0.000	0.222	0.00048	44.8	1.98	0.228	0.466	0.0375	2.18	0.000	0.660
3501a	Rubicon sandy loam	0.000	0.393	0.00972	2.18	0.128	0.388	0.0121	2.95	0.142	0.102	0.378	0.0105	2.81	1.16	1.14
3501b	Rubicon sandy loam	0.000	0.433	0.147	1.28	0.139	0.389	0.0572	1.83	−2.03	0.116	0.404	0.0752	1.62	−1.45	4.57
3503a	Pachapa fine sandy clay	0.000	0.340	0.0194	1.45	0.049	0.334	0.0132	1.84	−0.822	0.063	0.330	0.0118	2.06	−0.705	0.783
3504	Gilat sandy loam	0.000	0.432	0.0103	1.48	0.000	0.430	0.00973	1.50	−0.059	0.014	0.446	0.0117	1.50	1.50	6.96
4101a	Plainfield sand (210–250)	0.000	0.351	0.0236	12.30	0.020	0.346	0.0238	16.4	407.	0.020	0.348	0.0238	14.8	371	1.62
4101b	Plainfield sand (210–250)	0.000	0.312	0.0387	4.48	0.020	0.305	0.0380	5.92	−1.39	0.020	0.305	0.0380	5.91	−0.500	1.94
4102a	Plainfield sand (177–210)	0.000	0.361	0.0207	10.70	0.000	0.357	0.0205	11.2	26.2	0.020	0.357	0.0208	13.2	65.4	1.46
4102b	Plainfield sand (177–210)	0.022	0.309	0.0328	6.23	0.021	0.316	0.0333	5.94	−1.90	0.020	0.309	0.0328	6.11	−1.26	1.56
4103a	Plainfield sand (149–177)	0.000	0.387	0.0173	7.80	0.048	0.377	0.0174	17.4	105.	0.040	0.379	0.0174	14.3	71.6	1.87
4103b	Plainfield sand (149–177)	0.025	0.321	0.0272	6.69	0.026	0.321	0.0272	6.71	−1.59	0.026	0.321	0.0272	6.72	−1.30	1.63
4104a	Plainfield sand (125–149)	0.000	0.377	0.0145	10.60	0.070	0.361	0.0149	39.5	69284.	0.045	0.370	0.0148	18.6	311.	1.67
4104b	Plainfield sand (125–149)	0.000	0.342	0.0230	5.18	0.000	0.342	0.0230	5.11	−1.76	0.030	0.335	0.0232	6.96	−1.92	0.598
4130	Hygiene sandstone	0.000	0.256	0.00562	3.27	0.157	0.252	0.00809	11.0	0.000	0.111	0.248	0.00678	5.64	4.71	1.38

† ℓ = ½ and K_o = 1 for all soils.
‡ K_o = 1 for all soils.
§ Data from Moore (1939).

program was written so that the model parameters can be determined using only the retention data or both the retention and conductivity data. For the latter case, a set of optimal estimates for the model parameter vector (i.e., $\mathbf{b} = \{\theta_r, \theta_s, \alpha, m, n, \ell, K_s \text{ or } K_o\}$) is obtained where ℓ and K_s or K_o only occur in the equation describing the conductivity. The procedure minimizes the following objective function using Marquardt's maximum neighborhood method (Marquardt, 1963). This objective function, $O(\mathbf{b})$, has the general form

$$O(\mathbf{b}) = \sum_{i=1}^{N} \left\{ w_i \left[\theta_i - \hat{\theta}_i(\mathbf{b})\right] \right\}^2 + \sum_{i=N+1}^{M} \left\{ W_1 W_2 w_i \left[Y_i - \hat{Y}_i(\mathbf{b})\right] \right\}^2 \quad [7]$$

