Comparison of Models for Indirect Estimation of Water Retention and Available Water in Surface Soils

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ABSTRACT

Quantitative knowledge of the unsaturated soil hydraulic properties is required in most studies involving water flow and solute transport in the vadose zone. Unfortunately, direct measurement of such properties is often difficult, expensive and time-consuming. Pedotransfer functions (PTFs) offer a means to estimate soil hydraulic properties based on predictors like texture, bulk density, and other soil variables. In this study, we focus on PTFs for water retention and show that systematic errors in five existing PTFs can be reduced by using water content–based objective functions, instead of parameter value–based objective functions. The alternative analysis was accomplished by establishing offset and slope coefficients for each estimated hydraulic parameter. Subsequently we evaluated these and six other PTFs for estimating water retention parameters using the NRCS soils database. A total of 47 435 records containing 113 970 observed water contents were used to test the PTFs for mean errors and root mean square errors. No overall superior model was found. Models with many calibration parameters or more input variables were not necessarily better than more simple models. All models underestimated water contents, with values ranging from −0.0086 to −0.0279 $cm^3\ cm^{-3}$. Average root mean square errors ranged from 0.0687 $cm^3\ cm^{-3}$ for a PTF that provided textural class average parameters to 0.0315 $cm^3\ cm^{-3}$ for a model that also used two water retention points as predictors. Available soil water content for vegetation was estimated with errors ranging from 0.058 to 0.080 $cm^3\ cm^{-3}$, depending on the model and the definition of available water.

The hydraulic properties of the vadose zone exert a strong control over the movement of water and dissolved solutes between the soil surface and the groundwater table. However, because of their strong nonlinearity, direct measurement of the hydraulic properties (water retention and unsaturated hydraulic conductivity) is difficult, expensive, and subject to considerable experimental limitations. Our ability to obtain meaningful data is further complicated by the fact that the hydraulic properties often exhibit significant spatial variability. These problems indicate the need for PTFs as inexpensive and rapid tools to estimate soil hydraulic properties using indirect methods based on correlations between the hydraulic quantities and other more easily measurable soil or sediment variables, such as the particle-size distribution, bulk density, and/or organic matter content.

The wide variety of PTFs that have been developed in the past (for reviews see Rawls et al., 1991; Wösten et al., 2001) generally have a strong degree of empiricism in that they contain model coefficients that are calibrated on existing soil hydraulic databases. A PTF can be a simple look-up table that gives hydraulic parameters according to textural class (e.g., Carsel and Parrish, 1988), include linear or nonlinear regression equations (Rawls and Brakensiek, 1985; Minasny et al., 1999), or make use of neural network analysis (Pachepsky et al., 1996; Schaap and Bouten, 1996). Most PTFs are intended to be used when no, or at most limited, soil hydraulic data are available. One of the crucial requirements of PTFs is therefore their ability to give reasonable estimates for a wide range of soils. Other important issues include the required input data (which may limit the applicability of a PTF when not available), model complexity (which may determine the ease in which a PTF can be implemented in larger computer models or databases), and desired output data. The first objective of this study was to test 11 PTFs for estimating soil water retention parameters. While these PTFs generally have somewhat larger errors than PTFs that estimate specific retention points (e.g., Schaap and Bouten, 1996; Minasny et al., 1999), they enable the estimation of soil water contents at any pressure head, thus facilitating their use in numerical applications. The PTFs selected in this study were evaluated using the soil survey database of the USDA-NRCS (Soil Survey Staff, 1995) that contains pertinent data about 21 680 soil profiles across the United States. The PTFs were evaluated (i) using measured water contents at several soil water pressure heads and (ii) for their ability to estimate available water content, a parameter that is often required in large-scale hydrological studies.

Before testing the PTFs we first address one subtle issue regarding parameter-based PTFs. Our concern involves the fact that parametric PTFs are often developed using objective functions based on parameter values but evaluated in terms of water contents (the observed quantity). Parametric PTFs are generally constructed in three steps. First, water retention equations are chosen and fitted to observed water content–pressure head data, thereby yielding fitted retention parameters. The objective function used for fitting is usually defined in terms of squared differences between measured and observed water contents, here referred to as a "water content criterion." The second step in the development of para-

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Published in Vadose Zone Journal 3:1455–1463 (2004).

