

# A New Approach to Estimate Soil Hydraulic Parameters Using Only Soil Water Retention Data

**Navin K. C. Twarakavi\***

Dep. of Environmental Sciences  
Univ. of California  
Riverside, CA 92521

**Hiroataka Saito**

Tokyo University of Agriculture and Technology  
Dep. of Ecoregion Science  
Fuchu, Tokyo  
Japan 183-8509

**Jirka Šimunek**

Dep. of Environmental Sciences  
Univ. of California  
Riverside, CA 92521

**M. Th. van Genuchten**

U.S. Salinity Laboratory  
450 W. Big Springs Rd.  
Riverside CA 92507

Traditional approaches for estimating soil hydraulic parameters (such as the RETC code) perform well when experimental data for both the retention curve and hydraulic conductivity function are available; however, unsaturated hydraulic conductivity data are often unavailable. The objective of this work was to develop an approach to estimate robust soil hydraulic parameters from water retention curve data alone. The proposed approach, called the Multiobjective Retention Curve Estimator (MORE), is based on the Multiobjective Shuffled Complex Evolution Metropolis (MOSCEM-UA) algorithm and estimates an optimal parameter set by simultaneously minimizing two objective functions each representing water content and relative unsaturated hydraulic conductivity residuals. To address the lack of observed unsaturated hydraulic conductivity data, MORE transforms both predicted and observed water contents into the hydraulic conductivity space using a pore-size distribution model (e.g., the Mualem model) and also optimizes the soil hydraulic parameters in this fictitious space. We applied MORE to two cases. In the first case, MORE was used to estimate soil parameters using only retention curve data for 12 random soils selected from the UNSODA database. While the soil hydraulic parameters estimated using RETC and MORE fit the retention curve similarly, the MORE approach consistently decreased the error in fitting unsaturated hydraulic conductivities by as much as 5% compared with RETC. The second case involved using the parameters fitted using the MORE and RETC approaches to model a field-scale experiment. Compared with RETC, the error in predicted water contents decreased by 25% using parameters predicted by MORE. The MORE approach was shown to fit robust soil hydraulic parameters; however, the approach is relatively slower and more time consuming than RETC.

Abbreviations: MORE, Multiobjective Retention Curve Estimator; MOSCEM-UA, Multiobjective Shuffled Complex Evolution Metropolis.

The variably saturated flow process in soils is a highly nonlinear and dynamic phenomenon. Commonly used numerical models for variably saturated water flow use the classical Richards equation (Richards, 1931). The Richards equation is highly nonlinear due to the dependence of unsaturated hydraulic conductivity and water content on the capillary pressure head. Consequently, modeling variably saturated water flow involves solving the Richards equation along with a nonlinear soil hydraulic model (Gardner, 1958; Brooks and Corey, 1964; van Genuchten, 1980; Leij et al., 1997) that characterizes the relationships between the water content, capillary pressure head, and unsaturated hydraulic conductivity. Of all available soil hydraulic models, the van Genuchten–Mualem model (van Genuchten, 1980) is perhaps the most widely used model in simulation of vadose zone flow processes and, there-

fore, used in this study for representing the complex relationships between the hydraulic conductivity, the water content, and the pressure head.

Due to the multidimensionality of the parameter space, a common dilemma during parameter estimation in hydrologic processes is that there are a number of parameter sets that can fit the data equally well. The ultimate goal during the soil hydraulic parameter estimation is to obtain parameter estimates that are the most representative of flow processes in soils. An application of the van Genuchten–Mualem model in vadose zone flow modeling requires estimates of the following soil hydraulic parameters: the so-called shape parameters ( $\alpha$  and  $n$ ), saturated hydraulic conductivity ( $K_s$ ), saturated water content ( $\theta_s$ ), and residual water content ( $\theta_r$ ). Of the required parameter set,  $K_s$  and  $\theta_s$  can be estimated experimentally. The remaining parameters ( $\alpha$ ,  $n$ , and  $\theta_r$ ) have to be estimated indirectly by fitting the van Genuchten–Mualem model to the experimental retention and unsaturated hydraulic conductivity data using an optimization approach, such as the RETC code (van Genuchten et al., 1991). It has been traditionally assumed that a good estimate of the necessary soil hydraulic parameters is achieved when the estimated parameter set can accurately represent both the retention curve and hydraulic conductivity–pressure head relationships as well as the transient flow processes.

The RETC code is a widely used computer program for estimating the soil hydraulic parameters that represent the retention curve and the unsaturated hydraulic conductivity–pressure head

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\*Corresponding author (navink@ucr.edu).

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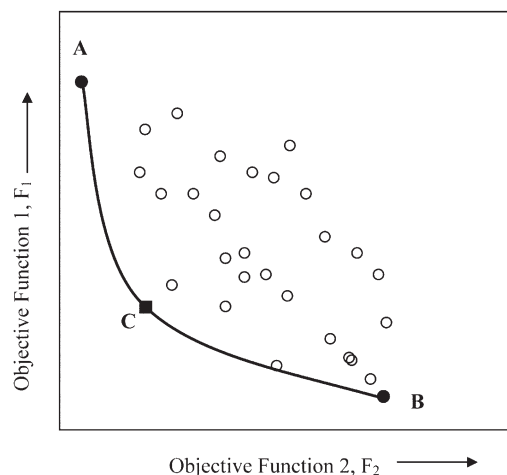
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relationships (van Genuchten et al., 1991). The RETC code uses a nonlinear least-squares optimization approach to estimate the unknown model parameters from observed retention, conductivity, or diffusivity data. The aim of this curve-fitting process is to find the set of parameters that best minimizes the sum of squared residuals, SSQ, between model predictions and data (van Genuchten et al., 1991). The SSQ reflects the degree of model bias (lack of fit) and the contribution of random errors. Note that the SSQ objective function is statistically synonymous with the RMSE. The RETC code minimizes the SSQ iteratively by means of a weighted least-squares approach based on Marquardt's maximum likelihood method (Marquardt, 1963).

