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ROSETTA: a computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions

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Abstract

Soil hydraulic properties are necessary for many studies of water and solute transport but often cannot be measured because of practical and/or financial constraints. We describe a computer program, ROSETTA, which implements five hierarchical pedotransfer functions (PTFs) for the estimation of water retention, and the saturated and unsaturated hydraulic conductivity. The hierarchy in PTFs allows the estimation of van Genuchten water retention parameters and the saturated hydraulic conductivity using limited (textural classes only) to more extended (texture, bulk density, and one or two water retention points) input data. ROSETTA is based on neural network analyses combined with the bootstrap method, thus allowing the program to provide uncertainty estimates of the predicted hydraulic parameters. The general performance of ROSETTA was characterized with coefficients of determination, and root mean square errors (RMSEs). The RMSE values decreased from 0.078 to 0.044 $cm^3\ cm^{-3}$ for water retention when more predictors were used. The RMSE for the saturated conductivity similarly decreased from 0.739 to 0.647 (dimensionless $\log_{10}$ units). The RMSE values for unsaturated conductivity ranged between 0.79 and 1.06, depending on whether measured or estimated retention parameters were used as predictors. Calculated mean errors showed that the PTFs underestimated water retention and the unsaturated hydraulic conductivity at relatively high suctions. ROSETTA's uncertainty estimates can be used as an indication of model reliability when no hydraulic data are available. The ROSETTA program comes with a graphical user interface that allows user-friendly access to the PTFs, and can be downloaded from the US Salinity Laboratory website: http://www.ussl.ars.usda.gov/.

Keywords: Soils; Hydraulic conductivity; Retention; Neural networks; Computer programs

1. Introduction

A broad array of methods currently exists to determine soil hydraulic properties in the field or in the laboratory (cf. Klute, 1986; Leij and van Genuchten, 1999). While measurements permit the most exact determination of soil hydraulic properties, they often require a substantial investment in both time and money. Moreover, many vadose zone studies are concerned with large areas of land that may exhibit substantial spatial variability in the soil hydraulic properties. It is virtually impossible to perform enough measurements to be meaningful in such cases, thus indicating a need for inexpensive and rapid ways to determine soil hydraulic properties.

Many indirect methods for determining soil hydraulic properties have been developed in the past (cf. Rawls et al., 1991; van Genuchten and Leij, 1992; Leij and van Genuchten, 1999). Most of these methods can be classified as pedotransfer functions (PTFs,

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after Bouma and van Lanen, 1987) because they translate existing surrogate data (e.g. particle-size distributions, bulk density and organic matter content) into soil hydraulic data. All PTFs have a strong degree of empiricism in that they contain model parameters that were calibrated on existing soil hydraulic databases. A PTF can be as simple as a lookup table that gives hydraulic parameters according to textural class (e.g. Carsel and Parrish, 1988; Wösten et al., 1995) or include linear or nonlinear regression equations (e.g. Rawls and Brakensiek, 1985; Minasny et al., 1999). PTFs with a more physical foundation exist, such as the pore-size distribution models by Burdine (1953) and Mualem (1976), which offer a method to calculate unsaturated hydraulic conductivity from water retention data. Models by Haverkamp and Parlange (1986) and Arya and Paris (1981) use the shape similarity between the particle- and pore-size distributions to estimate water retention. Tyler and Wheatcraft (1989) combined the Arya model with fractals mathematics, while Arya et al. (1999a,b) recently extended the similarity approach to estimate water retention and unsaturated hydraulic conductivity.

Practical applications of most PTFs are often hampered by their very specific data requirements. Some authors established PTFs that provided the best results for their data set, which sometimes produced models that require many input variables (cf. Rawls et al., 1991) or detailed particle-size distributions (Arya and Paris, 1981; Haverkamp and Parlange, 1986). However, users of PTFs are frequently confronted with situations where one or several input variables needed for a PTF are not available. Another problem is that PTFs provide estimations with a modest level of accuracy. It would therefore be useful if PTFs could accept input data with varying degrees of detail and if PTF predictions could include reliability measures.

Recently, neural network analysis was used to establish empirical PTFs (Pachepsky et al., 1996; Schaap and Bouten, 1996; Minasny et al., 1999; Pachepsky et al., 1999). An advantage of neural networks, as compared to traditional PTFs, is that neural networks require no a priori model concept. The optimal, possibly nonlinear, relations that link input data (particle-size data, bulk density, etc.) to output data (hydraulic parameters) are obtained and implemented in an iterative calibration procedure. As a result, neural network models typically extract the maximum amount of information from the data. Schaap et al. (1998) used neural network analyses to estimate van Genuchten (1980) water retention parameters and saturated hydraulic conductivity. To facilitate the practical use of the PTFs, they designed a hierachical structure to allow input of limited and more extended sets of predictors. The combination with the bootstrap method (Efron and Tibshirani, 1993) provided the reliability for the PTF estimations (Schaap and Leij, 1998).

Yet, while neural network-based PTFs may provide relatively accurate estimates, they contain a large number of coefficients that do not permit easy interpretation or publication in explicit form. To facilitate application of the PTFs, we have developed the computer program ROSETTA that implements some of the models published by Schaap et al. (1998); Schaap and Leij (1998) and Schaap and Leij (2000). The objectives of this paper are (i) to present the ROSETTA program in terms of hydraulic parameters, calibration data sets, selection of predictors, and characterization of model performance, and (ii) to discuss the uncertainty of estimated hydraulic parameters as a function of suction and texture.

2. Materials and methods

Much of this section has been published before in Schaap et al. (1998), Schaap and Leij (1998), and Schaap and Leij (2000). However, we describe the most important methodology here to provide the reader a concise documentation about the background of ROSETTA. This section will also present methodology that was not used in previous publications.