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Abbreviations: AWC, available water content; COS1, Cosby PTF based on univariate regression; COS2, Cosby PTF based on bivariate regression; ME, mean error; PTF, pedotransfer function; RBC, Rawls and Brakensiek PTF with Brooks–Corey parameters; RMSE, root mean square residual; RVG, Rawls and Brakensiek PTF with van Genuchten parameters; URMSE, unbiased root mean square residual; VER, Vereecken PTF; WOE, Wösten PTF.

metric PTFs is the selection of plausible predictors and an appropriate mathematical structure (tables, linear or nonlinear equations, or neural networks) that link the predictors to the fitted retention parameters. In the third step, the PTF coefficients are calibrated, generally using an objective function that is defined in terms of sum of squares of differences between fitted and estimated retention parameters (here called a "parameter criterion"). However, parametric PTFs are often evaluated with a water content criterion (e.g., mean errors or root mean square errors) that is based on observed water retention points. Due to the nonlinearity of the invoked hydraulic functions and the inherent imprecision of PTF estimates, a PTF that provides optimum estimates of parameters may not necessarily give optimum estimates in terms of water contents. For completeness we note that the term *fitted parameter* implies the result of an optimization of a retention function to observed water contents, while *estimated parameter* refers to a PTF estimate.

Scheinost et al. (1997) circumvented the water content vs. parameter criterion problem by calibrating parameter-based PTFs using an objective function that was defined in terms of a water content criterion. For this purpose they substituted simple expressions that estimated retention parameters from texture directly into the van Genuchten (1980) retention equation. The advantage of this approach is that the resulting equation can be optimized directly to a database of observed water retention characteristics. No fitted hydraulic parameters are necessary in this approach, yet they are generated automatically when the PTF is used. Minasny et al. (1999) adopted this method and found its accuracy equivalent to that of a neural network approach.

Unfortunately, because of the mathematical complexity of neural network optimization, it is difficult to employ the approach used by Scheinost et al. (1997) and Minasny et al. (1999) to the neural network models developed by Schaap and Leij (1998) and implemented in the computer program Rosetta (Schaap et al., 2001). Minasny and McBratney (2002) solved this problem by first calibrating a neural network PTF using the parameter criterion, and subsequently reoptimizing the calibrated neural network coefficients with a water content criterion by means of Levenberg–Marquardt optimization. Using this method, called the Neuro-m method, they obtained a 13% better performance than neural network results without the Neuro-m reoptimization.

As a second objective in this study we follow a different approach and assume that retention parameters that are optimal according to the parameter criterion differ only modestly from those that would be optimal according to the water content criterion. We propose the use of simple linear expressions to modify parameters of existing models in Rosetta such that they provide better estimates of the water contents. Although applicable to any parameter-based PTF, we will apply the parameter translation procedure only to the models in Rosetta, using the database that was used for its calibration. The proposed procedure is not applied to the other PTFs since we do not have access to their respective calibration databases.

PEDOTRANSFER FUNCTIONS EVALUATED IN THIS STUDY

This section briefly describes the most important characteristics of the PTFs that are evaluated in this study. Some of these characteristics are represented in Table 1; we refer the reader to the references for more in-depth descriptions of the PTFs. Most of the PTFs are also able to estimate the saturated hydraulic conductivity, and some even the unsaturated conductivity. However, performance for these properties will not be tested in this study since the NRCS database lacks the necessary conductivity data.