Previous studies have shown that RETC can be efficiently used to fit the retention curve and the unsaturated hydraulic conductivity function when experimental data are available for both properties (e.g., van Genuchten et al., 1991; Yates et al., 1992). While experimental data for the retention curve can be collected relatively easily, accurate measurements of unsaturated hydraulic conductivities are generally difficult and time consuming (Schaap and van Genuchten, 2005). Soil physicists, however, often find themselves in the predicament where they must estimate the soil hydraulic parameters that adequately represent the entire gamut of pressure head–water content–hydraulic conductivity relationships using only the retention curve data. When only retention curve data are available, RETC sometimes fits the retention curve at the cost of poorer characterization of the unsaturated hydraulic conductivity. For example, the van Genuchten–Mualem model, when fitted only to the experimental retention curve data, often results in a good fit of the retention curve but does not necessarily ensure a good description of the hydraulic conductivity–pressure head relationship (see below for illustrations). This is mainly due to the varying sensitivities of the retention curve and the unsaturated hydraulic conductivity function to the parameter set.



**Fig. 1.** Schematic of the location of the Pareto optimal solution of a multiobjective problem in the objective space. Circles represent various nonoptimal parameter sets that do not provide the best solution. Points A and B represent parameter sets that provide the best solution for individual objectives  $F_1$  and  $F_2$ , respectively. The line connecting Points A and B is the nondominated "Pareto optimal" set of solutions. Point C corresponds to the Pareto solution that may be regarded as the "best" possible solution.

In the past, many improvements have been suggested to the RETC code (e.g., Hollenbeck et al., 2000; Abbaspour et al., 2001); however, these improvements do not address conditions where only the soil water retention data are available. Similar to the RETC approach, these improved methods often result in parameter sets that inadequately represent the unsaturated hydraulic conductivity–pressure head relationship.

Traditional methods, such as RETC, for estimating the soil hydraulic parameters are formulated as a single-objective optimization problem. The classical single-objective optimization approach is based on the central assumption that the chosen single-objective function can adequately and correctly represent all errors that may be incurred due to the parameter set used in the model (Vrugt et al., 2003). Gupta et al. (1999) have convincingly pointed out that this may not be true, and that the single-objective function can sometimes contribute structural errors during model calibration that may even exceed measurement errors.

In this study, we developed a multiobjective optimization approach, called MORE, for estimating the soil hydraulic parameters that is designed to overcome the aforementioned weaknesses of the single-objective optimization in RETC. Multiobjective optimization is not an alien concept for soil physicists and has been explored in many previous studies (e.g., Neuman, 1973; Vrugt and Dane, 2005; Schoups et al., 2005; Mertens et al., 2006). The basic idea behind multiobjective optimization methods is finding parameter sets that simultaneously minimize multiple objective functions. The solution to this problem, however, will generally no longer be a single "best" parameter set but will consist of a group of possible solutions due to tradeoffs among different objective functions (Vrugt et al., 2003). A key characteristic of this so-called "Pareto set of solutions" is that each parameter set within the Pareto set of solutions is better than the others for at least one objective function, but none is better than the others for all objective functions.

Figure 1 gives an illustration of this concept. The Pareto set of solutions would also include the solutions for the individual objectives. For example, while Point A represents parameters that provide the best solution for the objective  $F_1$ , Point B represents the optimal parameter set for the objective  $F_2$ . Many algorithms are available for estimating the "optimal" parameter sets through multiobjective optimization, such as MOCOM-UA (Yapo et al., 1998) and MOSCEM-UA (Vrugt et al., 2003). One may select a "best" possible solution (represented by Point C) from the Pareto set of solutions by minimizing the normalized Euclidean measures of distance of the Pareto set to the origin (Vrugt et al., 2003). It is possible to estimate the same "best" possible solution using a weighted single-objective function; however, the relative values of weights would dominate the final "best" possible solution. It has been convincingly argued that the "best" solution has the smallest normalized distance. Throughout this study, the point on the Pareto set with the minimal normalized Euclidean distance to the origin has been selected as the "best" possible solution.

## MATERIALS AND METHODS

### Proposed Approach

For a one-dimensional scenario, the Richards equation is described mathematically as follows:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ K(b) \frac{\partial b}{\partial z} - K(b) \right] - S \quad [1]$$

where  $\theta$  is the volumetric water content,  $b$  is the soil water pressure head (L),  $t$  is time (T),  $z$  is the distance from a reference datum (L),  $K(b)$  is the unsaturated hydraulic conductivity ( $L T^{-1}$ ) as a function of  $b$  or  $\theta$ , and  $S$  represents flow from sinks and sources.

The van Genuchten–Mualem model, which is used to represent the functions  $K(b)$  and  $\theta(b)$  in the flow models, is described as

$$\theta(b) = \begin{cases} \theta_r + \frac{\theta_s - \theta_r}{(1 + |\alpha b|^n)^m} & b < 0 \\ \theta_s & b \geq 0 \end{cases} \quad [2a]$$

$$S_e(b) = \frac{\theta(b) - \theta_r}{\theta_s - \theta_r} \quad [2b]$$

$$K(b) = K_s S_e^l \left[ 1 - (1 - S_e^{1/m})^m \right]^2 \quad [2c]$$

$$m = 1 - 1/n \quad n > 1 \quad [2d]$$

where  $\theta(b)$  is the volumetric water content at pressure head  $b$ ,  $\theta_s$  and  $\theta_r$  are the saturated and residual volumetric water contents, respectively;  $S_e(b)$  is the scaled water content at pressure head  $b$  (L),  $K_s$  is the saturated hydraulic conductivity ( $L T^{-1}$ ),  $\alpha$  ( $L^{-1}$ ) and  $n$  are van Genuchten's shape parameters, and  $l$  is a tortuosity or pore-connectivity parameter estimated by Mualem (1976) to be 0.5. Equations [1] and [2] have been used with or without additional modifications to model variably saturated water flow and have been successfully extended into two and three dimensions (e.g., Šimunek et al., 1999; Preuss et al., 2004).