where θ_i and $\hat{\theta}_i$ are observed and calculated water contents,

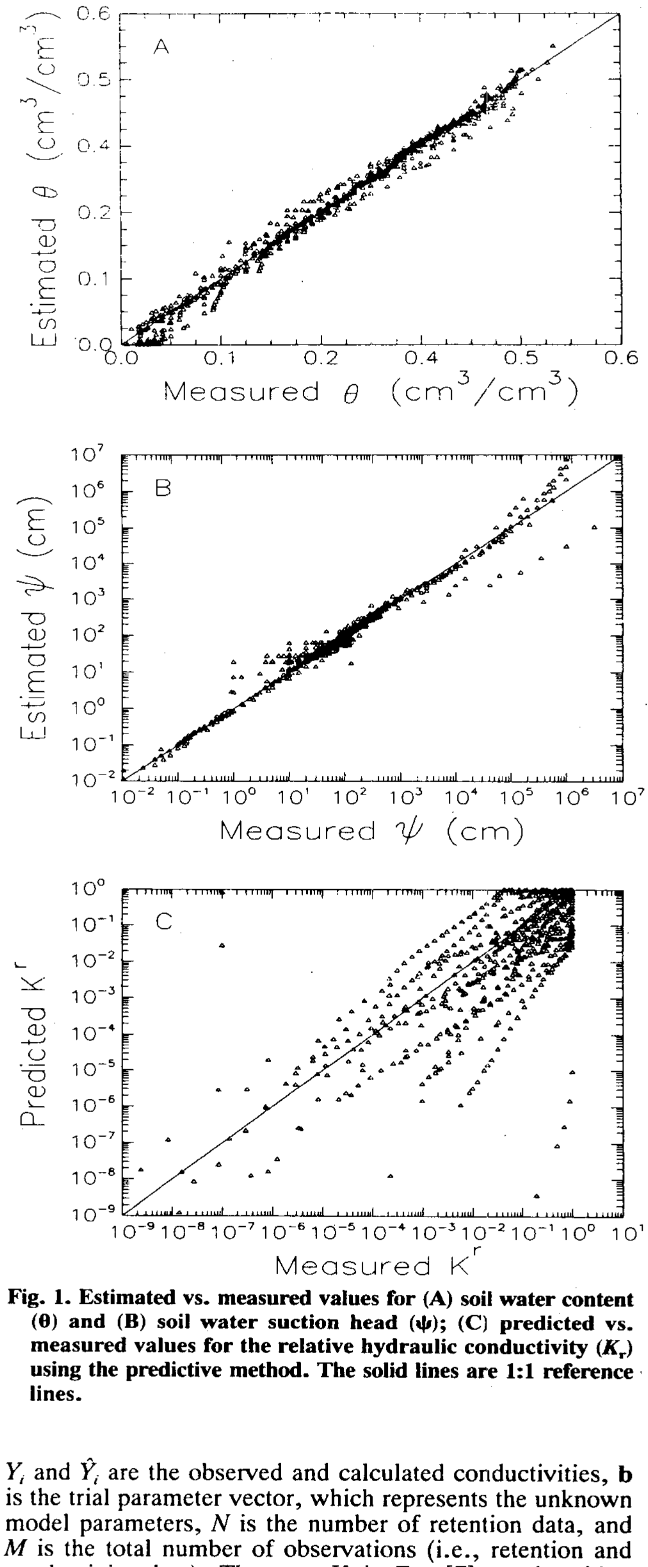

Fig. 1. Estimated vs. measured values for (A) soil water content (θ) and (B) soil water suction head (ψ); (C) predicted vs. measured values for the relative hydraulic conductivity (K_r) using the predictive method. The solid lines are 1:1 reference lines.

Y_i and $\hat{Y}_i$ are the observed and calculated conductivities, **b** is the trial parameter vector, which represents the unknown model parameters, N is the number of retention data, and M is the total number of observations (i.e., retention and conductivity data). The term Y_i in Eq. [7] can be either original conductivity values or their logarithms. In general, it is recommended that the logarithmically transformed conductivity values be used, since they better describe the conductivity across the entire range of observed values. The untransformed data give relatively more weight to the conductivity data near saturation, which may be useful when high accuracy is needed in this region.

The term w_i (where $i = 1,..., M$) in Eq. [7] are weighting coefficients that allow a single data value to be weighted more or less depending on a priori information and were set to unity. The coefficients W_1 and W_2 are also weighting coefficients. The weight factor W_1

$$W_1 = \frac{\frac{1}{N}\sum_{i=1}^{N} w_i\theta_i}{\frac{1}{M-N}\sum_{i=N+1}^{M} w_i|Y_i|} \qquad [8]$$

is automatically calculated and used by the program to give the water-content data approximately the same weight as the conductivity data. This keeps one data set from dominating the other due solely to the magnitude of its numerical values. The weighting factor W_2 is used to place more or less weight on the conductivity data during the optimization process. Since no a priori information was available, W_2 was set to unity.