2.1. Hydraulic parameters

ROSETTA is able to estimate van Genuchten (1980) water retention parameters and saturated hydraulic conductivity (K_s), as well as unsaturated hydraulic conductivity parameters based on Mualem's (1976) pore-size model. The retention function is given by

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

where $\theta(h)$ is the measured volumetric water content ($cm^3\ cm^{-3}$) at the suction h (cm, taken positive for

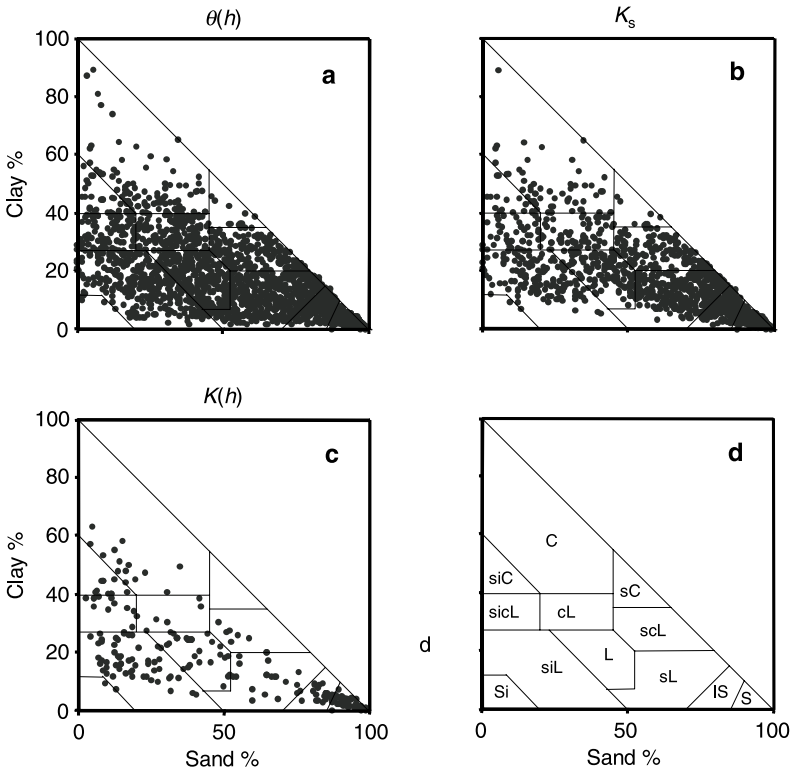

Fig. 1. Textural distribution of the samples for water retention (a), for the subset for saturated hydraulic conductivity (b), for the subset for unsaturated hydraulic conductivity (c). Fig. 1d depicts the textural classes. S: sand, lS: loamy sand, sL: sandy loam, scL: sandy clay loam, sC: sandy clay, L: loam, siL: silty loam, Si: silt, sicL: silty clay loam, siC: silty clay, cL: clay loam, C: clay.

increasing suctions). The parameters θ_r and θ_s are residual and saturated water contents, respectively, ($cm^3\ cm^{-3}$); α (>0, in cm^{-1}) is related to the inverse of the air entry suction, and n (>1) is a measure of the pore-size distribution (van Genuchten, 1980).

Combination of Eq. (1) with Mualem's (1976) pore-size model yields the following closed-form expression for unsaturated hydraulic conductivity (van Genuchten, 1980)

$$K(S_e) = K_0 S_e^L \{1 - [1 - S_e^{n/(n-1)}]^{1-1/n}\}^2 \quad (2)$$

where the effective saturation, S_e, is computed as

$$S_e = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} \quad (3)$$

K_0 is a fitted matching point at saturation ($cm\ day^{-1}$) while L (–) is an empirical parameter that is normally assumed to be 0.5 (Mualem, 1976). Eq. (2) can also be expressed in terms of h with the help of Eq. (1). Schaap and Leij (2000) found that fitted K_0 values were often about one order of magnitude lower than K_s, while fitted L were often negative, having an optimal value of -1. Although these findings suggest an increased level of empiricism in the Mualem model, they provide a far better description of unsaturated hydraulic conductivity data than the common practice of using $K_0 = K_s$ and $L = 0.5$ (see also Hoffmann-Riem et al., 1999; Kosugi, 1999). However, we should note that the use of $K_0 < K_s$ leads to an untenable situation near $S_e = 1$ or $h = 0$ cm because the hydraulic conductivity should be equal to K_s while Eq. (2) provides K_0. Schaap and Leij (2000) argue that Eq. (2) with fitted K_0 should be applied only at suctions of at least a few centimetre. The considerations above therefore require seven parameters (θ_r, θ_s, α, n, K_s, K_0 and L) to describe water retention, the saturated and unsaturated hydraulic conductivity.

2.2. Data set

In order to make the PTFs as widely applicable as possible, we obtained a large number of soil hydraulic data and corresponding predictive soil properties from three databases (Schaap and Leij, 1998). The data set thus assembled contained 2134 soil samples for water retention with a total of 20 574 $\theta(h)$ points. Most of the samples were derived from soils in temperate to subtropical climates of North America and Europe. Saturated hydraulic conductivity values were available for a subset of 1306 soil samples, while unsaturated hydraulic conductivity was known for 235 soil samples with a total of 4117 $K(h)$ points. The latter subset was solely derived from the database UNSODA (Leij et al., 1996; Nemes et al., 2001) with the requirement that at least five $K(h)$ data points were available; samples with chaotic data or with suction and conductivity ranges less than one order of magnitude were omitted. Fig. 1a–c gives the textural distributions of the datasets for water retention, K_s and unsaturated hydraulic conductivity. Fig. 1d provides the abbreviations of the USDA textural classes.