The MORE approach utilizes two objective functions to obtain a simultaneous fit of the retention curve and the unsaturated hydraulic conductivity function. The first objective function reflects the lack of fit of observed water contents, while the second objective function assesses the lack of fit of observed unsaturated hydraulic conductivities. The goal of the MORE methodology is to find the parameter set such that both objective functions,  $O(\mathbf{b})$ , described in Eq. [3] are minimized:

$$O(\mathbf{b}) = \begin{cases} \text{RMSE}[\theta_i, \hat{\theta}_i(\mathbf{b})] \\ \text{RMSE} \left\{ \log[k_i(\theta_i, \mathbf{b})], \log[\hat{k}_i(\hat{\theta}_i, \mathbf{b})] \right\} \end{cases} \quad [3]$$

where  $\mathbf{b} [= \alpha, n, \theta_s, \text{ and } \theta_r]$  is the set of optimized soil hydraulic parameters,  $\theta_i$  are the observed water contents,  $\hat{\theta}_i(\mathbf{b})$  are the fitted water contents as a function of the parameter set  $\mathbf{b}$ ,  $\hat{k}_i(\hat{\theta}_i, \mathbf{b})$  are the fitted relative hydraulic conductivities as a function of the parameter set  $\mathbf{b}$  and fitted water contents  $\hat{\theta}_i(\mathbf{b})$ , and  $k_i(\theta_i, \mathbf{b})$  are the apparent observed relative hydraulic conductivities as a function of the parameter set  $\mathbf{b}$  and observed water contents  $\theta_i$ . In the absence of observed relative conductivities,  $k_i(\theta_i)$ , apparent observed relative hydraulic conductivities,  $k_i(\theta_i, \mathbf{b})$ , are estimated using the parameter set  $\mathbf{b}$  and observed water contents,  $\theta_i$ , from Eq. [2a–2d]. It is assumed that  $k_i(\theta_i, \mathbf{b})$  closely reflects the actual relative hydraulic conductivity,  $k_i(\theta_i)$ , that could have been estimated experimentally. Similarly, fitted relative hydraulic conductivities,  $\hat{k}_i(\hat{\theta}_i, \mathbf{b})$ , are estimated using fitted water contents,  $\hat{\theta}_i(\mathbf{b})$ , and the parameter set  $\mathbf{b}$ . The optimization based on Eq. [3] thus simultaneously minimizes water content residu-

als in both the water content and the relative unsaturated hydraulic conductivity objective function spaces. A pore-size distribution model (e.g., Mualem, 1976) is used to project both fitted and observed water contents into the hydraulic conductivity space. Similar to the RETC approach, the RMSE is used in MORE as the objective function. Note that the RMSE objective function for the relative unsaturated hydraulic conductivities considers log-transformed values as unsaturated hydraulic conductivities that vary across many orders of magnitude.

Several assumptions are made in the MORE approach. Note that the water content data are projected into both the retention curve and hydraulic conductivity objective spaces in MORE. The second major assumption is that pore-size distribution models, such as the Mualem model, accurately transform water contents into relative hydraulic conductivities. This assumption is especially crucial, as the accuracy of the second objective function is entirely dependent on the validity of the pore-size distribution model for the soil under consideration.

The MOSCEM-UA algorithm is used to solve the multiobjective optimization problem posed in MORE. The algorithm in the MORE approach is essentially the same as the MOSCEM-UA algorithm (for a detailed description of the approach, see Vrugt et al., 2003). The only additions in the MORE approach are in the multiobjective vector estimation stage described above. Figure 2 shows the flow chart for calculating the multiobjective vector used in the MORE approach for a given parameter set and experimental retention data when the van Genuchten–Mualem model is considered.

Only a brief explanation of the procedure used in the MOSCEM-UA algorithm is presented here. The MOSCEM-UA algorithm starts with an initial population of points from the feasible parameter space defined by the user. For each individual of the population, values of the multiple objective functions are computed and the population is ranked and sorted based on their fitness. The fitness of each individual

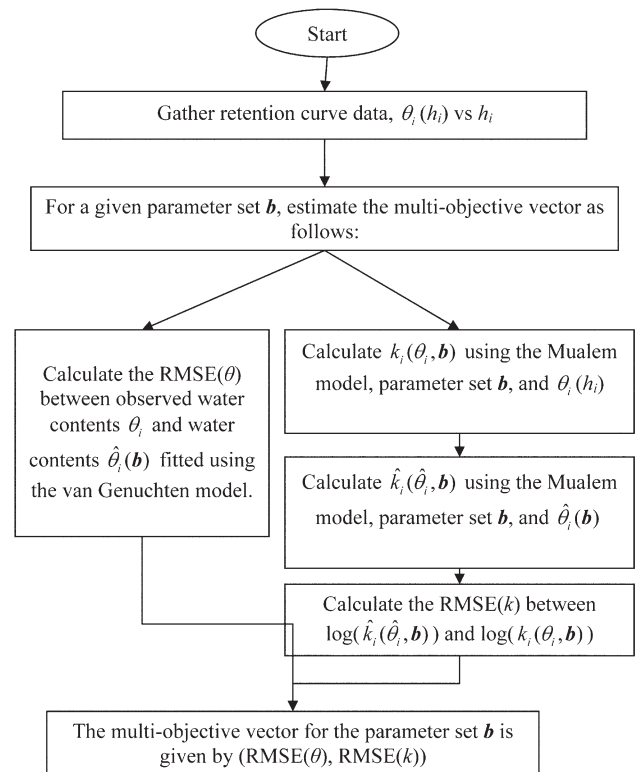


Fig. 2. A flowchart for calculating the multiobjective vector for a given parameter set in the Multiobjective Retention Curve Estimator (MORE) approach.