The parameters are adjusted until a minimum squared error is found, indicating an optimum set of values for **b**. In the most general case, **b** contains seven unknown coefficients:

$$\mathbf{b} = [\theta_r, \theta_s, \alpha, m, n, \ell, K_s \text{ or } K_o] \qquad [9]$$

The RETC program was used to find the optimal parameters vector **b** using several different methods for analyzing the data set. The first method used RETC to determine the optimal soil hydraulic parameters (i.e., θ_r, θ_s, α, and n) by the predictive method. The predictive method uses only the water-retention data and assumes $\ell = 0.5$ and K_s is equal to the measured K_{sat} value. This is the most common approach for using RETC and offers an advantage in that values of the unsaturated hydraulic conductivity can be obtained without requiring any known experimental conductivity data.

If the unsaturated hydraulic conductivity has been measured at only one water content (or pressure), which is not at saturation, it is possible to scale the estimated hydraulic conductivity using the method described by van Genuchten and Nielsen (1985) and, more recently, by Luckner et al. (1989). When combined with the predictive method described above, we call it the *scaled-predictive method*. This point-matching method can improve the predicted values of the conductivity by ensuring that the conductivity curve passes through a known (measured) value.

Using RETC, it is possible to use the water-retention and unsaturated hydraulic conductivity data simultaneously for estimating the soil hydraulic parameters. In this case, two additional parameters (i.e., ℓ and K_o) can be included in the analysis. The *simultaneous method with five parameters* included ℓ in the analysis. The *simultaneous method with six parameters* included ℓ and K_o in the analysis. For these cases, estimated and measured values are compared.

The final approach, termed the *predictive method with adjustable* ℓ, used the soil hydraulic parameters (θ_r, θ_s, α, and n) obtained from the predictive method and allowed RETC to find the optimum value for ℓ using the hydraulic-conductivity data. This approach provided estimates of the conductivity and allowed the effects on the conductivity due to ℓ to be determined.

RESULTS

Shown in Fig. 1 are scatter diagrams of the measured vs. estimated values for the water content, the soil water suction head, and the unsaturated relative hydraulic conductivity using the predictive method for all the data from Table 1. The solid line in each figure is a 1:1 line denoting the location where the measured and calculated values are equal. It is apparent that the measured vs. estimated values for the water content

Table 2. Statistics comparing measured and estimated water content and logarithmic pressure head.

	Mean sum of deviation	Mean sum of squares	Linear regression line	r^2
		Water content		
Predictive method	0.00172	0.000207	$-0.0058 + 1.015K_m$†	0.988
Simultaneous method, five parameters	0.00254	0.000766	$0.0095 + 0.975K_m$	0.948
Simultaneous method, six parameters	0.000262	0.000396	$-0.0035 + 0.986K_m$	0.975
		Suction head		
Predictive method	−0.0110	0.0673	$0.0844 + 0.963K_m$	0.949
Simultaneous method, five parameters	0.0665	0.147	$-0.0193 + 0.975K_m$	0.872
Simultaneous method, six parameters	0.0394	0.108	$0.0230 + 0.969K_m$	0.914

† K_m is the measured relative hydraulic conductivity.

Table 3. Statistics comparing measured, predicted, and estimated unsaturated hydraulic conductivity.

	Mean sum of deviation	Mean sum of squares	Linear regression line	r^2
Predictive method	0.0612†	0.120	$0.078 + 0.537K_m$‡	0.305
Simultaneous method, five parameters	0.0271†	0.0440	$0.054 + 0.903K_m$	0.683
Simultaneous method, six parameters	0.0140	0.101	$-0.005 + 0.970K_m$	0.550
Predictive method with scaling	0.0270	0.230	$0.021 + 0.839K_m$	0.296
Predictive method with fitted constant ℓ	0.0293†	0.0974	$0.049 + 0.446K_m$	0.293

† Null hypothesis rejected at the 0.01 probability level that the mean difference between the measured and estimated values of the unsaturated hydraulic conductivity is zero (i.e., that the estimates are biased).
‡ K_m is the measured relative hydraulic conductivity

Table 4. Statistics comparing measured and estimated $\log_{10}$-transformed hydraulic conductivity.

