

Improved Prediction of Unsaturated Hydraulic Conductivity with the Mualem-van Genuchten Model

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ABSTRACT

In many vadose zone hydrological studies, it is imperative that the soil's unsaturated hydraulic conductivity is known. Frequently, the Mualem-van Genuchten model (MVG) is used for this purpose because it allows prediction of unsaturated hydraulic conductivity from water retention parameters. For this and similar equations, it is often assumed that a measured saturated hydraulic conductivity (K_s) can be used as a matching point (K_o) while a factor S_e^L is used to account for pore connectivity and tortuosity (where S_e is the relative saturation and $L = 0.5$). We used a data set of 235 soil samples with retention and unsaturated hydraulic conductivity data to test and improve predictions with the MVG equation. The standard practice of using $K_o = K_s$ and $L = 0.5$ resulted in a root mean square error for $\log(K)$ (RMSE_K) of 1.31. Optimization of the matching point (K_o) and L to the hydraulic conductivity data yielded a RMSE_K of 0.41. The fitted K_o were, on average, about one order of magnitude smaller than measured K_s . Furthermore, L was predominantly negative, casting doubt that the MVG can be interpreted in a physical way. Spearman rank correlations showed that both K_o and L were related to van Genuchten water retention parameters and neural network analyses confirmed that K_o and L could indeed be predicted in this way. The corresponding RMSE_K was 0.84, which was half an order of magnitude better than the traditional MVG model. Bulk density and textural parameters were poor predictors while addition of K_s improved the RMSE_K only marginally. Bootstrap analysis showed that the uncertainty in predicted unsaturated hydraulic conductivity was about one order of magnitude near saturation and larger at lower water contents.

MANY STUDIES of water flow, transport of radionuclides, and chemical contaminants in soils rely on simulation models because the spatio-temporal scale of the problems often prohibits accurate and representative measurements. Although numerical models have become more and more sophisticated, their success and reliability are critically dependent on accurate information of hydrological system parameters. In this context, quantification of soil hydraulic properties is vitally important to model hydrological processes. However, in many cases measurements of soil hydraulic properties are difficult, in particular the unsaturated hydraulic conductivity.

As an alternative to measurements, one can use estimation methods that utilize physical or empirical relations between hydraulic properties and other soil variables. The advantage of such methods, also called pedotransfer functions, is that the input variables can be measured more easily—and, hence, are more widely available—than hydraulic properties. For the prediction of water retention and saturated hydraulic conductivity, this approach has led to a number of pedotransfer functions that use soil texture, bulk density, or other soil

variables as input (e.g., Rawls and Brakensiek, 1985; Ahuja et al., 1989; Vereecken et al., 1989; Schaap et al., 1998). Far fewer alternatives exist for unsaturated hydraulic conductivity. Although some pedotransfer functions are available (Saxton et al., 1986; Schuh and Bauder, 1986; Vereecken et al., 1990), pore-size distribution models by Burdine (1953) and Mualem (1976), among others, are more popular.

Generally speaking, the Burdine and Mualem models infer the pore-size distribution of a soil from its water retention characteristic. By making assumptions about continuity and connectivity of pores, integral expressions can be derived that describe unsaturated conductivity in terms of water content or pressure head. A general expression can be given as (after Hoffmann-Riem et al., 1999):

$$K(S_e) = K_o S_e^L \left(\int_0^{S_e} h^{-\beta} dS_e \int_0^1 h^{-\beta} dS_e \right)^{\gamma} \quad [1]$$

where K is the unsaturated hydraulic conductivity (cm day^{-1}), S_e is the relative saturation, h is the pressure head (cm), K_o is a hydraulic conductivity (cm day^{-1}) acting as a matching point, and L is a lumped parameter that accounts for pore tortuosity and pore connectivity. In this paper, we will consider the Mualem (1976) model in which $\gamma = 1$ and $\gamma = 2$.

van Genuchten (1980) defined the following water retention:

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

where θ is the volumetric water content ($\text{cm}^3 \text{cm}^{-3}$). The parameters θ_r and θ_s are residual and saturated water contents respectively ($\text{cm}^3 \text{cm}^{-3}$), α (>0 , in cm^{-1}) is related to the inverse of the air entry pressure, and n (>1) is a measure of the pore-size distribution (cf., van Genuchten, 1980; van Genuchten and Nielsen, 1985). Combination of Eq. [1] and [2] and for the Mualem parameters yields the following closed-form expression for $K(S_e)$:

$$K(S_e) = K_o S_e^L \{1 - [1 - S_e^{n(n-1)}]^{1-1/n}\}^2 \quad [3]$$

Equation [3] is frequently used to estimate unsaturated hydraulic conductivity using Eq. [2] (e.g., Powers et al., 1998; Vanderborght et al., 1998; Jones and Or, 1999; Wildenschild and Jensen, 1999), which requires that K_o and L must also be specified. Commonly, the saturated hydraulic conductivity, K_s , is used for K_o since it can be measured in a simple experiment. However, van Genuchten and Nielsen (1985) and Luckner et al. (1989) argued that K_s may not be an especially suitable

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matching point because K_s is sensitive to macropore flow, whereas unsaturated flow occurs in the soil matrix. They postulated that a matching point at slightly unsaturated conditions would yield better results. The term S_e^L in Eq. [3] is an empirical correction factor that was introduced by Burdine (1953) and Fatt and Dykstra (1951) to account for pore tortuosity (see Hoffmann-Riem, 1999 for a review). Mualem (1976) noted that L may be positive or negative. However, if S_e^L is to be interpreted in terms of pore continuity and tortuosity, S_e^L should always be smaller than 1 and hence $L > 0$ since $0 \leq S_e \leq 1$. Mualem (1976) found that $L = 0.5$ was an optimal value for a data set of 45 disturbed and undisturbed samples. For a subset of Mualem's data, Yates et al. (1992) found that L varied between -3.31 and values much greater than 100. For a data set of 75 samples, Schuh and Cline (1990) reported that L varied between -8.73 and 14.80 with increased variability for smaller mean particle diameters. The geometric mean of L was 0.63 with a 95% confidence interval between -0.88 and 2.44 . Using Eq. [2] with an exponent 1 instead of $1 - 1/n$, Vereecken (1995) determined that L had a positive correlation with the sand fraction and n parameter, and a negative correlation with K_s . Wösten et al. (1995) found that L was related to the organic matter content. Despite these insights, $K_o = K_s$ and $L = 0.5$ are the most common default values in predictive uses of Eq. [3].