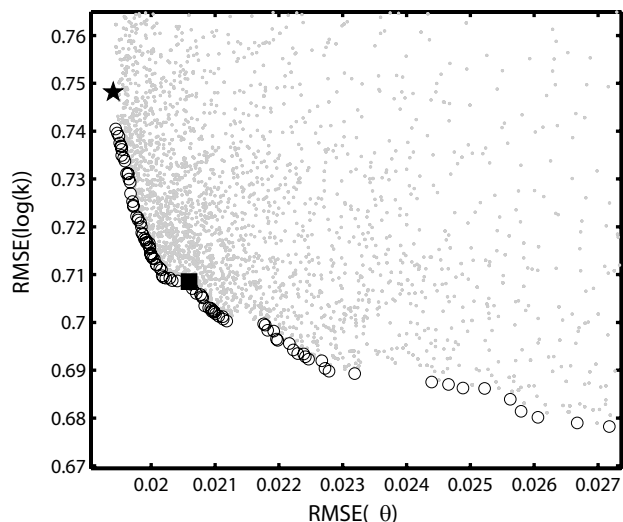


Fig. 3. Tradeoffs in the objective space of the Multiobjective Retention Curve Estimator (MORE) algorithm for the silt soil (UNSODA code no. 4670). Gray points represent different parameter sets considered by the MORE approach. Circles represent the final nondominated Pareto set after 10,000 function evaluations. The star symbol represents the parameter set estimated using RETC and the solid square symbol corresponds to the “best” possible parameter set estimated using the MORE approach;  $k$  is the relative hydraulic conductivity and  $\theta$  is the volumetric water content.

is based on how much the multiple objectives are minimized. The population (100 individuals were used in this study) is then partitioned into complexes (five in this study) and in each complex, parallel sequences of individuals are launched and new candidates are derived from the structure of the sequences and associated complexes. A Metropolis–Hastings algorithm is used to decide if the candidate points are acceptable and in case of acceptance, the worst member of the current complex is replaced. The procedure is continued until a prescribed number of iterations is reached (here 10,000), after which they are combined and new complexes are formed through the process of shuffling. This process converges to the Pareto set. From the estimated Pareto set, the nondominated Pareto set is selected. A Pareto set of parameters is said to be nondominated if no parameter

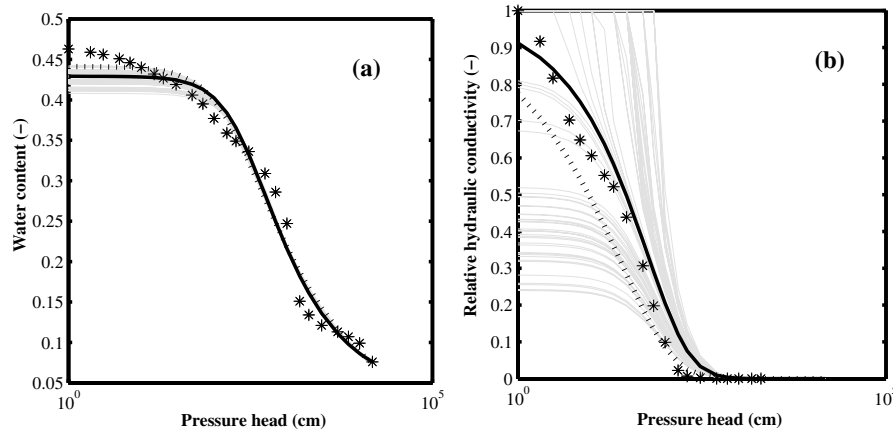


Fig. 4. Fitted (a) water content–pressure head and (b) relative unsaturated hydraulic conductivity–pressure head relationships obtained using parameter estimates from the Multiobjective Retention Curve Estimator (MORE) (solid line) for the silt soil (UNSODA code no. 4670). The points represent the experimental data. The dotted line is the solution based on RETC. Gray lines represent the several parameter sets corresponding to the nondominated Pareto set. Only retention data were used in parameter optimization by both RETC and MORE.

set exists that has the lowest values of all objective functions. The nondominated Pareto set is illustrated by a thick line in Fig. 1. From the nondominated Pareto set, the parameter set superior to other possible solutions is chosen as the “best” possible parameter set (represented by Point C in Fig. 1). The MORE approach was implemented in the MATLAB environment (The MathWorks, 1999) and was primarily based on the MOSCEM-UA algorithm (Vrugt et al., 2003). Figures 3 and 4 are practical examples of Fig. 1 and further illustrate the parameter sets obtained by the MOSCEM-UA algorithm.

The performance of MORE was evaluated using two case studies of varying complexity. The first case study compared the performance of RETC and MORE in estimating parameters for a variety of soils of different textures and structures randomly selected from the UNSODA database. The second case study involved estimating the soil hydraulic parameter set from experimental retention curve data for the Las Cruces one-dimensional variably saturated flow experiment (Wierenga et al., 1991). While the first case study involved laboratory measurements of core samples with smaller heterogeneity and fewer experimental data, the second case study involved a field-scale experiment with larger heterogeneity and more experimental data. HYDRUS-1D (Šimunek et al., 2005) was used to model the one-dimensional variably saturated water flow with parameters estimated from RETC and MORE in the second case study. To compare the observed data with those predicted using the MORE and RETC approaches, we used the RMSE statistic. The RMSE is a commonly used error statistic that is the square root of the mean of the squared residuals.

### Case 1: Selected Soils from the UNSODA Database

In comparing the performance of the MORE and RETC approaches for estimating parameters from soil water retention experimental data, we randomly chose 12 soils of different textures and structures from the UNSODA database (Leij et al., 1996; Nemes et al., 2001). These selected soils were chosen such that retention curve and unsaturated hydraulic conductivity data are available. Among these soils in the UNSODA database, many have similar retention curve and unsaturated hydraulic conductivity data. Most of these soils with similar retention curves and unsaturated hydraulic conductivity data shared the same sampling location. Care was taken to avoid such repetitions. Also, soils with obvious sampling and experimental errors were ignored. The selected soils, covering a wide range of textures and structures, are listed in Table 1. Although the MORE and RETC approaches were compared for their performance for all 12 selected soils, only one of these randomly selected soils is used here to illustrate in more detail the MORE approach.

Even though the selected soils had experimental data for both soil water retention and unsaturated hydraulic conductivity, only the retention curve data were used to estimate the soil hydraulic parameters. The estimated parameter set was then used to see how well the MORE and RETC approaches were able to characterize the unsaturated hydraulic conductivity by comparing the experimental unsaturated hydraulic conductivity data with predicted values. In other words, the experimental unsaturated hydraulic conductivities

were used only to evaluate the robustness of the “best” parameter sets estimated using MORE and RETC.