	Mean sum of deviation	Mean sum of squares	Linear regression line	r^2
Predictive method	0.0207†	0.0109	$-0.614 + 1.040K_m$‡	0.313
Simultaneous method, five parameters	0.00697	0.00348	$-0.072 + 0.945K_m$	0.946
Simultaneous method, six parameters	0.00781	0.00320	$-0.076 + 0.964K_m$	0.973
Predictive method with scaling	0.0145†	0.00780	$-0.375 + 0.870K_m$	0.736
Predictive method with fitted constant ℓ	0.00863†	0.00849	$-0.717 + 0.903K_m$	0.526

† Null hypothesis rejected at the 0.01 probability level that the mean difference between the measured and estimated values of the unsaturated hydraulic conductivity is zero (i.e., that the estimates are biased).
‡ K_m is the measured relative hydraulic conductivity.

and pressure are, in general, very close to the 1:1 line, indicating that the soil hydraulic parameters listed in Table 1 provide an adequate description of the water-retention relationship.

The unsaturated hydraulic conductivity, on the other hand, shows considerable variation around the 1:1 line, which indicates that the soil hydraulic parameters do not adequately describe this relationship. Except for a few outliers, most of the values fall within approximately two orders of magnitude in the wet region (measured perpendicular to the 1:1 line) and about two to four orders of magnitude in the dry range. For conductivity, there appears to be more points below the 1:1 line than above it, which is an indication that the estimates are biased. Tables 2 through 4 contain several statistics that summarize the behavior of these curves.

As expected, the predictive method provided the best characterization of the water-retention relationship. This is demonstrated by noting that the mean sum of squares is the smallest, the coefficient of determination is the largest, the linear-regression line has a near-zero constant and a slope close to unity, and the mean sum of deviation is acceptably small.

For the unsaturated hydraulic conductivity, however, the predictive method did not produce as good results as the simultaneous method with five or six parameters. This is shown by larger values of the mean sum of deviation and the mean sum of squares. Also, the regression line does not have a slope near unity and the coefficient of determination is approximately one-half as large as the values for the simultaneous methods. When the statistics were determined using the logarithmically-transformed conductivity (Table 4), there was an improvement in the slope of the regression line, but a comparison of the other statistics was essentially the same. The predictive method also produces a mean sum of deviation that indicates bias. The level of bias was determined by testing the null hypothesis, at the 0.01 probability level, that the mean difference between measured and estimated values for the unsaturated hydraulic conductivity is zero (Bhattacharyya and Johnson, 1977).

Shown in Fig. 2 is a scatter diagram using the simultaneous method with five parameters. This method uses both the water-retention and unsaturated relative hydraulic conductivity data in the analysis. The value for the K_0 parameter was set to unity and not allowed to change. It is apparent that there is an improvement in the estimation of the unsaturated hydraulic conductivity, compared with the predictive method. The cost of this improvement is a poorer characterization of the water-retention relationship. This can also be seen from the statistics in Tables 2 through 4 where, for the water content and pressure, there has been an increase in the mean sum of deviation and mean sum of squared deviation, and a decrease in the coefficient of determination. For the hydraulic conductivity, there has been a corresponding decrease in the mean sum of deviation and mean sum of squared deviation, and an increase in the coefficient of determination, indicating an improvement. These effects are more pronounced for the logarithmically-transformed conductivity than for the untransformed values (Tables 3 and 4). The estimates of the unsaturated hydraulic conductivity remain biased for this case, although the difference between the test statistic and critical value indicating a bias was smaller for this case than for the predictive method.

Shown in Fig. 3 are measured vs. estimated values for the water content and pressure and relative hydraulic conductivities using the simultaneous method with six parameters. In a manner similar to Fig. 2, comparing to the predictive case, the correspondence between the measured and estimated hydraulic conductivity has increased at a cost of a poorer characterization of the water-retention relationship. This is also demonstrated by comparing the values for the predictive method with the simultaneous method with six parameters (Tables 2–4).