The international database UNSODA has recently become available (Leij et al., 1996) and allows a more detailed investigation of pore-size models than was previously possible. Using 200 soils from the UNSODA database, Kosugi (1999) evaluated the standard Burdine ($L = 2$, $\beta = 2$, $\gamma = 1$) and Mualem ($L = 0.5$, $\beta = 1$, $\gamma = 2$) versions of Eq. [1] in conjunction with a lognormal function for water retention (Kosugi, 1994). The measured conductivity closest to saturation was used as a matching point. Kosugi (1999) found that usage of the standard parameters led to considerable errors in the description of unsaturated hydraulic conductivity. Much better results were obtained if L , β or γ were optimized. Kosugi (1999) developed two models to predict relative unsaturated hydraulic conductivity from water retention parameters. The first model used optimal values for the entire data set ($L = -0.3$, $\beta = 1.8$) whereas the second model used $L = -0.8$ and utilized a power function between β and a distribution parameter in the retention equation. Compared with the standard Burdine and Mualem models, the variance between measured and predicted relative hydraulic conductivities decreased by about 90%. Although this is a considerable improvement in the ability to estimate unsaturated hydraulic conductivity, Kosugi's models estimate relative hydraulic conductivity data. Predictive uses of Kosugi's models therefore need additional measurements or estimates of a matching point.

The objective of this paper is to develop predictive expressions for K_o and L for the Mualem-van Genuchten model (Eq. [3]) and compare their effectiveness and reliability with those of the standard model of Mualem (1976), where $K_o = K_s$ and $L = 0.5$. To this end, we

will fit both K_o and L to the unsaturated conductivity data of 235 samples from the UNSODA database. We set β and γ to 1 and 2, respectively. In this way, we can keep Eq. [3] mathematically simple and avoid strong correlations among fitted L , β or γ , which would complicate any further modeling efforts. We will investigate the correlation structure among K_o , L , and potential predictors such as retention parameters, K_s , soil texture and bulk density and we will develop predictive models for K_o and L using a combined bootstrap-neural network approach (Schaap et al., 1999). Neural networks were used because of their ability to find patterns in complex data. The bootstrap was used to quantify the uncertainty in predicted K_o and L , and therefore uncertainty in $K(S_e)$, due to variability and ambiguity in the data set. Such information is useful for interpreting the reliability of predictions and essential when predicted K_o and L are used in stochastic analyses of water flow in unsaturated soils.

THEORY

Because unsaturated hydraulic conductivity can vary many orders of magnitude, it is convenient to write Eq. [3] into a logarithmic form:

$$\log_{10}[K(S_e)] = \log_{10}(K_o) + L \log_{10}(S_e) + 2 \log_{10}\{1 - [1 - S_e^{n/(n-1)}]^{1-1/n}\} \quad [4]$$

This formulation makes it easier to plot unsaturated hydraulic conductivity and, more importantly, it minimizes a bias towards high conductivities when Eq. [4] is fitted to experimental data. Furthermore, Eq. [4] makes it easier to understand the effects of K_o and L on the shape of $K(S_e)$.

The effect of K_o on the shape of $K(S_e)$ can be easily understood as a scaling of $K(S_e)$. The roles of the second and third terms on the right hand side of Eq. [4] are more complex. Figures 1a through c show the sensitivity of the second term (Fig. 1a) and the relative conductivity ($\log_{10}(K_r) = \log_{10}[K(S_e)/K_o]$, which is equal to the sum of the second and third term) to variations in L for $n = 2.5$ (Fig. 1b) and $n = 1.2$ (Fig. 1c). The second term in Eq. [4] diverges at low S_e for different L and has a positive slope for positive L (Fig. 1a). The third term always increases with S_e but is invariant for L and is therefore represented by the curves at $L = 0$ in Fig. 1b and 1c. This term is dependent on the n parameter of Eq. [2] and, indirectly, also on α because S_e must be computed with Eq. [2]. The combination of the second and third terms in Fig. 1b and c demonstrate that higher values of L lead to a stronger reduction in $K(S_e)$ at low S_e and vice versa. Although the contribution of the second term is the same for both values of n , there seems to be a difference in sensitivity of $\log_{10}(K_r)$ to L for $n = 2.5$ and $n = 1.2$. This effect is apparent because it results from the range that we used to plot $\log_{10}(K_r)$, which was chosen to contain most of the measurements. In practice, however, only the hydraulic conductivity of soils with high n (predominantly sandy soils) can be measured over the full S_e scale. Differences in sensitivity to L may therefore occur for different n .

Figure 1b further demonstrates that if L becomes more negative, $K(S_e)$ may increase with decreasing S_e . This effect is physically unrealistic but it occasionally occurs while fitting Eq. [4] because of random or systematic errors in the unsaturated hydraulic conductivity data. To ensure continuously increasing $K(S_e)$ we used the constraint $L > -2 - 2/(n - 1)$