Rosetta (Models H1 through H5)

Rosetta (Schaap et al., 2001) may be used to estimate water retention parameters in van Genuchten's (1980) equation, given by

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

where $\theta(h)$ is the measured volumetric water content ($cm^3\ cm^{-3}$) at pressure head h (cm, in this study taken positive for unsaturated conditions), the parameters θ_r and θ_s are residual and saturated water contents, respec-

Table 1. Overview of the most important characteristics of the pedotransfer functions evaluated in this study.†

		Required input									
Model	Reference	Sand	Silt	Clay	ρ_b	OC	Hor	θ_{330}	$\theta_{15\,000}$	Nc	Output	NRCS
												%
H1	Schaap et al. (2001)	x		x						48	VG	100.00
H2		x	x	x						52	VG	100.00
H3		x	x	x	x					58	VG	100.00
H4		x	x	x	x			x		64	VG	99.97
H5		x	x	x	x			x	x	70	VG	99.97
RBC	Rawls and Brakensiek (1985)	x		x	x					35	BC	99.99
RVG		x		x	x					35	VG	99.99
COS1	Cosby et al. (1984)	x		x						6	BC	100.00
COS2		x	x	x						9	BC	100.00
VER	Vereecken et al. (1989)	x		x	x	x				15	VG	97.85
WOE	Wösten et al. (1999)		x	x	x	x	x			44	VG	97.85

† ρ_b, bulk density; OC, organic C or organic matter; Hor, horizon; θ_{330} and $\theta_{15\,000}$, water contents at 330 and 15 000 cm pressure; Nc, number of model coefficients; Output, type of retention function (VG: van Genuchten, BC: Brooks–Corey); NRCS, percentage of the 47 435 selected NRCS records for which a particular model could be run. See text for further explanation.

tively ($cm^3\ cm^{-3}$); α (>0, in cm^{-1}) is related in an approximate manner to the inverse of the air entry pressure, and n (>1) is a pore-size distribution parameter (van Genuchten, 1980). The parameter m is equal to $1 - 1/n$.

Rosetta uses a hierarchical approach that allows users to estimate water retention parameters (θ_r, θ_s, logθ, log$n$) using limited to more extended sets of predictors (Schaap et al., 1998, 2001). The first model (H1) is a class PTF, consisting of a look-up table that provides parameter averages for each USDA soil textural class (see also Table 1). The second model (H2) uses sand, silt, and clay percentages as input and, as opposed to H1, provides hydraulic parameters that vary continuously with texture. The third model (H3) includes bulk density as an additional predictor, while the fourth model (H4) also uses the water content at 330-cm pressure head. The last model (H5) includes the water content at 15 000 cm pressure in addition to the input variables of H4. The choice of pressure heads in models H4 and H5 was determined by their availability in the NRCS database (Soil Survey Staff, 1995). Model H1 provides the mean values of θ_r, θ_s, logα, and log$n$ for each of the 12 USDA textural classes. This model thus contains 48 model coefficients (12 classes $\times$ 4 parameters). Models H2 through H5 provide the same parameters and contain a larger number of coefficients without a well-defined meaning (Schaap and Bouten, 1996). The objective function used for the calibration minimized the variance of all hydraulic parameters simultaneously according to

$$O_p = \sum_{i=1}^{4} \sum_{j=1}^{N} (\zeta_{i,j} - \zeta'_{i,j})^2 \qquad [2]$$

where N is the number of samples and ζ and ζ' are fitted and estimated parameters (θ_r, θ_s, $\log_{10}\alpha$, $\log_{10}n$, indexed by i), respectively.

Modified Rosetta Models (Models H1m through H5m)

We employ a parameter modification procedure based on the hypothesis that the parameter estimates obtained with Models H1 through H5 can be modified to Models H1m through H5m, such that a minimum error in terms of water contents can be obtained. We assume that a simple linear translation of the estimated parameters is sufficient to reach the minimum variance between estimated and observed water contents. For this purpose, each of the estimated retention parameters ζ'_i is modified to ζ''_i according to

$$\zeta''_i = a_i + b_i\zeta'_i \qquad [3]$$

Each retention parameter and each PTF H1m through H5m has its own parameters a_i and b_i. Using the original calibration database employed for models H1 through H5 with 2134 samples and 20 574 individual retention points (Schaap and Leij, 1998; Schaap et al., 2001; a textural distribution is given in Fig. 1), we simultaneously optimized parameters a_i and b_i for all four retention parameters for each PTF using the objective function