Comparing the simultaneous method using five parameters with the method using six parameters shows an improvement in the characterization of both the water-retention and hydraulic-conductivity relationships when six parameters are used. Also, for the simultaneous method with six parameters, no biasing was found in the conductivity regardless of whether or not the conductivity data were logarithmically transformed.

Figure 4A shows a scatter diagram for a case where the soil hydraulic parameters from the predictive method were used and the estimates of the relative hydraulic conductivity were scaled using the method described by Luckner et al. (1989). This method uses one value

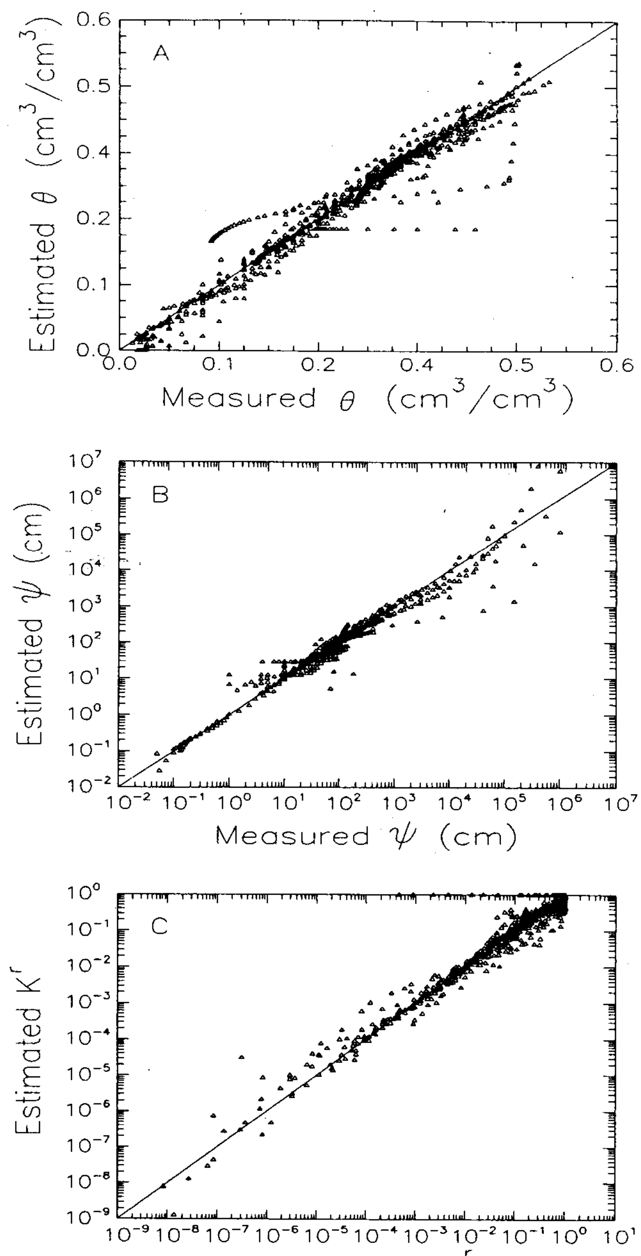

Fig. 2. Estimated vs. measured values for (A) soil water content (θ) and (B) soil water suction head (ψ); (C) predicted vs. measured values for the relative hydraulic conductivity (K_r) using the simultaneous method with five parameters. The solid lines are 1:1 reference lines.

of the hydraulic conductivity measured near but not at saturation as a matching point. Using this technique improved the correspondence between the measured and estimated values of the hydraulic conductivity, compared with the predictive (without matching point) method shown in Fig. 1C. The greatest improvement is near saturation, where there is a decrease in the variation around the 1:1 line. In the drier regions, the scaling technique does not seem to have much effect on the estimates. One advantage of using the predictive method with scaling is the reduction in bias. For the transformed and untransformed conductivities there