## Case 2: Las Cruces Trench Experiment

The second case study involved modeling of the one-dimensional infiltration for the Las Cruces trench site experiment (Wierenga et al., 1989, 1991). The Las Cruces trench site experiment was a comprehensive field study conducted in southern New Mexico. The primary purpose of the study was to develop a data set for validating and testing numerical models. For this purpose, the study site was heavily instrumented with tensiometers, neutron probes, and solute samplers for collecting water contents, pressure heads, and solute concentrations. More than 500 soil samples (undisturbed and disturbed) were taken at the experimental site and analyzed in the laboratory for bulk density and to find the saturated hydraulic conductivity and soil water retention curve. The experimental infiltration study involved application of water to a 4-m-wide area using closely spaced drips with an average surface flux of 1.82 cm d<sup>-1</sup> for the 86 d of the experiment. During the experiment, no surface ponding was observed. To reduce the disruption of the experimental conditions by rain and evaporation, the irrigated area and the surroundings were covered by a pond liner. To evaluate the data set, Wierenga et al. (1991) developed a simple one-dimensional numerical model assuming uniform soil conditions. Similar to HYDRUS-1D, the model was based on the Richards equation (Eq. [1]) for one-dimensional variably saturated water flow. For modeling purposes, Wierenga et al. (1991) assumed the equivalent saturated hydraulic conductivity ( $K_s$ ) as a geometric mean of laboratory-measured values from all soil samples. The retention curve parameters were estimated from the laboratory data using an approach similar to RETC (Wierenga et al., 1991). Water contents were observed along the depth on Days 19 and 35 after the experiment was started.

Similar to the work done by Wierenga et al. (1991), the one-dimensional simulation of the infiltration in the Las Cruces experiment was performed with the MORE-estimated soil hydraulic parameters. Initial pressure heads ( $h_1 = -100$  cm) in the soil profile were the same as those used in Wierenga et al. (1991). While a constant water flux was used as the upper boundary condition ( $q_0 = 1.82$  cm d<sup>-1</sup>), free drainage was assumed at the lower boundary. Also, similar boundary conditions and equivalent saturated hydraulic conductivity ( $K_s = 270.1$  cm d<sup>-1</sup>) were used. The retention curve parameters were estimated using again the RETC and MORE approaches. Except for the retention curve parameters, all remaining parameters and initial and boundary conditions were kept the same. This allowed us to compare the effectiveness of the RETC and MORE approaches in estimating parameter sets for variably saturated flow models.

## RESULTS AND DISCUSSION

### Case 1: Selected Soils from the UNSODA Database

One selected soil (undisturbed core sample of silt collected from Hannover, Germany; UNSODA code no. 4670) was initially used to analyze and demonstrate the MORE approach. For the selected soil, the RETC code was used to estimate the

soil hydraulic parameters from only the retention data. The optimized retention parameters were as follows:  $\theta_s = 0.441$ ,  $\theta_r = 0.000$ ,  $\alpha = 0.005$  cm<sup>-1</sup>, and  $n = 1.41$ .

The MORE approach was then used to obtain the soil hydraulic parameters using multiobjective optimization. Figure 3 shows the evolution of the “best” parameter set in the objective space using the MORE approach. Figure 3 is similar to Fig. 1, which illustrates the concept of the Pareto optimality. Figure 3 also shows the location of the RETC solution and the “best” possible solution obtained by MORE in the objective space. From the nondominated Pareto set of solutions, the “best” possible parameter set (illustrated by Point C in Fig. 1) was chosen as follows:  $\theta_s = 0.429$ ,  $\theta_r = 0.030$ ,  $\alpha = 0.004$  cm<sup>-1</sup>, and  $n = 1.56$ .

The estimated parameter sets obtained by RETC and MORE were then used to predict the retention curves and hydraulic conductivity–pressure head functions using Eq. [2]. Figure 4 compares observed water contents and relative hydraulic conductivities with the corresponding soil hydraulic functions obtained from MORE and RETC. It is clear that RETC fits water contents much better than it predicts relative hydraulic conductivities. Relative unsaturated hydraulic conductivities are clearly underestimated when parameters estimated only from the retention curve are used. An underprediction of relative hydraulic conductivities would translate into a prediction of flow rates slower than in reality during model simulations. On the other hand, the MORE approach shows a significantly improved correspondence between measured and predicted relative unsaturated hydraulic conductivities (Fig. 4b), despite the fact that measured hydraulic conductivities were not used in the optimization process. Although the MORE approach predicts the hydraulic conductivity function significantly better than the RETC approach, the retention curves fitted by the two approaches differ only slightly (Fig. 4a). Figures 5a and 5b show contour plots of the RMSE between the observed and estimated water contents and relative hydraulic conductivities, respectively, for different combinations of the  $\alpha$  and  $n$  parameters. Figure 5 also shows the location of the RETC and MORE solutions. One can immediately observe the dissimilarity of the two error surfaces. For example, the hydraulic

**Table 1. Summary of 12 soils selected from the UNSODA database for the first case study. Note that the silt soil (no. 4670, in italics) was used for a thorough analysis of the Multiobjective Retention Curve Estimator (MORE) approach.**

UNSODA no.	Texture	Structure	Experimental data points	
			Soil water retention	Unsaturated hydraulic conductivity
			no.	
4672	silt loam	fine to moderate polyhedral	25	25
2242	sandy loam	granular	11	12
1400	clay	angular	28	10
4011	loamy sand	granular	24	11
1382	sandy clay loam	angular	46	10
4661	sand	single grain	25	25
4670	<i>silt</i>	<i>blocky</i>	25	25
1490	silt loam	blocky	39	10
1361	silty clay	crumb angular	45	10
1371	silty clay loam	angular	48	10
1270	–	slightly welded	5	8
2740	clay loam	angular	6	13

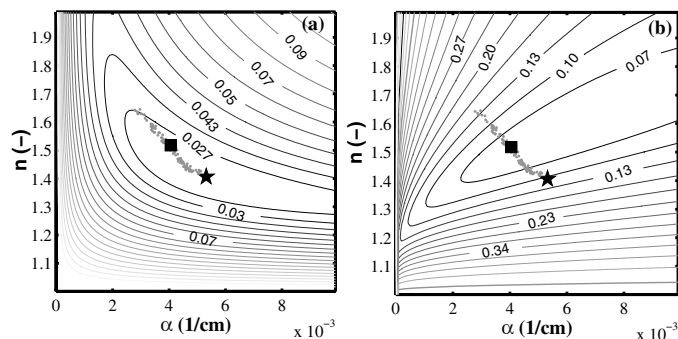


Fig. 5. Contour plots of the RMSE between the observed and fitted (a) water contents and (b) log of relative hydraulic conductivities as a function of shape parameters  $\alpha$  ( $\text{cm}^{-1}$ ) and  $n$  for the silt soil (UNSODA code no. 4670). The star symbol represents the parameter set estimated using RETC and the solid square symbol corresponds to the “best” possible parameter set estimated using the Multiobjective Retention Curve Estimator (MORE) approach. Gray points are the final nondominated Pareto set estimated by the MORE approach. Only retention data were used in parameter optimization by both RETC and MORE.