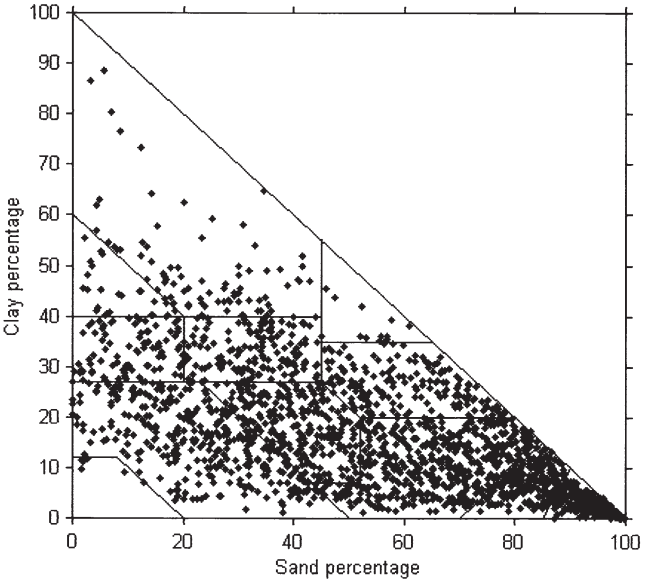

Fig. 1. Textural distribution of the 2134 samples used to calibrate Models H1 through H5. The textural classes are given in Fig. 2.

$$O_i = \sum_{i=1}^{M} \sum_{i=1}^{N} [\theta_{i,j} - \theta'(h_j, \theta''_{r,i}, \theta''_{s,i}, \alpha''_i, n''_i)]^2 \qquad [4]$$

where M is the number of water retention characteristic, N the number of measured points for each retention characteristic, and θ and θ' are measured and estimated (with modified parameters) water contents, respectively. The offset parameter a_i for θ_r was set to zero to constrain θ_r to positive residual water contents. Higher-order alternatives (e.g., polynomials) to Eq. [3] were also considered but were more difficult to optimize and often yielded nonunique coefficients. Although the outlined procedure leads to different retention parameter values, we stress that all parameters retain their traditional meaning.

Rawls and Brakensiek (RBC and RVG)

Rawls and Brakensiek (1985) presented a multivariate PTF for estimating parameters of the Brooks and Corey (1964) equation, given by

$$\theta(h) = \begin{cases} \theta_s & h \le h_b \\ \theta_r + (\theta_s - \theta_r)\left(\dfrac{h_b}{h}\right)^{\lambda} & h > h_b \end{cases} \qquad [5]$$

where h_b is the air entry pressure head, and λ a pore-size distribution parameter comparable to n in Eq. [1]. Input variables to the model, here identified as RBC, are porosity, and sand and clay percentages. The saturated water content was not directly estimated with this PTF but set equal to the porosity, ϕ. In this study the porosity is derived from the bulk density (ρ_b) as $\phi = 1 - \rho_b/2.65$, where 2.65 is the assumed density of the solid phase ($g\ cm^{-3}$). In addition to the RBC model, Rawls and Brakensiek (1985) presented a conversion of Brooks–Corey parameters to van Genuchten parameters, assuming the approximations $\alpha = 1/h_b$ and $n = \lambda + 1$. This version of the RBC model will be referred to as RVG. Although Rawls and Brakensiek (1985) indicated that

their models were valid for sand contents between 5 and 70% and clay contents between 5 and 60%, we applied their models to all selected data. Reasons for this were that the differences in errors were minor (not further shown here) and because otherwise only 71.5% of the selected NRCS data could be evaluated. Although no explicit statement was found in Rawls and Brakensiek (1985) and related publications, we assume that their calibration database contained several thousands of samples from agricultural soils in the USA.

Cosby (COS1 and COS2)

Cosby et al. (1984) presented two PTFs based on univariate or bivariate regression, identified as COS1 and COS2, respectively. The models are very simple—they contain only six or nine regression parameters in total—and estimate parameters of the Campbell (1974) water retention equation. For the purposes of this study we inverted the Campbell equation to yield the Brooks–Corey (1964) equation, but with θ_r in Eq. [5] set to 0. Cosby et al. (1984) calibrated their PTFs using data derived from Holtan et al. (1968) and Rawls et al. (1976), totaling 1448 soil samples.