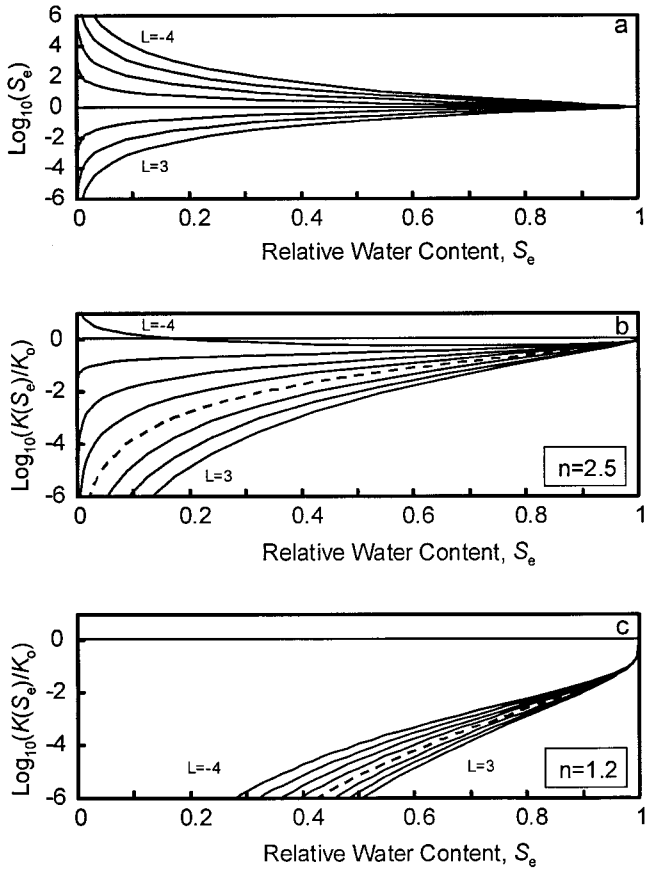


Fig. 1. Effect of variations in L on unsaturated conductivity terms in Eq. [4]: $L \log_{10}(S_e)$ (a) and $\log_{10}[(K(S_e)/K_0)]$ for $n = 2.5$ (b) and $n = 1.2$ (c). The dashed lines in (b) and (c) indicate the position of the third term of Eq. [4] ($L = 0$).

(Hoffman-Riem et al., 1999; Durner et al., 1999). Marginal differences resulted from usage of this constraint.

The sharp increase in hydraulic conductivity near saturation in Figure 1c is caused by the nonzero slope of Eq. [2] near $h = 0$ for $n < 2$. We refer to Vogel and Cislserova (1988) for a more detailed discussion of using Eq. [2] and [3] near saturation for low n .

MATERIALS AND METHODS

Data Set

The UNSODA database was compiled by Leij et al. (1996) from many international sources. UNSODA consists of 791 soil samples with water retention, saturated and unsaturated hydraulic conductivity data measured in the field or laboratory, as well as particle size distribution and bulk density data. We used a subset of 235 laboratory samples that had at least six $\theta - h$ pairs and at least five $K - h$ pairs. Samples with chaotic data or with limited retention or conductivity ranges were omitted. Almost all samples were from temperate zones in the northern hemisphere (Belgium, 47; France, 1; Germany, 54; India, 1; Japan, 9; the Netherlands, 13; Switzerland, 54; United Kingdom, 11; USA, 22; former USSR, 23). Figure 2 provides the textural distribution of the samples and their classification in four textural groups: Sands (100), Loams (41), Silts (58) and Clays (36).

Water retention data were determined with 12 different techniques which can be generalized in five groups: pressure based methods (pressure, vacuum suction), hanging water col-

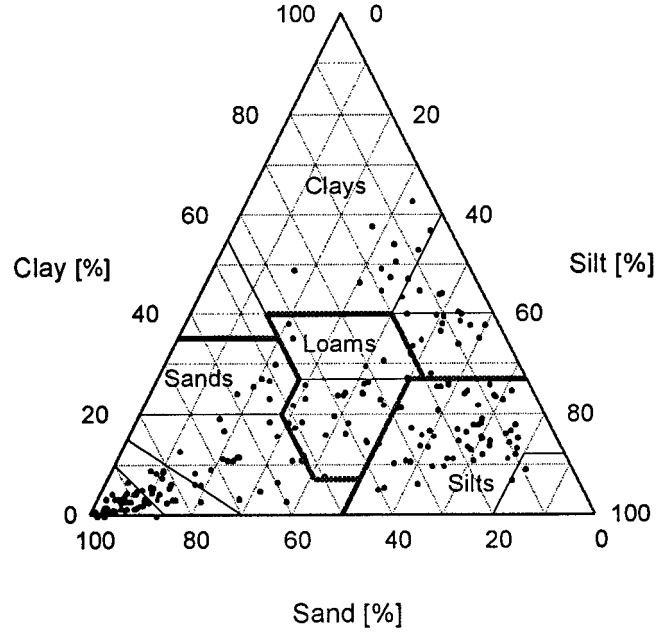


Fig. 2. Textural distribution of the 235 samples and the classification in four textural groups.

umn, tensiometer based (combined with TDR, gravimetric, volumetric, gamma ray attenuation methods), and the sand box. Thirteen methods were used to determine $K - h$ data, they can be generalized in pressure methods (pressure and suction), infiltration (sprinkling infiltrometer, falling head method), evaporation methods (including the hot air method), and the instantaneous profile method. In many cases, a combination of methods was used to determine the water retention or conductivity characteristics over an extended pressure head range.

Fitting Retention and Conductivity Parameters to Hydraulic Data

Equations [2] and [4] were fitted to measured data with the Simplex or Amoeba algorithm (Nelder and Mead, 1965; Press et al., 1988). Because we used parameters from Eq. [2] to predict unsaturated hydraulic conductivity with Eq. [4], we did not carry out simultaneous optimizations of Eq. [2] and [4] (cf., Yates et al., 1992). Instead, we first optimized Eq. [2] and then used the α n parameters to compute S_e and optimize K_0 and L in Eq. [4].

Some samples had insufficient retention points to describe the entire retention curve. To avoid fitted parameters with unreasonable values (e.g., $\theta_s > 1$), we imposed the following constraints during the optimization: $0.0 < \theta_s < 0.3 \text{ cm}^3 \text{ cm}^{-3}$; $0.6 \phi < \theta_s < \phi \text{ cm}^3 \text{ cm}^{-3}$ (where ϕ is the total porosity); $0.0001 < \alpha < 1.000 \text{ cm}^{-1}$; $1.0001 < n < 10$. The objective function that was minimized is given by:

$$O_w(p) = \sum_{i=1}^{N_w} (\theta_i - \theta'_i)^2 \quad [5]$$

where θ_i and θ'_i are the measured and predicted water contents respectively, N_w is the number of measured water retention points for each sample and p is the parameter vector $\{\theta_s, \alpha, n\}$.