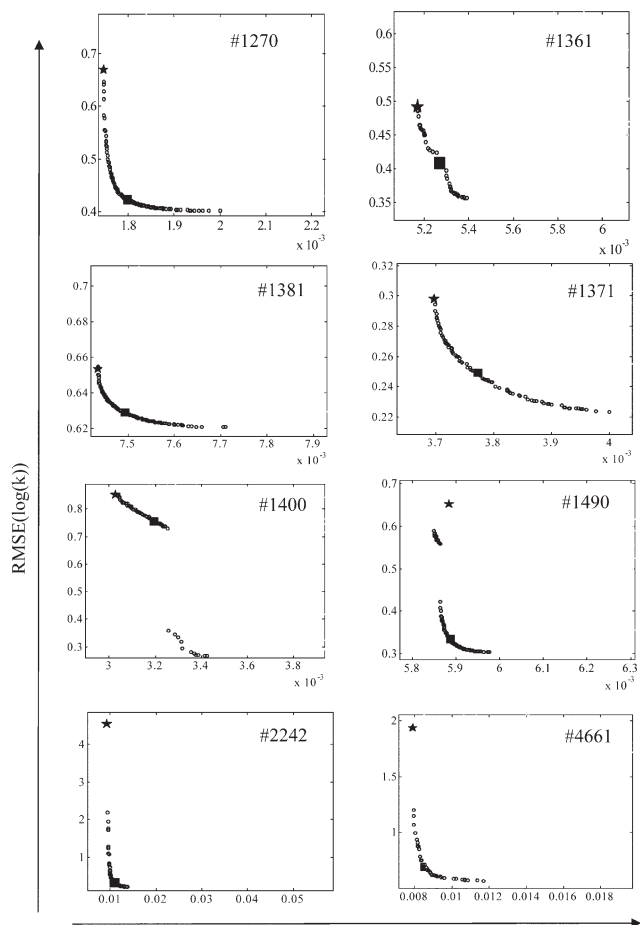


Fig. 6. Tradeoffs in the objective space of the Multiobjective Retention Curve Estimator (MORE) algorithm for selected soils. Gray points represent different parameter sets considered by the MORE approach. Circles represent the final nondominated Pareto set after 10,000 function evaluations. The star symbol represents the parameter set estimated using RETC and the solid square symbol corresponds to the “best” possible parameter set estimated using the MORE approach;  $k$  is the relative hydraulic conductivity and  $\theta$  is the volumetric water content.

conductivity is relatively more sensitive to the  $n$  parameter than to the  $\alpha$  parameter. Figure 5 further illustrates that retention and hydraulic conductivity functions have different minima. While the estimated RETC parameter set is located well inside the global minimum for water contents, it is not necessarily in the region of the global minimum for relative hydraulic conductivities. Similar observations have been reported in previous studies (e.g., Yates et al., 1992). Yates et al. (1992) analyzed the RETC code for a range of soils from the UNSODA database and noted that estimates of the unsaturated hydraulic conductivity were, on average, less accurate. Because of the often poor characterization of the unsaturated hydraulic conductivity, one may expect that RETC may lead to parameter estimates that are less representative of the flow characteristics of the medium. Compared with the RETC solution, the MORE solution is better placed in the region of global minima for both the water content and relative hydraulic conductivity. We emphasize here again that no measured hydraulic conductivity data were used in optimizing the soil hydraulic parameters and that these measured data were used only to evaluate the solutions obtained by the two methods.

It should be noted that the MOSCEM-UA algorithm on which the MORE approach is based has a set of user-input values. These include the number of complexes, the number of function evaluations, and the size of the population. In our analysis of the various soils selected from the UNSODA database, approximately 10,000 function evaluations were sufficient to attain a robust Pareto set of solutions. The sensitivity of the MORE code to the number of complexes and population size was analyzed and is reported in Table 2. Similar to the observation made by Vrugt et al. (2003), the number of Pareto points generated by the MORE approach is relatively insensitive to the population size and the number of complexes. The “best” possible solution was also relatively insensitive to the population size and number of complexes. Similar observations were made during the sensitivity analysis of the remaining selected soils from the UNSODA database.

The MORE approach seemed to consistently provide better results than the RETC code for a variety of soils. Figure 6 shows the tradeoff in the objective space of the MORE approach for several selected soils. One may note that the Pareto set is relatively uniformly distributed. Any gaps that may be observed in the Pareto set distribution (Soil no. 1490, for example) are due to poor representation of the data by the model. Table 3 lists the “best” parameter sets estimated by the MORE and RETC approaches, while Table 4 lists the RMSE estimates between fitted and observed water contents and predicted and observed unsaturated hydraulic

Table 2. The total number of nondominated PARETO points after 10,000 function evaluations with the Multiobjective Retention Curve Estimator (MORE) approach for the silt soil (UNSODA no. 4670) as a function of population size 10, 20, 50, or 100 and the number of complexes.

Complexes	Nondominated Pareto points			
	10	20	50	100
	no.			
1	84	148	114	83
2		153	110	88
5			108	98
10				100

conductivities. Even though unsaturated hydraulic conductivity data were not used in either the RETC or the MORE approaches, the parameter sets generated by MORE showed an improved characterization of the hydraulic conductivity–pressure head relationship. The RMSE for fitted retention curves was almost identical for both approaches, while the RMSE for the predicted hydraulic conductivity function was often much lower for the MORE approach than for the RETC approach. Only in one case did the RETC approach provide a lower RMSE than the MORE approach.