Vereecken (VER)

Vereecken et al. (1989) presented several regression equations for estimating parameters in a modified van Genuchten curve in which $m = 1$ and $n > 0$ (Eq. [1]). The model we selected (referred to as VER) uses sand and clay percentages, bulk density, and organic C content as input. Another model by Vereecken et al. (1989) relied on principal component analysis of the textural distribution, but it could not be tested in this study because the required data were not available. We note here that estimates of the α and n parameters in Vereecken et al. (1989) are based on natural logarithms, not base 10 logarithms, as suggested in the publication. The VER model was calibrated using data from duplicate samples derived from 182 soil horizons in northern Belgium.

Wösten (WOE)

Based on an analysis of the European soil hydraulic database HYPRES, Wösten et al. (1999) presented a PTF for estimating van Genuchten parameters. The multivariate model with 44 parameters estimates θ_s, α, and n (as well as parameters in the Mualem–van Genuchten equation) using silt, clay, organic matter content, bulk density, and the Boolean variable "topsoil" vs. "subsoil." In this study θ_r was set to 0.01 (Wösten et al., 1999) and the organic matter content was estimated by multiplying the organic C content with 1.72 (Nelson and Sommers, 1982). Wösten et al. (1999) classified all A and E horizons as topsoils. For the purposes of this study we assumed topsoils for all samples taken at depths shallower than 30 cm.

THE NRCS SOIL CHARACTERIZATION DATABASE

The NRCS soil characterization database (Soil Survey Staff, 1995) contains detailed data of 21 680 soil profiles across the USA and served to test all PTFs selected for this study. The data are available on a soil horizon basis, totaling 136 620 records involving some 250 possible attributes covering a broad range of soil physical, chemical, and mineralogical characteristics. No single record contains a complete set of data and, unfortunately, only a limited number of water contents are available. Water retention at 15 000 cm is available for 90.1% of the samples in the NRCS database, while the 330 cm water content is available for 37.1% of the cases. Water contents at 60, 100, 1000, and 2000 cm are only available for a small fraction of the database. All retention data were measured using pressure plates, with the 60-, 100-, and 330-cm water contents obtained on undisturbed clods (w6cld, w10cld, w3cld, respectively, in Soil Survey Staff 1995). The water contents at 1000, 2000, and 15 000 cm (w1bair, w2bair, w15ad, respectively, in Soil Survey Staff, 1995) were measured on initially air-dry sieved samples. We refer the reader to Soil Survey Staff (1996) for more information. Water contents in the NRCS database are given on a gravimetric basis and were converted to volumetric units using the bulk density measured at 330 cm pressure (db_13b, Soil Survey Staff 1995).

To test the selected PTFs we required that at least soil texture, bulk density, and the 330- and 15 000-cm water contents were available. As shown in Table 1, not all data could be used for all PTFs. Most often this was due to missing organic C data (needed for the VER and WOE models), low or extremely high bulk densities (densities <0.5 and >2.0 g cm^{-3} were excluded) or inconsistent data (e.g., sometimes the volumetric water content at 330 cm was smaller than that at 15 000 cm). Occasionally unrealistically high volumetric water contents were found (e.g., >1 cm^3 cm^{-3}), presumably due to data entry errors in the NRCS database. To prevent unreasonable results, we required that all volumetric water contents should be smaller than 0.6 cm^3 cm^{-3}, a reasonable assumption given that the smallest available pressure head in the NRCS database was 60 cm. Together with other constraints on the data, this left 47 435 records and 113 970 water retention points for testing of the PTFs. We note that most retention points were located at 330- and 15 000-cm pressure heads; values at 60, 100, and 1000 cm were available for only 2.7, 15.4, and 0.7% of the selected records, respectively. A textural distribution of the selected NRCS data appears in Fig. 2. Note that these data are presented in the somewhat unusual unit of number of samples per square percentage. Plotting all individual points as in Fig. 1 would have made the graph unreadable.