The parameters K_0 and L in Eq. [4] were subject to the constraints $0.001 \text{ (cm day}^{-1}\text{)} < K_0 \leq K_s$ and $-2 - 2/(n - 1) < L < 100$. The lower constraint for K_0 was never violated; the upper constraint was necessary for 66 samples, mainly

because of missing conductivity data near the wet end which would otherwise have led to $K_o > K_s$. The following objective function was minimized:

$$O_K(p) = \sum_{i=1}^{N_k} [\log_{10}(K_i) - \log_{10}(K'_i)]^2 \quad [6]$$

where K_i and K'_i are the measured and predicted hydraulic conductivity respectively, N_k is the number of measured $K(h)$ data points and $p = \{K_o, L\}$. As mentioned earlier, logarithmic values of K_i were used in Eq. [6] to avoid bias towards high conductivities in the wet range.

The goodness of fit of Eq. [2] and [4] was quantified with the root mean square error:

$$\text{RMSE}_{w,K}(p) = \sqrt{\frac{O_{w,K}(p)}{N_{w,K} - n_p}} \quad [7]$$

where $N_{w,K}$ is the number of water retention or hydraulic conductivity measurements and n_p is the number of parameters that were optimized. Results of Eq. [7] will be presented as averages for each textural group and as averages for all 235 samples. Because logarithmic values were used for K_i , RMSE_K results are dimensionless.

Prediction of K_o and L

The results from the previous section will show how well Eq. [4] describes existing unsaturated hydraulic conductivity data. Our goal, however, is to evaluate how well we can predict unsaturated hydraulic conductivity when these data are not available. To this end, we need to estimate K_o and L from potential predictors like sand and clay percentages, bulk density, θ_s , θ_s , α , n , and/or K_s . We computed Spearman rank correlations (e.g., Press et al., 1988) to investigate the correlation structure among fitted K_o , L , and these predictors. Spearman rank correlations were chosen over linear correlations because the variables were not always normally distributed.

Subsequently, we developed neural network models to estimate K_o and L from the potential predictors. Neural networks have previously been used to predict water retention and saturated hydraulic conductivity and, for the sake of brevity, we refer to Pachepsky et al. (1996), Schaap et al. (1998), and Schaap and Leij (1998) for details. The primary reason to use neural networks is that they can discover and implement complex nonlinear relations among variables (Hecht-Nielsen, 1991; Haykin, 1994). Similar to Schaap and Leij (1998), we used feed-forward backpropagation networks with one hidden layer, containing six nodes, and sigmoidal transfer functions. Instead of minimizing the variance of fitted and predicted K_o and L during the neural network optimization (cf., Schaap and Bouten, 1996), we used Eq. [6] as an objective function. Although computationally more intensive, this choice was motivated by the difference in sensitivity of Eq. [4] to different values of n and L , as discussed earlier. The change in objective function led to RMSE_K values that were about 10% lower.

The neural network analysis was combined with the bootstrap method (Efron and Tibshirani, 1993) to study the uncertainty in predicted K_o and L . As was shown by Schaap and Leij (1998) for water retention and K_s , uncertainty and ambiguity in a data set used for model calibration leads to uncertainty in predicted hydraulic parameters. The theory behind the bootstrap method assumes that multiple alternative realizations of a population can be simulated from a single data set. By calibrating a (neural network) model on each of these alternative data sets, slightly different models result—leading to uncertainty in the prediction. The alternative data sets have the same size as the original data set and are generated by random

sampling with replacement. Therefore, in a data set of N samples, each sample has a chance of $1 - [(N - 1)/N]^N$ to be selected once or multiple times. Because some samples are selected more than once, each alternative data set contains about 63% of the original data. Neural networks were calibrated on each of the alternative data sets and validated with the 37% of the samples that were not selected. We will present only the validation results in this study.

The bootstrap method was combined with the TRAINLM routine of the neural network toolbox (Demuth and Beale, 1992) of MATLAB¹ (version 5.0, MathWorks Inc., Natick, MA). The neural network code was modified to avoid local minima in the objective function. We used 100 bootstrap data sets resulting in 100 neural network models. In effect, each prediction yielded 100 values for K_o and L , which were subsequently summarized with means and standard deviations.

As error criteria, we will present coefficients of determination (R^2) between predicted and fitted K_o and L . Further, we will compute RMSE_K values (Eq. [7]) of our model predictions. Although it is not necessary to correct model predictions for the number of model parameters (n_p), we will still carry out these corrections to be able to compare the RMSE_K values of the predictions with those of the optimizations.

RESULTS AND DISCUSSION

Optimization Results

An overview of average values and standard deviations of optimized water retention and hydraulic conductivity parameters and measured K_s values are given in Table 1. Values are reported for each textural group and the total data set of 235 samples. For the water retention curve, we found average RMSE_w values between 0.0096 and 0.0141 $\text{cm}^3\text{cm}^{-3}$. Contrary to our expectation, average $\log_{10}(\alpha)$ were higher for the Loams than for the Sands while we also found that the Loams had lower $\log_{10}(n)$ values than the Clays.