### Case 2: Las Cruces Trench Experiment

The RETC and MORE algorithms were used to estimate the retention curve parameters by fitting the retention curve data for the Las Cruces Trench experiment. Figure 7 shows the tradeoffs between different possible parameter sets in the objective space when fitting the retention curve and the unsaturated hydraulic conductivity function. The RETC solution and the “best” possible solution from MORE are also compared in the objective space. Application of the RETC code to the retention curve data for the undisturbed and disturbed soils (>500 soil samples) resulted in the following retention curve parameter values:  $\theta_s = 0.321$ ,  $\theta_r = 0.083$ ,  $\alpha = 0.055 \text{ cm}^{-1}$ , and  $n = 1.51$ . Note that the estimated values from the RETC code are the same as those used by Wierenga et al. (1991). The MORE algorithm led to the following “best” parameter set:  $\theta_s = 0.323$ ,  $\theta_r = 0.084$ ,  $\alpha = 0.038 \text{ cm}^{-1}$ , and  $n = 1.65$ . The MORE solution is considerably different from the RETC solution in terms of the estimated parameter values. Of particular interest is the value of  $n$ , which has a significant influence on the shape of the unsaturated hydraulic conductivity. It should be noted that in Fig. 7, while  $\text{RMSE}(\theta)$  compares the observed and predicted water contents,  $\text{RMSE}(k)$  compares the apparent observed and predicted relative hydraulic conductivities (which were calculated from the optimized parameter set and observed and predicted water contents). Vrugt et al. (2003) suggested that it is desirable to have a smooth nondominated Pareto set, which is clearly the case in Fig. 7. The estimated retention curve parameters obtained with the RETC and MORE algorithms were then used to predict water content profiles at two different times for which observation data were available. The modeling was done using HYDRUS-1D (Šimunek et al., 2005). Figure 8 compares predicted water content profiles calculated with parameters obtained using the RETC and MORE approaches against observed water contents for Days 19 and 35. The parameter set estimated using MORE provides a better estimate of water contents than the parameter set obtained by

**Table 3. The final parameter sets (residual and saturated volumetric water contents,  $\theta_r$  and  $\theta_s$ , respectively, and shape parameters  $\alpha$  and  $n$ ) estimated by the RETC and Multiobjective Retention Curve Estimator (MORE) approaches for the randomly selected soils from the UNSODA database.**

UNSODA soil no.	RETC				MORE			
	$\theta_r$	$\theta_s$	$\alpha$	$n$	$\theta_r$	$\theta_s$	$\alpha$	$n$
			$\text{cm}^{-1}$				$\text{cm}^{-1}$	
4672	0.000	0.391	0.007	1.15	0.000	0.392	0.007	1.16
2242	0.161	0.548	0.024	4.75	0.140	0.551	0.024	4.09
1400	0.000	0.449	0.004	1.09	0.000	0.448	0.003	1.09
4011	0.057	0.415	0.021	1.70	0.052	0.415	0.022	1.66
1382	0.000	0.344	0.017	1.11	0.000	0.345	0.015	1.12
4661	0.037	0.408	0.102	1.82	0.036	0.408	0.101	1.81
4670	0.000	0.441	0.005	1.41	0.030	0.429	0.004	1.56
1490	0.000	0.399	0.008	1.19	0.007	0.400	0.008	1.20
1361	0.165	0.433	0.004	1.26	0.192	0.430	0.004	1.32
1371	0.208	0.407	0.003	1.38	0.219	0.405	0.002	1.44
1270	0.066	0.169	0.002	1.67	0.064	0.169	0.002	1.63
2740	0.000	0.710	0.107	1.17	0.000	0.707	0.099	1.17

RETC. In other words, it may be concluded that the parameter set estimated using MORE is more representative of the flow processes than the one estimated using RETC. One may also observe that the errors in predicted water contents are higher for Day 19 than for Day 35. It is interesting to see an improved prediction of the wetting front with the MORE parameters. A simple error analysis of the predicted water contents was performed for Days 19 and 35 (Table 5). The error statistics indicate a considerable improvement in predicted water contents using the parameter set from MORE. The errors in predicted water contents were reduced by 25% using the MORE approach. The cumulative distribution functions of the errors in predicted water contents for Days 19 and 35 are plotted in Fig. 9. Also, the maximum error in predictions was reduced for both days from 0.13 to 0.08 by using the soil hydraulic parameters from MORE. The cumulative distribution function for MORE is initially steeper than the RETC, indicating prevalence of smaller deviations between observed and calculated water contents for the latter.

**Table 4. Root mean squared errors between observed water contents or unsaturated hydraulic conductivities and corresponding fitted values calculated using the parameter sets estimated by the RETC and Multiobjective Retention Curve Estimator (MORE) approaches.**

UNSODA no.	RMSE			
	RETC		MORE	
	Water content	Unsaturated hydraulic conductivity	Water content	Unsaturated hydraulic conductivity
4672	0.004	3.100	0.004	2.970
2242	0.011	0.536	0.011	0.359
1400	0.003	0.852	0.003	0.816
4011	0.010	0.902	0.010	0.832
1382	0.007	1.297	0.008	1.218
4661	0.008	1.661	0.008	1.652
4670	0.019	0.809	0.021	0.764
1490	0.006	0.815	0.006	0.825
1361	0.005	0.493	0.005	0.409
1371	0.004	0.298	0.004	0.250
1270	0.002	0.717	0.002	0.679
2740	0.031	3.789	0.011	3.590