The parameters in Eqs. (1) and (2) were fitted to water retention and unsaturated hydraulic conductivity data with the simplex or amoeba algorithm (Nelder and Mead, 1965; Press et al., 1988). The objective function for water retention was

$$O_w(\mathbf{p}) = \sum_{i=1}^{N_w} (\theta_i - \theta_i')^2 \tag{4}$$

where θ_i and θ_i' are the measured and estimated water contents, respectively. N_w is the number of measured water retention points for each sample and $\mathbf{p}$ is the parameter vector (θ_r,θ_s,α,n). For the optimization of unsaturated hydraulic conductivity parameters, we minimized

$$O_k(\mathbf{p}) = \sum_{i=1}^{N_K} [\log_{10}(K_i) - \log_{10}(K_i')]^2 \tag{5}$$

where K_i and K_i' are the measured and estimated hydraulic conductivity, respectively, N_K is the number of measured $K(h)$ data points and $\mathbf{p} = (K_0, L)$. Logarithmic values of K_i were used in Eq. (5) to avoid bias towards high conductivities in the 'wet' range. We used log-transformed values of α, n, K_s and K_0 to account for their approximately lognormal distributions.

2.3. Model calibration

Because different numbers of samples were available for water retention, the saturated and unsaturated hydraulic conductivity, we developed separate PTFs for each of these characteristics. For the estimation of the water retention parameters (θ_r,θ_s,α,n) and K_s, we followed a hierarchical approach with limited or more extended sets of predictors (Schaap et al., 1998). The first model (H1) is a class PTF, consisting of a lookup table that provides parameter averages for each USDA textural class. The second model (H2) uses sand, silt, and clay as input, and in contrast to H1, provides hydraulic parameters that vary continuously with texture. The third model (H3) includes bulk density as a predictor while the fourth model (H4) also uses water content at 330 cm suction ($h =$ 33 kPa). The last model (H5) includes a water content at 15 bar suction ($h = 1500$ kPa) in addition to the input variables of the fourth model. The choice of suctions in models H4 and H5 was determined by their availability in the NRCS database (Soil Survey Staff, 1995).

Schaap and Leij (2000) showed that the hierarchical approach was not possible for unsaturated hydraulic conductivity because K_0 and L were poorly related to texture and bulk density. However, the same study showed that K_0 and L could be estimated from fitted water retention parameters (θ_r,θ_s,α and n). This PTF (model C2) thus requires such data to be available. To accommodate situations where this is not the case, we investigated how well we can estimate K_0 and L using estimated retention parameters obtained from models H1 to H5. These models are denoted as C2-H1–C2-H5 and allow K_0 and L to be estimated in a pseudo-hierarchical manner.

While model H1 is a simple table with average hydraulic parameters for each textural class, all other models involve a combination of neural networks and the bootstrap method. The neural networks for water retention parameters and K_s were calibrated using the following objective function

$$O_{nn}(\mathbf{c}_{nn}) = \sum_{i=1}^{N_s} \sum_{j=1}^{N_p} (\eta_{i,j} - \eta_{i,j}')^2 \tag{6}$$

where $\mathbf{c}_{nn}$ represents the coefficient matrices of the artificial neural network; N_s is the number of calibration samples. The number of parameters, N_p, equals 4 for the water retention models and 1 for K_s model, while η and η' are the fitted and estimated parameters, respectively. For the neural network models for unsaturated conductivity, an objective function similar to Eq. (5) was used. In this case, conductivities were computed by evaluating Eq. (2) at the water contents for which measurements were available (Schaap and Leij, 2000).

Models H2–H5 and model C2 were combined with the bootstrap method (Efron and Tibshirani, 1993) for two reasons. First, it allowed an uncertainty estimate to be assigned to each model prediction. For example, for a texture of 60% sand, 30% silt, and 10% clay, model H2 predicts a saturated hydraulic conductivity of 1.56 log cm - day^{-1} plus or minus a standard deviation of 0.11 log cm day^{-1}. For a coarser texture of 80% sand, 15% silt and 5% clay, the estimates are 1.99 ± 0.079 log cm day^{-1}, making this prediction more reliable than the previous one. The uncertainty estimates are useful because they quantify the reliability of model estimates — even when no independent hydraulic measurements are available. The second reason for using the bootstrap method was the possibility to carry out calibration and testing of the individual neural networks on complementary subsets of the data. This was possible because the bootstrap randomly selects data with replacement causing $1 - [(N-1)/N]^N$ samples (about 63%) to be selected into each calibration data set. This selection procedure leaves out 37% of the data, which can subsequently be used to test the neural network model. The repetition of calibration-testing procedure for the alternative selections of data ensured a minimal bias towards noise and artifacts in the data.

PTFs H2–H5 and C2 each consist of 60 (water retention) or 100 (saturated and unsaturated conductivity) neural network models. Because they are based on different alternative data selections, each neural network inside a PTF provides slightly different estimates. ROSETTA reports the average of the 60 or 100 estimates as the prediction of a PTF. The standard deviation characterizes the uncertainty of the prediction.

2.4. Characterization of model performance

While testing on a completely independent data set is desirable, we chose to test ROSETTA on the calibration data set because a data set of similar size and characteristics was not available. Further, Schaap and Leij (1998) demonstrated that the performance of a PTF depends on the data sets on which a PTF is calibrated and tested. Usage of an independent data set for testing might introduce artifacts specific to that dataset and make characterization of ROSETTA's properties ambiguous. Finally, the bootstrap procedure ensured robust models that provided similar results for calibration and validation (see Section 2.3 and Schaap and Leij, 1998).