For the hydraulic conductivity curve, we found RMSE_K values between 0.393 to 0.481, corresponding to an error of about 0.4 orders of magnitude. The relatively small variation in RMSE_K indicated that Eq. [4] described log hydraulic conductivity equally well for all textural groups. Average K_o values were almost an order of magnitude lower than average K_s , which may be attributed to macropore flow that is included in K_s but not in K_o , which is inferred from unsaturated conductivity data (cf., van Genuchten and Nielsen, 1985; Luckner et al. 1989). The results in Table 1 indicate that setting $K_o = K_s$ in Eq. [4] leads to an overestimation of unsaturated hydraulic conductivity. At the same time, however, we have to realize that using K_o as a matching point will lead to a hydraulic conductivity that is too low at or near saturation since at $h = 0$ the hydraulic conductivity should be equal to K_s . This indicates that Eq. [4] cannot describe the shape of the measured conductivity characteristics near saturation. With the present data set it is impossible to use a bi-modal pore structure (e.g., Durner, 1994) to account for effects of macro-porosity on retention and conductivity curves. The results in this paper thus only pertain to conditions

¹ Trade names are provided for the benefit of the reader and do not imply endorsement by the USDA.

Table 1. Average hydraulic parameters for each soil textural group, with standard deviations in parentheses. Except for K_s , all parameters were optimized.

	N	θ_r	θ_s	$\log_{10}(\alpha)$	$\log_{10}(n)$	RMSE _w	$\log_{10}(K_o)$	L	RMSE _K
		$\text{cm}^3 \text{cm}^{-3}$		cm^{-1}		$\text{cm}^3 \text{cm}^{-3}$	cm day^{-1}		
All	235	0.055 (0.073)	0.442 (0.101)	-1.66 (0.52)	0.214 (0.209)	0.0122	1.92 (0.81)	1.03 (1.04)	-3.09 (8.75) 0.410
Sands†	100	0.052 (0.043)	0.396 (0.056)	-1.58 (0.37)	0.349 (0.228)	0.0122	2.24 (0.79)	1.29 (1.06)	-1.28 (3.17) 0.395
Loams‡	41	0.056 (0.091)	0.512 (0.132)	-1.39 (0.50)	0.076 (0.047)	0.0119	2.03 (0.64)	1.42 (0.98)	-6.97 (9.57) 0.398
Silts§	58	0.031 (0.058)	0.428 (0.078)	-1.92 (0.52)	0.139 (0.141)	0.0141	1.70 (0.61)	0.82 (0.80)	-1.22 (10.17) 0.403
Clays#	36	0.098 (0.109)	0.512 (0.108)	-1.75 (0.64)	0.114 (0.112)	0.0096	1.31 (0.80)	0.26 (0.94)	-5.96 (12.40) 0.481

† Sand, loamy sand, sandy loam, sandy clay loam.

‡ Loam, clay loam.

§ Silty loam, silt.

Clay, sandy clay, silty clay, silty clay loam.

away from saturation (suctions stronger than a few centimeters).

We found negative L for all textural groups with the lowest values for the Loams and Clays. Although not all individual samples had a negative L , the fact that $S_e^L > 1$ for negative L makes it impossible to interpret S_e^L in Eq. [4] as a simple reduction factor that accounts for pore tortuosity and connectivity (Mualem and Dagan, 1976). Because K_o is constant for all S_e of a sample, the negative L seem to compensate the third term in Eq. [4]. This term is equivalent to the curve for $L = 0$ in (cf. Fig. 1a–1c) and it could be argued that it drops off too quickly with decreasing S_e because of the factor 2, which follows from γ in Eq. [1]. However, using a different water retention model, Kosugi (1999) reported negative L values even after setting $\gamma = 1$. Apparently, negative L are found irrespective of the chosen water retention model and the β and γ configuration of Eq. [1]. This therefore seems to point to a failure in the pore-tortuosity or pore-interaction concepts in models defined by Eq. [1]. Likewise, Hoffmann-Riem et al. (1999) concluded that models based on Eq. [1] should not be interpreted as being physically based. In the remainder of the study we will therefore treat K_o and L as empirical parameters.

Although we found negative L values for many samples, the results in Table 1 by themselves do not prove that using a negative L leads to substantially lower RMSE_K (Eq. [7]) compared with a fixed value $L = 0.5$ (Mualem, 1976). We therefore varied L between -3 and 3 in steps of 0.5 while we fitted K_o and computed the average RMSE_K for each soil textural group and the entire dataset (Fig. 3). The Sands have a clear minimum RMSE_K of 0.60 at $L = -1$, which is substantially lower than at $L = 0.5$ where the RMSE_K is 1.21. The other textural groups also have lower RMSE_K values at negative L but with smaller decreases relative to $L = 0.5$. The more gradual slopes of the RMSE_K curves for these groups are caused by their lower n values and limited S_e range of the measurements. These factors cause that the shape of Eq. [4] is less sensitive to variations in L (cf. Table 1, Fig. 1b and 1c). For all samples (All), the optimum value is also $L = -1$. This value does not agree with the value of -3.09 in Table 1 because in that case both K_o and L were optimized and the reported L is an average for all 235 samples. Because all RMSE_K curves are near-optimal at $L = -1$, it makes sense to use this value for all samples. It should be noted, how-

ever, that the optimal fixed value of L might depend on ratio of coarse textured soils (with $L \approx -1$) and fine textured soils ($L < -1$) in the data set. Furthermore, by fixing L and only optimizing K_o we must make a concession to the goodness of fit. Average RMSE_K for all samples at $L = -1$ is 0.75 (Fig. 3), whereas it is 0.41 when both K_o and L were optimized (Table 1).

Correlation Structure of the Hydraulic Parameters

Table 2 shows the Spearman correlations among the potential predictors (sand and clay percentages, bulk density, θ_r , θ_s , α , n , and K_s) and K_o and L for all 235 samples (All). Significance levels at $P = 0.05$, 0.01, and 0.001 indicate where the Null Hypothesis (no correlation present) should be rejected. We also show truncated matrices for the four textural groups with the correlations between K_o , L , and the potential predictors. The correlation structures of the omitted parts are largely similar to the matrix of all 235 samples but they are less significant due to a reduced number of samples. Correlations for the case where we fitted only K_o and assumed $L = -1$ are not shown because these were largely similar to the results in Table 2.