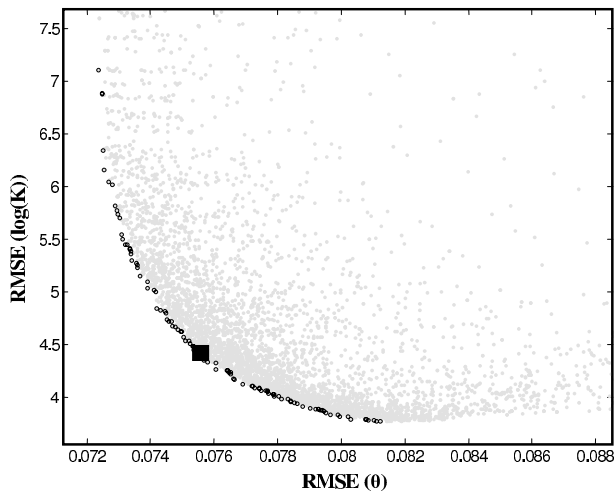


Fig. 7. Evolution of the tradeoff curve in the objective space of the Multiobjective Retention Curve Estimator (MORE) algorithm for the Las Cruces trench experiment. Gray points represent different parameter sets considered by the MORE approach. Circles represent the final nondominated Pareto set after 10,000 function evaluations. The solid square symbol corresponds to the “best” possible parameter set estimated using the MORE approach;  $k$  is the relative hydraulic conductivity and  $\theta$  is the volumetric water content. The solution set estimated by RETC is less optimal than the MORE solution and is beyond the limits of the plot.

## CONCLUSIONS

We have presented a new approach, called MORE, for estimating soil hydraulic parameters when only retention data are available. This approach provides the optimal parameter set by simultaneously and independently minimizing two objective functions that represent water content and relative hydraulic conductivity residuals. When observed hydraulic conductivities are not available, the MORE approach transforms both predicted and observed water contents into the hydraulic conductivity space using Mualem’s pore-size distribution model and also optimizes the soil hydraulic parameters in this fictitious space. By doing so, it accounts for the effect the fitted retention function exerts on predicted unsaturated hydraulic conductivities.

We have demonstrated the applicability of the MORE algorithm using two case studies, both of which showed an improve-

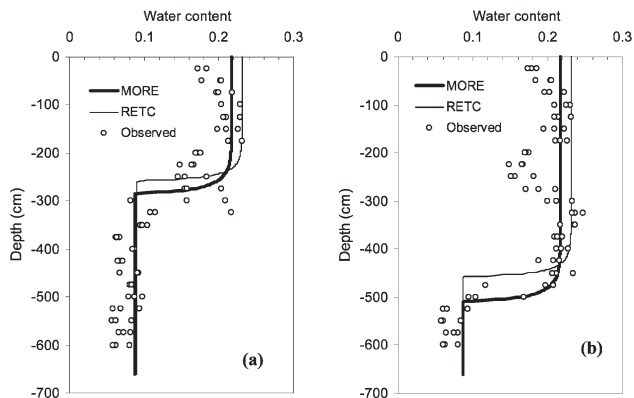


Fig. 8. Water content measured and predicted using HYDRUS-1D with the soil hydraulic parameters optimized by the RETC and Multiobjective Retention Curve Estimator (MORE) approaches for (a) Day 19 and (b) Day 35 for the Las Cruces trench experiment.

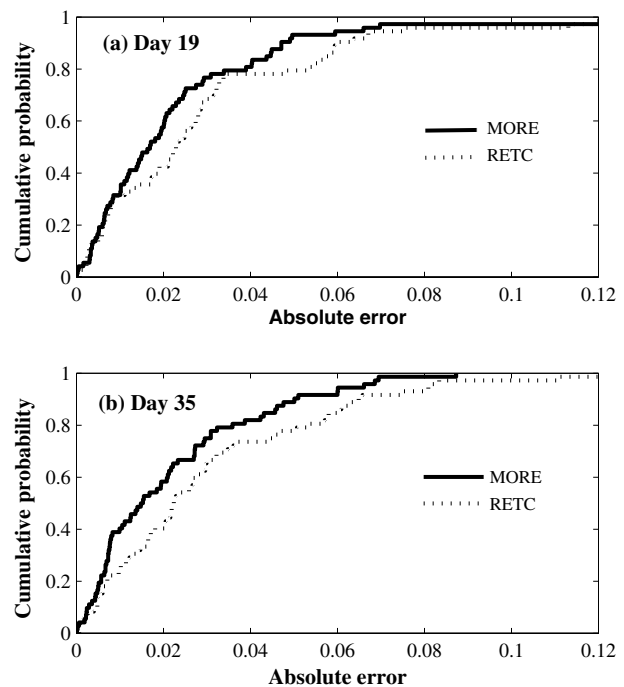


Fig. 9. Cumulative distribution functions for absolute errors in predicted water contents for (a) Day 19 and (b) Day 35 for the Las Cruces trench experiment.

ment in descriptions of unsaturated hydraulic conductivities and soil water flow characterization. The MORE approach is a promising approach for improving the estimation of soil hydraulic parameters, despite some minor drawbacks. For example, MORE tends to be slower than RETC due to the higher computational demand.

The performance of both approaches was also compared for the van Genuchten–Burdine model and for conditions of different data availability. It was found that when both retention and hydraulic conductivity data are available, the performance of RETC and MORE is similar. In scenarios where only retention data are available (which is the most common case in modeling studies), the MORE approach estimates the soil hydraulic parameters better than RETC since, in addition to retention data, it also considers their transformation into the hydraulic conductivity space.

During the development of MORE, a number of philosophical questions were encountered that may be of interest for future research. One of the key issues was the uniqueness of the soil hydraulic parameters and its dependence on the type of modeling problem. In modeling scenarios involving multiple components, such as movement of water, solute, and heat, it would be interesting to analyze whether multiple objectives representing different components need to be considered during the parameter estimation. For example, in a coupled water

Table 5. Summary statistics (RMSE and mean absolute error, MAE) of errors in water contents predicted by the RETC and Multiobjective Retention Curve Estimator (MORE) approaches at different times for the Las Cruces trench experiment.

Parameter	RMSE		MAE	
	RETC	MORE	RETC	MORE
Water content, Day 19	0.040	0.033	0.030	0.026
Water content, Day 35	0.039	0.030	0.029	0.022



and heat transport modeling (such as Saito et al., 2006), the third objective representing the thermal conductivity may need to be included in MORE. The MORE approach has been initially written in the MATLAB environment (The MathWorks, 1999) and will be integrated into the RETC code in the near future. Interested readers may contact the authors for using the MORE code.

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