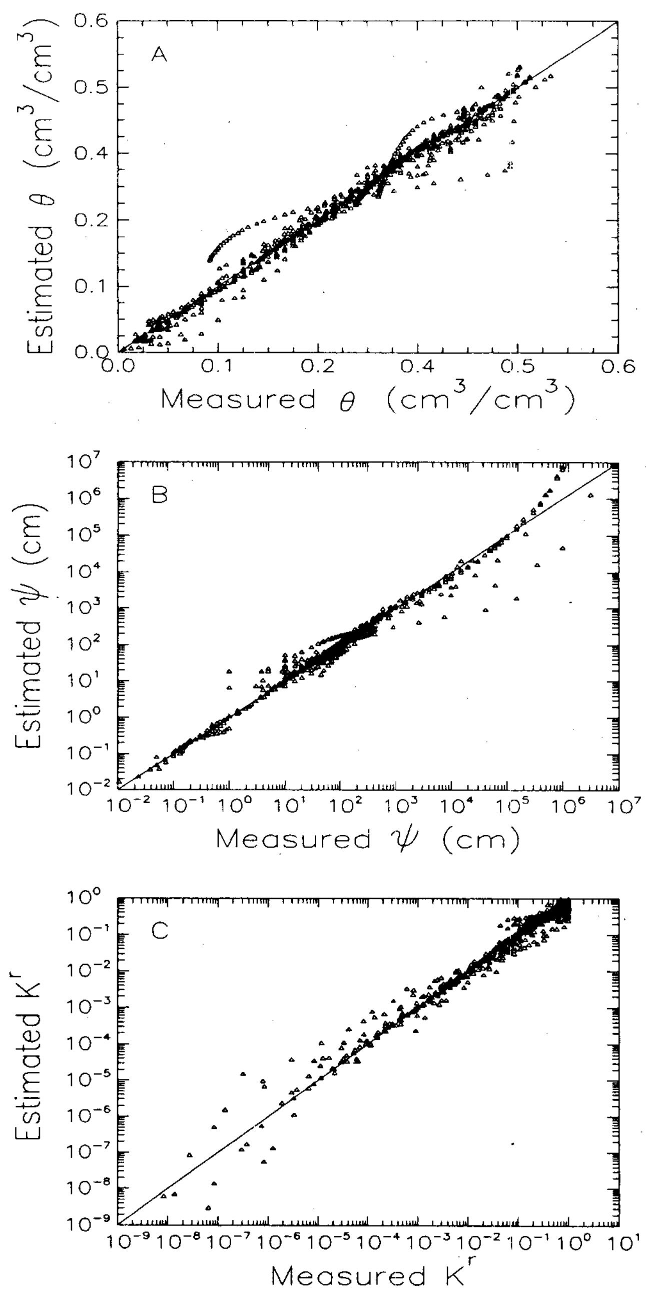

Fig. 3. Estimated vs. measured values for (A) soil water content (θ) and (B) soil water suction head (ψ); (C) predicted vs. measured values for the relative hydraulic conductivity (K_r) using the simultaneous method with six parameters. The solid lines are 1:1 reference lines.

is a 30 and 56% reduction in the bias, respectively, compared with the predictive method without scaling.

Figure 4B demonstrates the effect of using only Mualem's ℓ parameter (i.e., exponent in the tortuosity factor) to improve the characterization of the unsaturated hydraulic conductivity. For this example, the soil hydraulic parameters θ_r, θ_s, α, and n have the same values as determined from the predictive method (Fig. 1). For this data set, it appears that the correspondence between the estimated and measured values of the conductivity were somewhat improved, compared with the predictive method, especially in the moderately wet range (i.e., 10^{-4} to 10^{-3} range) but