The correlation matrix for the entire data set shows that most variables have significant correlations ranging from 0.14 to 0.84 (absolute values). Some of these corre-

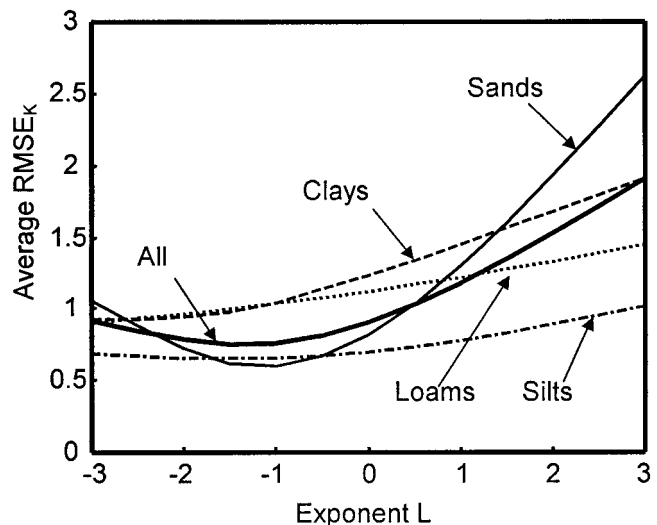
**Fig. 3.** RMSE_K curves for various values of L for the five textural groups.

Table 2. Spearman correlation matrix for all 235 samples (All) and truncated versions for the K_o and L parameters of the four textural groups (Sands, Loams, Silts, Clays).

		% sand	% clay	Bulk d.	θ_r	θ_s	α	n	K_s	K_o	L
All ($N = 235$)	%sand	1.00									
	%clay	-0.80***	1.00								
	Bulk d.	0.29***	-0.36***	1.00							
	θ_r	0.16*	-0.14*	-	0.92						
	θ_s	-0.34***	0.46***	-0.46***	-	1.00					
	α	0.27***	-	-0.13*	-	0.23***	1.00				
	n	0.58***	-0.68***	0.28***	0.55***	-0.31***	-	1.00			
	K_s	0.46***	-0.46***	-0.23***	-	0.14*	0.30***	0.39***	1.00		
	K_o	0.34***	-0.30***	-0.24***	-0.18**	0.24***	0.57***	-	0.53***	1.00	
	L	0.26***	-0.41***	-	-	-0.15*	-0.29***	0.47***	0.28***	0.25***	1.00
Sands ($N = 100$)	K_o	-	-0.34***	-	-0.27**	-	0.54***	-	0.57***	1.00	
	L	0.23*	-0.45***	-	-	-	-	0.24*	0.45***	0.59***	1.00
Loams ($N = 41$)	K_o	-0.37**	-	-0.35**	-	0.68***	0.52***	-	0.64***	1.00	
	L	-0.31*	-	-	-	-	-0.40**	0.57***	-	-	1.00
Silts ($N = 58$)	K_o	-	-	-0.56***	-0.49***	0.49***	0.49***	-	0.28*	1.00	
	L	-	-	-	-	-	-0.39**	0.41**	-	0.26*	1.00
Clays ($N = 36$)	K_o	-	0.36*	-0.48**	-0.37*	-	0.54***	-0.52**	0.85***	1.00	
	L	-	-	-	-	-	-0.38*	0.50**	-	-	1.00

*, **, *** Significant at the 0.05, 0.01, 0.001 probability levels, respectively.

lations are artificial and result from implicit constraints. For example, sand and clay percentages are forced to have a correlation because the sum of sand and clay should never exceed 100%. Likewise, the negative correlation between bulk density and θ_s can be understood because the total porosity is determined by the bulk and particle densities while θ_s should be smaller or equal to the porosity. The autocorrelation of θ_r is not equal to 1 because θ_r had to be constrained to 0.0 for more than 100 samples when we fitted Eq. [2] to the retention data. Therefore, these samples obtain the same rank, resulting in a reduction in the Spearman correlation.

Table 2 shows that K_o has a significant positive correlation with K_s . This is partly caused by the constraint $K_o \leq K_s$ that we imposed during the optimization of Eq. [4] in which we forced $K_o = K_s$ if the optimal value of K_o was greater than K_s . However, Table 2 shows that the correlation is not near 1; in fact, it is quite poor for the Silt group (0.28). Table 1 already showed that fitted K_o values were considerably lower, while standard deviations were higher, than measured K_s . This indicates that K_o cannot be calculated from K_s with a simple reduction factor. The K_o parameter shows a positive correlation with α for all textural groups which is easily explained by the fact that larger α indicate larger average pore sizes. Negative correlation coefficients are found for bulk density, except in the case of the Sand group. Lower bulk densities increase the pore space and therefore, potentially, increase the conductive path for water flow. Similarly, negative correlations are also found for θ_r ; in this case, lower θ_r values effectively increase hydraulically active pore space. Conversely, θ_s has a positive correlation coefficient with K_o for the Loams and the Silts because higher θ_s values increase the amount of potentially mobile water. Note that, if significant, the correlation coefficients between θ_r , θ_s and bulk density, and K_o are higher for the individual textural groups than for all 235 samples. This finding points to possibly complex relations between K_o and its predictors. Correlations of sand and clay percentages with K_o are more ambiguous than correlations with retention parameters and usually small or insignificant.

In the case of L , we find positive correlation coeffi-

cients with n for all textural groups as was also reported by Vereecken (1995) for a combination of Mualem's (1976) model with a different retention function. This correlation implies that when n decreases, L decreases, causing the hydraulic conductivity to decrease less with S_e (cf. Fig. 1a-c). Because L is predominantly negative and seems to compensate the third term in Eq. [4], it is difficult to interpret physically this correlation. The parameter α exhibits a weaker correlation with L , except for the sands where no significant correlation was found. The negative correlation means that smaller α values lead to larger values of L and a stronger reduction in hydraulic conductivity. Because small values of both α and n are normally associated with finer textures, it seems that α and n have opposite effects on L . A significant correlation between L and bulk density, sand, or clay is absent for most or all textural groups.