EVALUATION CRITERIA

Three criteria were used to quantify errors in the PTF estimates of the water contents. The most commonly used criterion in PTF-related work is probably the root mean square residual (RMSE), defined as

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\theta' - \theta)^2} \qquad [6]$$

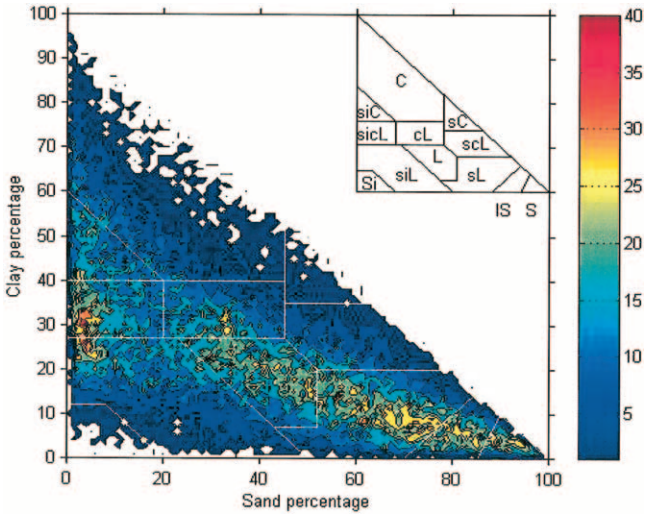

Fig. 2. Textural distribution of 47 435 samples used to evaluate the pedotransfer functions selected for this study. Displayed is the number of samples at intervals of 1, 5, 10, 15, 20 samples per square percentage. S, sand; lS, loamy sand; sL, sandy loam; scL, sandy clay loam; sC, sandy clay; L, loam; siL, silty loam; Si, silt; sicL, silty clay loam; siC, silty clay; cL, clay loam; C, clay.

where N is the size of the (sub)set of observations for which the RMSE is computed, and θ_i and θ_i' are measured and estimated water contents, respectively. The value of θ_i' is computed by evaluating the appropriate retention function at the observed pressure head with the estimated retention parameters. The RMSE may be viewed as giving the accuracy of the model in terms of standard deviations.

When systematic errors exist, the RMSE values are biased and do not reflect the true zero-mean variance. Systematic errors are often an artifact of the calibration database (Schaap and Leij, 1998) and could render a comparison of PTFs based on RMSE values difficult. We therefore decompose the RMSE into a mean error and an unbiased RMSE (Hastie et al., 2001).

Mean errors (ME) may be used to quantify systematic errors between measurements and model estimations:

$$\mathrm{ME} = \frac{1}{N}\sum_{i=1}^{N}(\theta' - \theta) \qquad [7]$$

ME values are negative when the PTF underestimates water contents. Unbiased RMSE (URMSE) values were used by Tietje and Hennings (1996) and have the mean errors removed according to

$$\mathrm{URMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}[(\theta' - \mathrm{ME}) - \theta]^2} \qquad [8]$$

URMSE values should always be equal to or smaller than the corresponding RMSE values; RMSE, ME, and URMSE values in this study are all given in cubic centimeters per cubic centimeter.

RESULTS AND DISCUSSION

Modification of the Parameters Estimated by Models H1 through H5

Figure 3 shows the mean errors for nine pressure head classes available in the calibration database (between boundaries at 0, 3, 10, 30, 100, 300, 1000, 3000, 10 000, and 30 000 cm) for the original H1 through H5 models (Fig. 3a) and after parameter modification (Fig. 3b). Also shown are the results of the direct fit of the van Genuchten equation (Eq. [1]) to the data (FIT). The direct fit shows no large systematic errors in this pressure range, indicating that water retention can be described adequately with Eq. [1]. However, the mean errors of H1 through H4 before modification were considerable (between −0.045 and 0.025 $cm^3\ cm^{-3}$). Water contents for pressure heads smaller than 3 cm were underestimated, overestimations are present between 3 and 10 cm, and strong underestimations are found beyond 30 cm. The patterns exhibited by H1 through H3 are virtually identical, indicating that the algorithm used for PTF development (textural class averages for H1 vs. a neural network approach for H2 and H3) is not the cause of the systematic errors. Models H4 and H5 have less severe systematic errors since they use one or two measured retention points as input. The parameter modification procedure removed most systematic errors for pressure heads higher than 30 cm (Fig. 3b). However, the systematic errors were not removed near saturation; that is, the underestimations between 0 and 3 cm and the overestimations between 3 and 10 cm remained. The modified PTFs H1m through H5m estimate retention near saturation with a pressure-dependent database average bias between −0.02 and 0.02 $cm^3\ cm^{-3}$.