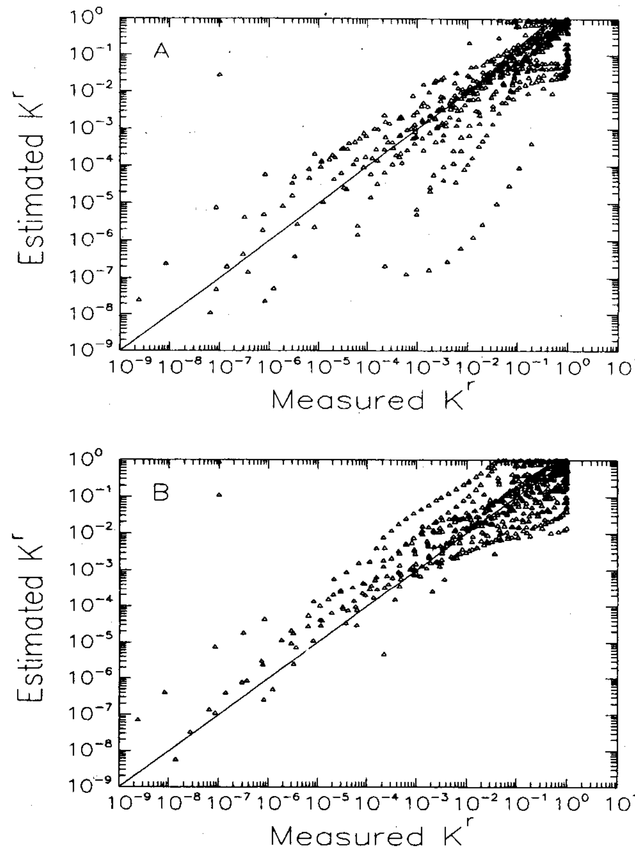

Fig. 4. Estimated vs. measured values for the relative conductivity (K_r) using (A) the predictive method with scaling and (B) predictive method with fitted empirical constant ℓ. The solid lines are 1:1 reference lines.

this method appears to be somewhat ineffective, compared with the simultaneous methods (i.e., compare with Fig. 2C and 3C). The insensitivity of this method near saturation was expected since a power function of the effective saturation will be approximately unity for all values of the exponent in this region. This is also evident from Tables 3 and 4 where the statistics summarizing Fig. 4B show some improvement for the logarithmically-transformed conductivity, compared with the untransformed conductivity. This improvement is due to the more equal weighting for all water-constant levels that occurs when the conductivity is logarithmically transformed.

CONCLUSIONS

The RETC program has been used to analyze 36 moisture-characteristic curves from 23 different soils. The nonlinear least-squares optimization method employed by RETC offers an efficient method for obtaining values for the soil hydraulic parameters that can be used for predicting or estimating the unsaturated hydraulic conductivity, depending on the available information. The predictive method provides soil hydraulic parameters that, on the average, most accurately describe the water-retention relationship, compared with the other methods described here. However, the estimates of the unsaturated hydraulic conductivity are, on average, the least accurately characterized and biased. Figure 1C indicates that the biasing is not large and, given that the biasing was determined under the assumption that the experimental values of the conductivity were error free, may be an artifact of the data set. Since the experimental data probably contain some measurement error, the biasing should not be considered an indication that the method is invalid. To do so, further study would be required and many more soils considered.

The simultaneous method with five and six parameters produces soil hydraulic parameters that most accurately describe both the water-retention and hydraulic-conductivity relationships. Using the mean sum of deviation, mean sum of squared deviation, and the coefficient of determination as criteria, the simultaneous method using six parameters was found to be the best method overall, but differences from using either five or six parameters with logarithmically transformed data are slight. However, using the simultaneous methods causes a decreasing correspondence between the measured and estimated water-retention relationship, compared with the predictive method.

The use of a matching point to improve the correspondence between measured and estimated conductivity has the advantage that only one value for the unsaturated hydraulic conductivity needs to be measured. The major disadvantage, for the soils considered here, is that the improvement between the measured and estimated values is not as great as with the simultaneous methods, especially in the drier region. If one such value for the unsaturated hydraulic conductivity is available, however, it is advantageous to use it for scaling purposes. For the soils used here, the scaling method improved the coefficient of determination by about a factor of 2 (as measured by the logarithmically-transformed conductivity, see Table 4).

It was found that the predictive method with fitted ℓ was somewhat ineffective in improving the correspondence between the measured and estimated conductivity, compared with the simultaneous methods, but there was some improvement when compared with the predictive method for the case where the conductivity was logarithmically-transformed. For the untransformed conductivity, there was little improvement in the correspondence, compared with the predictive method. This indicates that an independent means for determining ℓ may not prove valuable in enhancing the agreement between measured and estimated values. For the data used here, only about a 20% reduction in the mean sum of squared error and about a 70% increase in the r^2 value for the logarithmically-transformed conductivity will result, with no improvement for the untransformed conductivity. A 200% increase in r^2 will result if the simultaneous method with five parameters is used.

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