Prediction of K_o and L with Neural Networks

Three models for predicting K_o and L were tested. Model A reflects the traditional Mualem-van Genuchten model (van Genuchten, 1980) with $K_o = K_s$ and $L = 0.5$. In the case of Model B, we constructed neural network models that predicted only K_o while assuming that $L = -1$. Model C predicts both K_o and L . Based on the results in Table 2, we used four different sets of predictors for Models B and C: (i) sand and clay percentages and bulk density, (ii) retention parameters $\{\theta_r, \theta_s, \alpha, n\}$, (iii) retention parameters and K_s , and (iv) Sets 1 and 3 combined. Models B and C were indexed according to these four sets of predictors (i.e., B1...B4, C1...C4).

Table 3 shows that the RMSE_K of Model A is more than one order of magnitude, with a very high value for the Clays (1.70). Models B1 and C1 yielded somewhat lower RMSE_K values by using sand, silt, clay, and clay (SSCBD) as predictors. Models B2 and C2 clearly show that water retention parameters make more effective predictors, as was already inferred from the correlation matrices in Table 2. Results for Models B3 and C3 show that adding K_s to the retention parameters increased the coefficients of determination of K_o . However, com-

Table 3. Coefficients of determination and RMSE_K results for predictions of unsaturated hydraulic conductivity according to models A, B, and C.

Model	Input	R ²		RMSE _K				
		log ₁₀ (K _o)	L	All	Sands	Loams	Silts	Clays
A	K_o = K_s, L = 0.5	–	–	1.31	1.22	1.35	1.20	1.70
Flexible K_o, L = –1								
B1	SCBD†	0.29	–	1.16	1.04	1.54	0.93	1.40
B2	0,0,α n	0.51	–	0.95	0.90	1.30	0.73	1.08
B3	0,0,α n K_s	0.64	–	0.96	0.88	1.26	0.78	1.16
B4	SCBD0,0,α n K_s	0.63	–	0.95	0.87	1.22	0.78	1.13
Flexible K_o and L								
C1	SCBD	0.27	0.08	1.18	1.16	1.48	0.86	1.43
C2	0,0,α n	0.48	0.45	0.84	0.91	0.88	0.69	0.86
C3	0,0,α n K_s	0.56	0.43	0.82	0.86	0.92	0.68	0.82
C4	SCBD0,0,α n K_s	0.53	0.40	0.79	0.83	0.84	0.67	0.81

† SCBD: sand, clay and bulk density.

parison with Models B2 and C2 shows that RMSE_K were only marginally reduced, if at all. Models C2, C3, and C4 had lower RMSE_K than the B2, B3, and B4 models, especially for the Loams and Clays. These findings suggest that both K_o and L should be predicted and should not be fixed to predetermined values.

Table 4 shows that the correlation structure for K_o and L as predicted with Model C4 is largely similar to that of fitted K_o and L (Table 2) suggesting that the correlation structure is preserved in the model predictions. A small correlation between L and bulk density appeared in the neural network results while the correlation between fitted L and K_o in Table 2 disappeared. Similar results were found for C2 and C3.

Although Model C4 performed the best in terms of RMSE_K, the differences with Models C2 and C3 were relatively small. Given the fact that C2 requires only retention parameters to predict K_o and L, this model is preferable because n is required in Eq. [3] while α and n are also needed to compute S_e with Eq. [2]. It is interesting to note that Model C2 uses less data than Model A (K_s is not required), yet it has a RMSR_K that is about half an order of magnitude lower. Comparison of our results with those of the AB and FN models reported in Table 3 of Kosugi (1999) shows that Model C2 performs better. Assuming that Kosugi (1999) also used an average of 18.5 K(S_e) observations per sample (his and our data sets were derived from UNSODA and partially overlap), the converted RMSE_K results for Model AB and FN are 1.11 and 0.94 respectively, whereas Model C2 had an error of 0.84. Still, the RMSE_K of Models C2, C3, and C4 are significantly higher (approximately 0.8) than the RMSE_K of the direct fit to the measured K – h data (0.41, Table 1). The results for direct fit are essentially averages for *individual* samples and are insensitive to variations among samples due to systematic differences in, for example, measurement methods (cf. Stolte et al., 1994). The neural network models, however, attempt to implement relations that are valid for *all* the samples in the calibration data set.

Consequently, the RMSE_K of the model predictions are sensitive to systematic and random differences that exist from sample to sample.

Finally, Fig. 4 shows the predictions of Models A, B2, and C2 for the average hydraulic parameters of the sands and clays in Table 1. The inserts in Fig. 4 provide the values of the estimated K_o and L parameters as well as their uncertainty, which was generated with the bootstrap method. Figure 4 also shows the 90% confidence interval for Model C2 as shaded areas. These intervals were generated by evaluating Eq. [4] at many values of S_e for each of the K_o and L pairs following from the 100 bootstrap–neural network analyses that were performed to create C2. Especially for the sand, Model A predicts systematically higher K(S_e) values at S_e > 0.15 for the sand and S_e > 0.45 for the clay than Model B2 or C2. Below these values, Model A predicts smaller K(S_e) than B2 or C2. The overprediction of Model A follows from the use of K_o = K_s. The underprediction at small S_e is caused by setting L to 0.5 which causes a steeper drop in K(S_e) than Models B2 and C2, which have smaller L values (cf., Fig. 1a–c). Predictions by Models B2 and C2 are largely similar. The confidence intervals of C2 show that even though Model C2 has a near-optimal minimum RMSE_K, the uncertainty in predicted K(S_e) can still be large. For example, the confidence intervals increase from less than one order of magnitude near saturation to about two orders of magnitude at low S_e. We note that this uncertainty does not directly relate to variability found in the field but rather reflects variability and ambiguity in the data set that was used. Schaap and Leij (1998) showed that using larger data sets generally leads to smaller confidence intervals.