Three error measures were used to characterize ROSETTA. To test the match between predicted and fitted parameters we computed the coefficient of determination (R^2). The root mean square error (RMSE) between measured and estimated water contents, saturated and unsaturated hydraulic conductivities was computed as

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\zeta_i' - \zeta_i)^2} \tag{7}$$

In addition, we computed the mean error (ME) to quantify systematic errors with

$$\mathrm{ME} = \frac{1}{N}\sum_{i=1}^{N}(\zeta_i' - \zeta_i) \tag{8}$$

The symbols ζ and ζ' denote measured or estimated $\theta(h)$, $\log K_s$, or $\log K(h)$ values;N is the number of measurements for which the RMSE and ME values were calculated. The values for RMSE and ME will be given with the subscripts w, s, and u to denote water retention, saturated, and unsaturated hydraulic conductivity, respectively. Estimated water retention or unsaturated hydraulic conductivity values were calculated by evaluating the hydraulic functions at the suctions of the measurements. Because logarithmic values were used for K_s and $K(h)$, the corresponding RMSE and ME values are dimensionless; the units of $\mathrm{RMSE_w}$ and $\mathrm{ME_w}$ are in cm^3 cm^{-3}. In this study, we computed the RMSE and ME values over all available data (i.e. $N_w = 20\,574$ for retention, $N_s = 1306$ for K_s, and $N_u = 4117$

Table 1
R^2 and RMSE values for the five hierarchical models that predict water retention parameters and saturated hydraulic conductivity. SSC: percentages sand, silt and clay; BD: bulk density; θ_{33}, θ_{1500}: water contents at 330 and 15 000 cm suction. The $RMSE_w$ for the direct fit to water retention data is also shown

Model	Input	Water retention					Saturated conductivity	
		R^2				$RMSE_w$ ($cm^3\ cm^{-3}$)	R^2 log K_s	$RMSE_s$ (ME_s) (–)
		θ_r	θ_s	log α	log n			
H1	Textural class	0.066	0.143	0.203	0.452	0.078	0.427	0.739 (−0.001)
H2	SSC	0.086	0.178	0.238	0.473	0.076	0.461	0.717 (−0.001)
H3	SSCBD	0.094	0.581	0.265	0.495	0.068	0.535	0.666 (0.000)
H4	SSCBD θ_{33}	0.121	0.605	0.417	0.599	0.047	0.640	0.586 (−0.004)
H5	SSCBD $\theta_{33}\theta_{15\,000}$	0.387	0.600	0.577	0.760	0.044	0.647	0.581 (−0.002)
Direct fit to data		–	–	–	–	0.012	–	–

for $K(h)$). To investigate how the RMSE and ME values vary with suction, we also computed these values for 10 suction classes between 0, 3.2, 10, 32, 100, 320, 1000, 3200, 10 000, 32 000, and 10 000 cm.

We like to note that the R^2, RMSE and ME values differ from Schaap et al. (1998), Schaap and Leij (1998) and Schaap and Leij (2000). Previously, we averaged R^2 and RMSE values computed for each of the 60 or 100 neural networks inside each PTF (see Section 2.3). This approach was necessary to evaluate the merits of using different sets of predictors. The program ROSETTA, however, reports averages and standard deviations of 60 or 100 sets of estimated hydraulic parameters, as generated by the neural networks inside models H2–H5. To better reflect the errors that result from practical use of Roseta, it is necessary to compute the R^2, RMSE, and ME statistics based on the averages of the estimated hydraulic parameters, rather than providing average error values. To this end, we ran ROSETTA for the entire data set, without considering independent calibration and validation sets. In addition, we do not reduce the degrees of freedom in the computation of RMSE and ME. Previously, such a correction was necessary to compare the RMSE of PTFs with the RMSE of a direct fit of Eq. (1) or (2) to the data. However, a correction for the degrees of freedom is not necessary when the PTFs are applied.

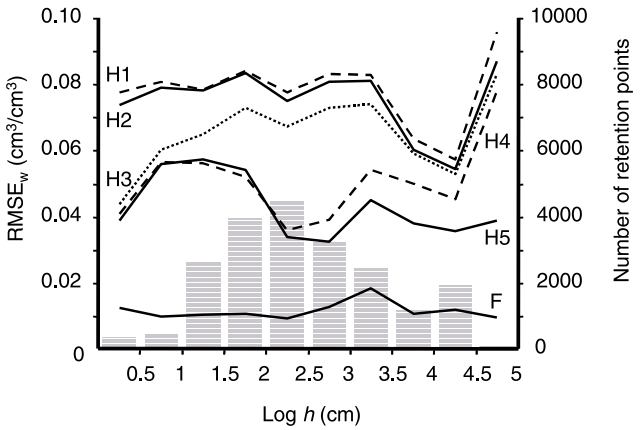

Fig. 2. $RMSE_w$ (lines, left axis) of the direct fit to water retention data (F) and the five hierarchical models (H1–H5). The number of retention points for each suction class is also shown (bars, right axis).

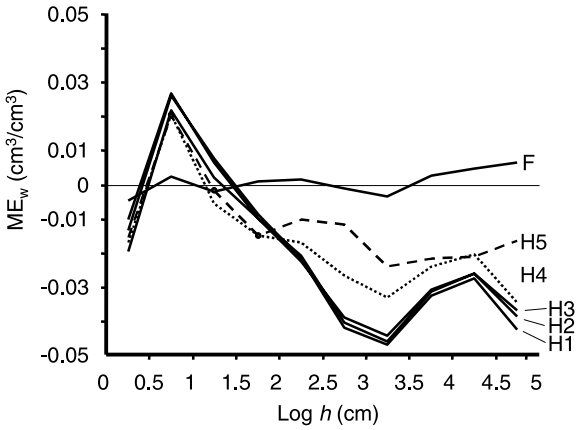

Fig. 3. ME_w of the direct fit to water retention data (F) and the five hierarchical models (H1–H5). A negative value indicates an underestimation of water contents.