Table 2 provides the coefficients found for the parameter modifications (Eq. [3]) as well as ME and RMSE values for the original and modified models. By far the strongest effect is seen for the parameter n in Eq. [1]; the slope coefficient for this parameter ranges from 0.655 for Model H2 to 0.877 for Model H5. These results indicate that the modified $\log_{10}n$ values were reduced substantially with regard to the original values. The effect of this change is that, especially for higher pressure heads, estimated water contents will be higher than before, which in turn, leads to smaller underestimations (Fig. 3b). Smaller changes in offset and slope (relative to 0 and 1, respectively) were found for the other retention parameters. Most likely these changes account for correlations that are commonly present among water retention parameters—when n is modified, changes in the other parameters are necessary to maintain a good match with observed water retention data. Table 2 shows that mean errors are one (H5 vs. H5m) to almost two orders (H1 vs. H1m) of magnitude smaller for the modified parameters compared with the original estimates. Corresponding RMSE values were reduced modestly: approximately 0.005 (H5m) to 0.008 (H2m) $cm^3\ cm^{-3}$ compared with the original models. Expressed in percentages the reductions in RMSE ranged between 8% (H1m and H2m) and 13% (H4m). These reductions are very similar to those found by Minasny and McBratney (2002) for the Neuro-m method for reoptimization of neural network–based PTFs. Because of the reduced errors (especially for ME), we will use Models H1m through H5m in the remainder of this study rather than H1 through H5.

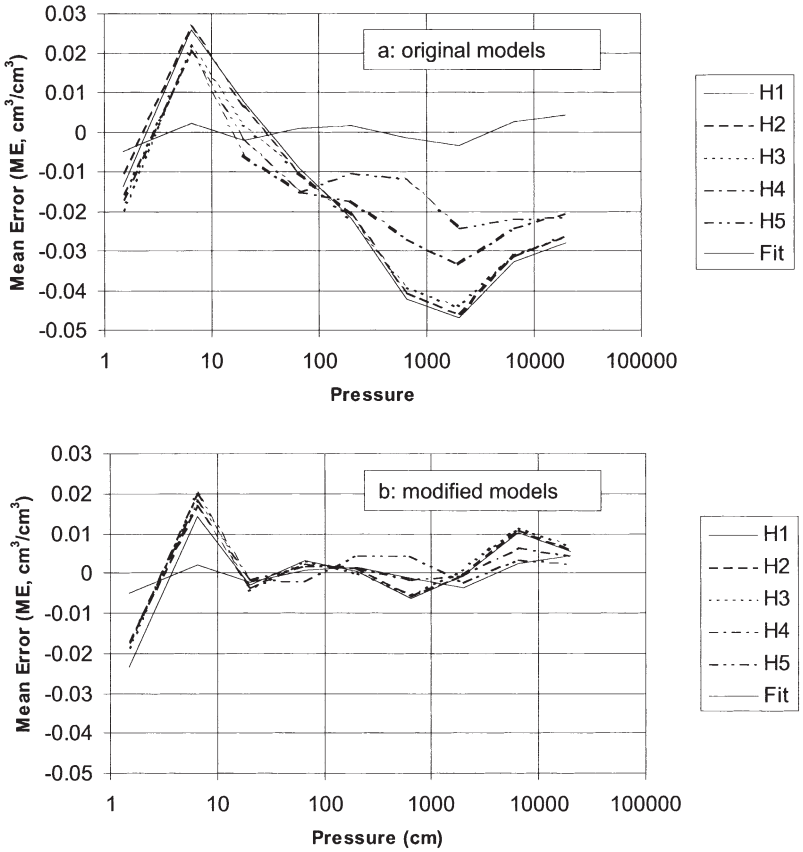

Fig. 3. Mean errors for the H1 through H5 models in Rosetta (a) before and (b) after parameter transformation. The mean errors were computed for nine pressure head classes with boundaries at 0, 3, 10, 100, 300, 1000, 3000, 10 000, and 30 000 cm. The results were plotted at the midpoint of each pressure class (e.g., 1.5, 6.5, 20, 65 cm). For reference, the direct fit to the original retention data is also shown (FIT).