While our models provide an improved prediction of unsaturated hydraulic conductivity, we would like to reiterate that because of the one order of magnitude difference between K_o and K_s our models only apply for situations away from saturation, i.e., for suctions of at least a few cm of pressure head. Near saturation, our

Table 4. Spearman correlation matrix for predicted K_o and L of model C4 for all 235 samples.

Model	%sand	%clay	Bulk d.	θ _r	θ _s	α	N	K _s	K _o	L
C4										
All data	K_o	0.45***	–0.39***	–0.29***	–0.22***	0.25***	0.70***	–	0.67***	1.00
	L	0.19**	0.50***	0.18**	–	–0.26***	–0.48***	0.56***	0.37***	1.00

*, **, *** Significant at the 0.05, 0.01, 0.001 probability levels, respectively.

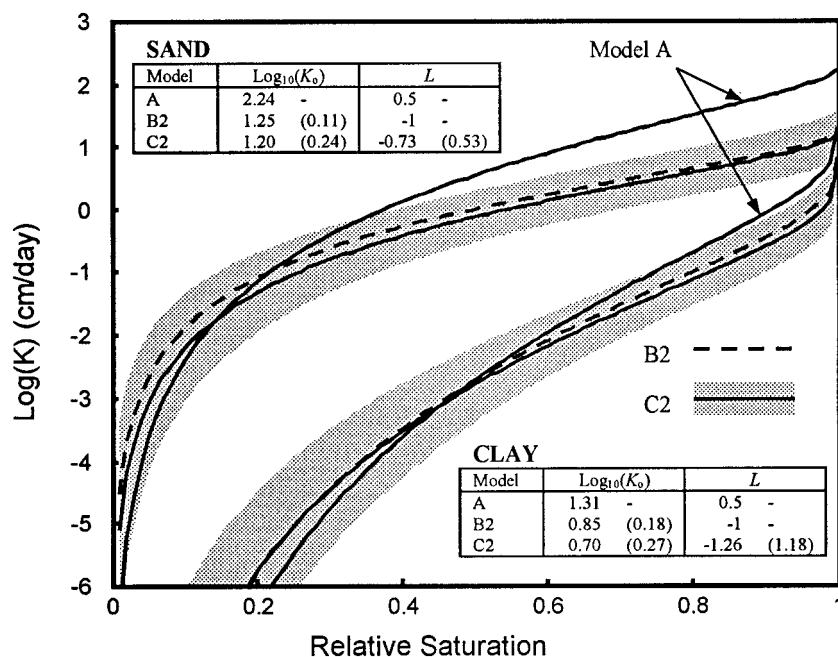


Fig. 4. Predicted unsaturated hydraulic conductivities for the sand and clay retention parameters listed in Table 1 for Model A, B2, and C2. Predicted K_o and L parameters for Models B2 and C2 are listed in the tables with their uncertainties as generated by the bootstrap method in parenthesis. The shaded area's indicate the 90% confidence interval of the predicted hydraulic conductivities for Model C2.

predicted K_o and L probably lead to an underestimation of the hydraulic conductivity because effects of macropore flow are not included in the Mualem–van Genuchten model. Future work should therefore focus on this subject.

Model C2 is implemented in Rosetta, a Windows 95/98 program that permits the prediction of retention, saturated, and unsaturated hydraulic parameters with pedotransfer functions. Rosetta is available at: <http://www.ussl.ars.usda.gov/models/rosetta/rosetta.htm>; verified January 31, 2000.

SUMMARY AND CONCLUSION

The results of our study showed that the predictive use of the Mualem–van Genuchten model, Eq. [4] with $K_o = K_s$ and $L = 0.5$, leads to relatively poor predictions of unsaturated hydraulic conductivity ($\text{RMSE}_K = 1.31$). The unsaturated hydraulic conductivity is overpredicted in the wet range and underpredicted in dry range. When we fitted Eq. [4] to hydraulic conductivity data, we found that K_o was, on average, almost one order of magnitude smaller than K_s while L was often negative, with smaller values for finer textured soils. The difference between K_o and K_s can be attributed to effects of macroporosity which does affect K_s but which hardly has an effect on unsaturated hydraulic conductivity. The negative values for L make a physical interpretation of the Mualem (1976) model difficult because they imply that the tortuosity decreases and/or the connectivity increases with decreasing water contents. In the light of $K_o < K_s$, the negative values can be understood as correction factors that cause a more gradual drop in conductivity than positive values for L . The results in the present study and those of Kosugi (1999) indicate that neither K_o nor L can be interpreted as physically meaningful parameters

and should be considered only as empirical shape factors of the Mualem–van Genuchten model. This, ultimately, suggests that the models proposed by Mualem (1976) or Burdine (1953) give a too-simplified conceptualization of the hydraulic conductivity of a porous medium. Still, as was shown by Kosugi (1999) and the current study, these pore-size distribution models can be used to successfully predict unsaturated hydraulic conductivity from water retention parameters.

Using Spearman rank correlation matrices, we showed that K_o and L have low correlations with sand and clay percentages and bulk density. Water retention parameters were better and more consistent predictors of K_o and L . A neural network model that predicted both K_o and L from retention parameters (θ_r , θ_s , α , n) yielded a RMSE_K of 0.84, which was a substantial improvement over the traditional Mualem–van Genuchten model. Uncertainty analysis with the bootstrap method suggested that the data set created a large degree of uncertainty in the prediction of unsaturated hydraulic conductivity. Near saturation, the uncertainty was less than one order of magnitude, at lower water contents the uncertainty grew to two orders of magnitude. The uncertainty intervals can probably be reduced when the models would be based on more unsaturated hydraulic conductivity characteristics. Effects of macroporosity are not included in the model; such effects need to be accounted for when our models are to be used near saturation.

ACKNOWLEDGMENTS

This study was jointly supported by NSF, NASA (EAR – 9804902), and the ARO (39153 – EV). The authors would like to thank Holger Hoffmann-Riem for discussions and comments on an earlier version of the manuscript. Two anonymous

reviewers are thanked for their valuable comments. We especially thank Wolfgang Durner for his thoughts.

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