3. Results

3.1. Model characteristics

An overview of the performance of the hierarchical models for estimation of water retention parameters and K_s is given in Table 1. Not surprisingly, the results show that correlations between fitted and estimated parameters increase and RMSE values decrease when more predictors are used (H1–H5). Residual water content is difficult to estimate with all models, while saturated water content is difficult to estimate without information about bulk density. The correlation for α increases considerably when one or two retention points are added to the predictors (H4 and H5). The n parameter and K_s generally have the highest correlations showing a gradual increase in R^2 from model H1 to H5.

Table 2
R^2 and $RMSE_k$ values for estimated unsaturated hydraulic conductivity for the MVG model with $K_0 = K_s$ $L = 0.5$, and for model C2 where K_0 and L were estimated from fitted (C2-Fit) or estimated (models C2-H1–C2-H5) retention parameters. The $RMSE_k$ for the direct fit to hydraulic conductivity data is also shown

Model	R^2		$RMSE_K$
	K_0	L	
MVG ($K_0 = K_s$, $L = 0.5$)	–	–	1.40
C2-Fit	0.605	0.548	0.79
C2-H1	0.070	0.001	1.06
C2-H2	0.073	0.007	1.02
C2-H3	0.093	0.012	1.05
C2-H4	0.187	0.019	1.01
C2-H5	0.271	0.327	0.90
Direct fit to data	–	–	0.41

Fig. 2 shows the $RMSE_w$ of models H1–H5 for 10 suction classes as well as the number of water retention points in each class (bars). The $RMSE_w$ of the direct fit of Eq. (1) to the data (F) provides the minimum possible error because no PTF can estimate water retention better than this fit. Models H1 and H2 show a very similar pattern in errors across the entire suction range. This would indicate that there is not much to be gained by using sand, silt or clay percentages as predictors (H2) instead of textural classes (H1). However, model H2 provides continuously varying prections, whereas model H1 exhibits discrete jumps at texture class boundaries. Model H3 shows a considerable improvement near saturation and a better performance until $h = 3200$ cm (i.e. $\log h = 3.5$). Including a water content at 330 cm (H4) lowers $RMSE_w$ between 10 and 10 000 cm, whereas addition of a water content at 15 bar provides a further improvement beyond 100 cm. Because there were only 28 data points with suctions $> 32\,000$ cm the increase in $RMSE_w$ for this suction range may be due to statistical effects.

Fig. 3 shows a similar picture for ME_w; negative numbers denote underestimation by the models. Clearly, the direct fit to the data (F) closely adheres the line of $ME_w = 0$, indicating that Eq. (1) adequately describes retention data over the entire suction range. All models underestimate water retention near saturation ($h < 3.2$ cm suction or $\log h < 0.5$) and overestimate water contents between 3.2 and 10 cm suction; all models underestimate water retention beyond 32 cm. Models H1–H3 all behave similarly, while models H4 and H5 make smaller systematic errors for $h > 100$ cm suction. The systematic errors are probably due to the fact that the neural networks were optimized in terms of Eq. (6) but evaluated according to Eq. (8). Additionally, the nonlinearity of Eq. (1) probably causes a non normal distribution of errors. MEs for K_s are essentially equal to zero (Table 1).

Results for three methods to estimate unsaturated hydraulic conductivity appear in Table 2. The first

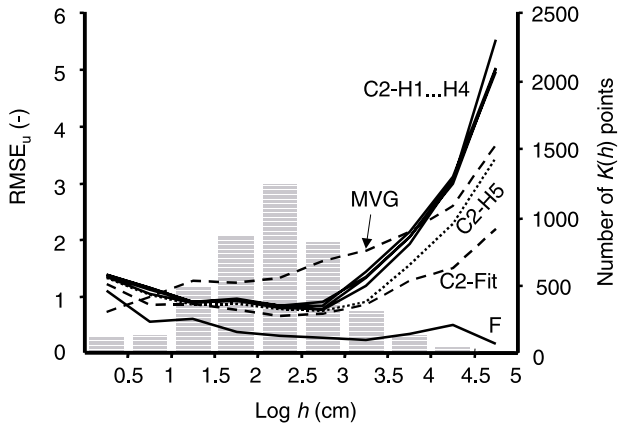

Fig. 4. RMSE$_u$ (lines, left axis) for the direct fit to conductivity data (F), for model C2 using fitted retention parameters (denoted as C2-Fit), model C2 using estimated retention parameters from the hierarchical approach (C2-H1–C2-H5). The MVG model with $K_0 = K_s$ and $L = 0.5$ is shown as MVG. The number of conductivity points per suction class is also shown (bars, right axis).

method is the traditional Mualem–van Genuchten (MVG) model (Eq. (2)) with $K_0 = K_s$ and $L = 0.5$. The second method (C2-Fit) is model C2 of Schaap and Leij (2000) that estimates K_0 and L from fitted retention parameters. This model presumes the availability of fitted retention data. The third method also uses model C2 but with estimated retention parameters derived from models H1 to H5 as input (denoted as C2-H1–C2-H5).

The MVG model clearly provides the poorest estimations of $K(h)$ with an average RMSE$_u$ of 1.40 (i.e. 1.4 order of magnitude). Schaap and Leij (2000) showed that its estimation was especially poor for clayey soils (RMSE$_u$ = 1.70). model C2-Fit has an RMSE$_u$ that is almost half an order of magnitude lower (0.79), while it also has a more uniform performance over all textural classes (see Table 3 in Schaap and Leij, 2000). As models C2-H1–C2-H5 rely on estimated input data, they do not perform as well as model C2-Fit; however, they are better than the MVG model. For example, model C2-H5 has an RMSE$_u$ value that is only slightly higher than that of C2-Fit (0.90 vs. 0.79). Note, however, that the correlations for K_0 and L of models C2-H1–C2-H4 are extremely poor and only slightly better for model C2-H5.

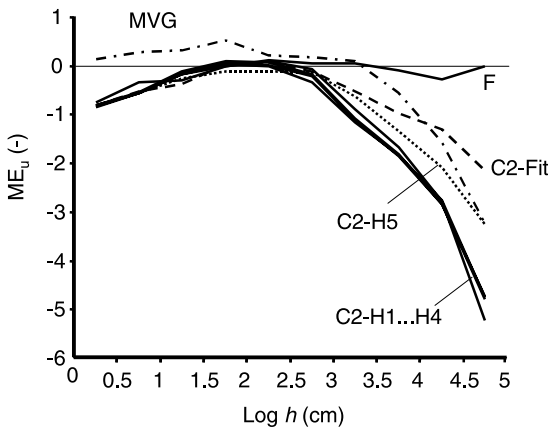

Fig. 5. ME$_u$ for the direct fit to conductivity data (F), for model C2 using fitted retention parameters (C2-Fit), model C2 using estimated retention parameters from the hierarchical approach (C2-H1–C2-H5). The MVG model with $K_0 = K_s$ and $L = 0.5$ is shown as MVG.

Fig. 4 shows the RMSE$_u$ for 10 suction classes as well as the number of conductivity measurements in each class (bars). The direct fit of Eq. (2) to the data (F) indicates the minimum attainable error for all models with a flexible K_0 and L. We note that the direct fit has a relatively large error near saturation. As expected, model C2-Fit has the best overall performance. Model C2-H5 has a very similar performance between $h = 10$ and 3200 cm ($1 < \log h < 3.5$), while models C2-H1–C2-H4 have similar performances in the range between $h = 10$ and 1000 cm. The MVG model has the worst overall performance, except for near saturation where it performs better than all other models because its matching point is K_s and not K_0. The RMSE$_u$ of all models strongly increases beyond 3200 cm where few data points are available.

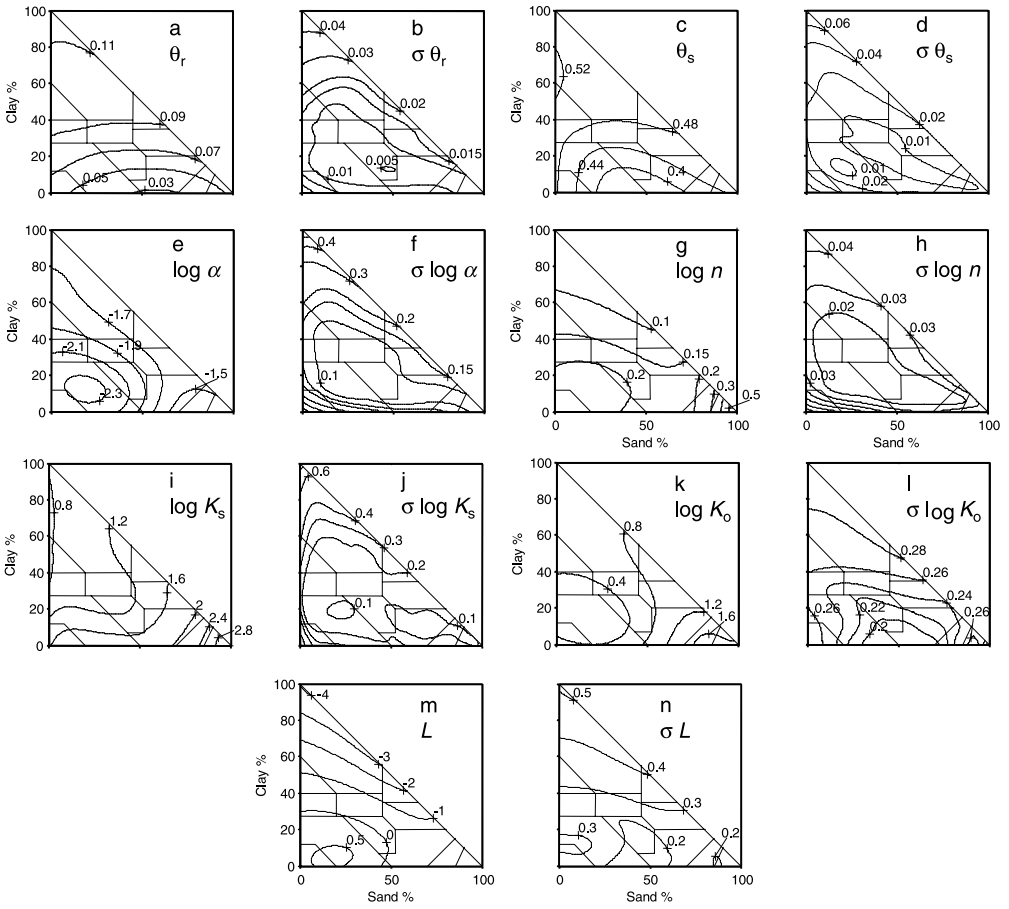

Fig. 6. Distributions of estimated parameter values (a, c, e, g, i, k, m) and associated uncertainties (b, d, f, h, j, l, n) for model H3 and a bulk density of 1.3 g cm^{-3}. Each graph provides the parameter; σ denotes the standard deviation of a parameter. See text for explanation.

Fig. 5 shows the ME for the 10 suction groups; negative values indicate an underestimation of unsaturated hydraulic conductivity. The MVG model overestimates conductivity until $h = 3000$ cm, after which it underestimates conductivity. Models C2-Fit and C2-H1–C2-H5 are all based on fitted K_0 and L, and therefore, they show similar problems of underestimating conductivity between 0 and 32 cm. Again, model C2-Fit has the best performance, followed by model C2-H5. The MEs are near zero between 32 and 1000 cm, but the error rapidly becomes more negative beyond 1000 cm. This effect could be due to the sparse data in this suction range. It is also possible that the problem is the inaccurate estimation of L, which controls the slope of the conductivity curve under dry conditions (Schaap and Leij, 2000).

3.2. Uncertainty estimates

The R^2, RMSE, and ME values can only be estimated when measured hydraulic data are available. When PTFs are applied, such data are typically at hand, thus leaving the user uncertain about the reliability of the PTF. Because we used the bootstrap method for the calibration of the models in ROSETTA, it is possible to estimate standard deviations of the predicted parameters. Although the standard deviation is different from the previously discussed errors, it allows a unique model and input data-specific assessments of the reliability of the parameter estimates. Fig. 6a–n provides predictions by models H3 and C2-H3 for the seven hydraulic parameters and their standard deviations (σ) as a function of texture and a

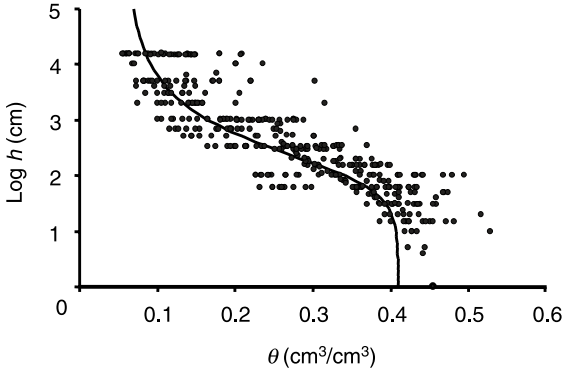

Fig. 7. Water retention data for 47 loam samples (totaling 412 points) with a bulk density range between 1.3 and 1.4 g cm^{-3}. The curve represents the estimation with model H3.

bulk density of 1.3 g cm^{-3}. The parameter values show trends that concur with empirical knowledge. For example, values for α, n and K_s decrease when textures become finer, while at the same time θ_r becomes larger. The standard deviations generally show a pattern that reflects the distribution of data in Fig. 1a–c. The uncertainty increases when less data points are available, such as the silt and clay regions of the textural triangle. Likewise, uncertainties increase when the models are used beyond the calibration range of other predictors in models H1–H5 (results not shown). Fig. 8a–n depict a specific example and should not be used as a general indication of parameter values or uncertainty estimates. Results are most likely different for other bulk densities and for the other models in ROSETTA.

4. Discussion

Even with the best predictive models, i.e. H5 for retention and C2-Fit for unsaturated conductivity, the correlations between estimated and fitted or measured hydraulic parameters were modest at best (cf. Tables 1 and 2). The differences between RMSE and ME values of estimation and direct fits (Figs. 2–5) further suggest that the models in this study could be improved upon. However, the direct fits only give the theoretically minimum attainable errors for PTFs because Eqs. (1) and (2) were fitted to individual characteristics. Therefore, the fit ignores any effects that cause variation among hydraulic properties, such as variability in physical soil properties or systematic differences among measurement methodologies. In contrast, the PTFs are supposed to be valid for the ensemble of all characteristics. This problem is illustrated in Fig. 7, which shows retention data for a narrow selection of 47 loam samples with bulk densities between 1.3 and 1.4 g cm^{-3}. The average retention curve, as estimated by H3, is also shown. We expect to see measured retention data in a narrow band, but the figure shows that there is a considerable scatter. This variation may be caused by predictors other than texture and bulk density or by systematic differences in measurement methodologies.

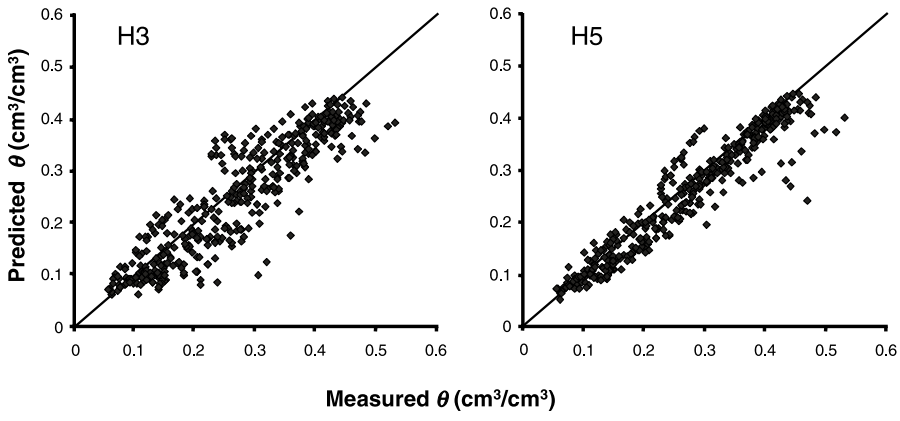

Fig. 8. Estimated vs. measured water contents for model H3 and H5 for 47 loam samples with bulk densities between 1.3 and 1.4 g cm^{-3} (cf. Fig. 8).

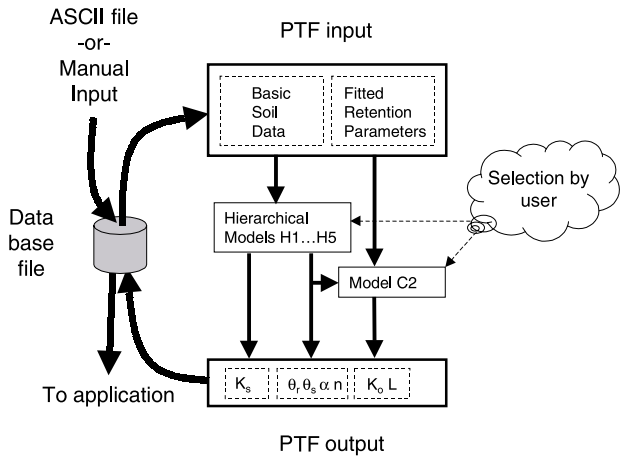

Fig. 9. Schematic overview of the structure of ROSETTA.

Improved PTFs were obtained by Vereecken et al. (1989) and Schaap and Bouten (1996), among others, who used more particle size fractions. Additional predictors can also be used to improve the performance of the models, such as organic matter content, porosity, particle density, soil chemical parameters, soil structure, mineralogy, and pedality (Rawls et al., 1991). However, using more predictors also requires that they be available for both the calibration of PTFs and their actual application. Of course, the determination of additional predictors may take a considerable effort, thereby diminishing the very reason why one would want to use PTFs instead of relying on the direct measurement of hydraulic properties. From this perspective, the inclusion of measured water retention points (Ahuja et al., 1989; Messing 1989; Williams et al., 1992; Schaap and Bouten, 1996) is a pragmatic way to improve the prediction of hydraulic properties by PTFs. One or two water retention points can be viewed as lumped parameters that contain implicit information on hydraulic properties not provided by soil texture or bulk density. In many cases, one or two retention points can be measured relatively quickly or are available in national databases such as the NRCS database, which contains more than 120 000 soil horizons for the USA (Soil Survey Staff, 1995). Using the same data as in Fig. 7, we plotted estimated vs. measured retention points for model H3 and H5 in Fig. 8. While the agreement with the measured data is not perfect, the estimations by model H5 are much better than the estimations by model H3. In the many situations where retention points are simply not available, models H1–H3 may still make acceptable estimations — also considering that these models were calibrated on the same data as models H4 and H5.

The ability of the hydraulic functions (Eqs. (1) and (2)) to match the hydraulic data is another important factor. Figs. 2 and 3 demonstrated that fits of Eq. (1) described water retention data well. For hydraulic conductivity however, we see that the direct fit of Eq. (2) has already large $RMSE_u$ near saturation and a predominantly negative ME_u (Figs. 4 and 5). This indicates that Eq. (2) is incapable of simultaneously fitting the wet and the dry part of the unsaturated hydraulic conductivity curve. As a result, all models based on fitted K_0 and L will perform poorly near saturation. Schaap and Leij (2000) found that the fitted K_0 was often about one order of magnitude lower than the measured K_s value, thus causing a discontinuity in hydraulic conductivity if Eq. (2) is evaluated at saturation. They interpreted this difference in terms of macropores that predominantly influenced K_s and properties of the soil matrix that determined K_0. An improved version of Eq. (2) may need to consider the effects of macropores. Unfortunately, such an effort will be hampered by the limited number of hydraulic conductivity measurements near saturation (Fig. 4).

5. Description of ROSETTA

Named somewhat whimsically after the Rosetta Stone that allowed translation of ancient Egyptian hieroglyphs into Old Greek, ROSETTA allows user-friendly access to models H1–H5 for water retention and saturated hydraulic conductivity and models C2-Fit and C2-H1–C2-H5 for unsaturated hydraulic conductivity. In this section, we will review the most important features of ROSETTA. More information about various aspects of the program and file specifications may be obtained through the help system which can be accessed from anywhere within the program. ROSETTA is primarily a Windows®[1] based application which uses a Microsoft ACCESS 97®[1] database file to store its data and estimations. The Microsoft ACCESS software, however, is not needed to run ROSETTA. Command-line versions of ROSETTA (currently without database support) are available for the MS-DOS®[1] and the LINUX operating systems. ROSETTA can be downloaded freely from the world-wide-web site: .

The flow of data inside ROSETTA is illustrated in Fig. 9. Input data can be entered manually or as a formatted ASCII file. Input and output data are stored in various tables in the same database file and accessed by the program as needed. Basic soil data (sand, silt, and clay percentages, bulk density and the water contents at 330 and 15 000 cm suction) are used by the hierarchical models (H1–H5) to estimate water retention parameters and K_s. Model C2 uses fitted retention parameters to estimate K_0 and L (i.e. C2-Fit), but is also able to use estimated retention as input as illustrated by the model combinations C2-H1–C2-H5 in this study.

The user interface of ROSETTA (not shown) consists of three menu-controlled and easy to understand screens. The first screen provides general database information, i.e. number of records in the database. The second screen serves to make estimations of the seven hydraulic parameters with models H1–H5 and C2-H1–C2-H5. The third screen allows estimations of K_0 and L from fitted retention parameters using model C2-Fit.

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

6. Concluding remarks

This study presents the computer program ROSETTA which implements a number of PTFs for estimation of water retention parameters, the saturated and unsaturated hydraulic conductivity as well as associated uncertainties. The models were characterized in terms of their calibration data sets and the accuracy of their estimations. For the estimation of water retention and saturated hydraulic conductivity, it turned out that the hierarchical models performed reasonably well if more predictors were used (texture, bulk density and one or two retention points). The estimations were less accurate when fewer predictors were used, however, such predictions by these models may still be useful when no data are available. The PTFs provide uncertainty estimates of predicted hydraulic parameters allowing an assessment of ROSETTA's reliability, even when no independent hydraulic data are available.

A previous study (Schaap and Leij, 2000) established models that estimated unsaturated hydraulic conductivity parameters from fitted retention parameters. This study showed that it was also possible to get reasonable estimations of unsaturated hydraulic conductivity using estimated retention parameters derived from the hierarchical models. However, some problems remain in the estimation of unsaturated hydraulic conductivity, notably the poor performance near saturation. Although the new models are better than the 'traditional' MVG model ($K_0 = K_s$ and $L = 0.5$) for suctions higher than a few centimeter, they are unable to deal with a transition from saturated to unsaturated hydraulic conductivity.

ROSETTA offers a user-friendly graphical interface and combines the PTFs with a simple database management structure to facilitate parameter estimates and data management. The program is available at the US Salinity Laboratory's World-Wide-Web site.

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