Evaluation of PTFs on Data from the NRCS Database

Table 3 shows ME and URMSE results for the 11 PTFs for six different pressure heads for the NRCS soil characterization database. Also shown are the average ME, URMSE, and RMSE errors, weighted according to the number of observations for each pressure head. Note that only few observations were available for the 60- and 1000-cm pressure heads, whereas more observations were available for 100 and 2000 cm (7562 and 10431 data points, respectively). Most or all water contents at 330 and 15 000 cm could be used for our analysis.

The weighted ME values show that all models underestimated water retention with values ranging from -0.0279 cm^3 cm^{-3} for H1m to -0.0043 cm^3 cm^{-3} for COS2. This underestimation may be a result of an overestimation of measured volumetric water contents, which were derived from gravimetric water contents and the bulk density at a pressure head of 330 cm (see the section about the NRCS database). For individual water retention points the most negative ME (-0.0421 cm^3 cm^{-3}) was found for the RVG model at 330 cm, while the largest ME (0.0118 cm^3 cm^{-3}) was found for Model H5m at 60 cm. Table 3 also substantiates setting θ_s to the porosity, ϕ, in the RBC and RVG models. Both models show negative ME values at 60 cm. If we had accounted for air entrapment (e.g., by assuming $\theta_s = \beta\phi$, with $\beta < 1$), a more negative ME would have resulted. Table 3 also shows that setting θ_r to zero (COS1, COS2) or to a small value (WOE) does not lead to large ME values at 15 000 cm. The COS1 and COS2 models even slightly overestimated water contents at this pressure head. The COS1 and VER models were also tested by Kern (1995) using a smaller subset of the NRCS database for pressure heads at 100, 330, and 15 000 cm. Our ME values for the COS1 model are somewhat smaller

Table 2. Translation coefficients for Models H1 through H5 for the van Genuchten (1980) water retention parameters for Rosetta's calibration database (Schaap and Leij 1998). Mean errors (ME) and biased root mean square residuals (RMSE) for original and modified models are also shown. The offset parameter for θ_r was set to zero (see text).

	Offset parameters (a_i)			Slope parameters (b_i)				Original		Modified	
	θ_s	$\log_{10}\alpha$	$\log_{10}n$	θ_r	θ_s	$\log_{10}\alpha$	$\log_{10}n$	ME	RMSE	ME	RMSE
H1	−0.013	0.198	−0.003	0.957	1.008	1.086	0.696	−0.022	0.078	0.0003	0.072
H2	−0.048	0.159	0.004	0.969	1.103	1.050	0.655	−0.021	0.076	0.0006	0.070
H3	0.002	0.162	0.003	0.995	1.000	1.028	0.660	−0.022	0.068	0.0008	0.060
H4	0.011	0.067	0.006	1.156	0.974	1.039	0.796	−0.019	0.047	0.0010	0.041
H5	−0.020	−0.040	−0.003	1.220	1.045	0.956	0.877	−0.013	0.044	0.0013	0.039

Table 3. Mean error (ME) and unbiased root mean square errors (URMSE) for six retention points. Also listed are the number of available water contents per pressure (N_{obs}) and the weighted ME, URMSE, and (biased) RMSE errors (in italics) for the characteristics. Negative ME values indicate underestimated water contents.

Pressure (cm):	60	100	330	1000	2000	15000	Weighted error	
N_{obs}:	1288	7309	47162	352	10429	47435		
				ME				
				cm³ cm⁻³				
H1m	−0.0057	−0.0198	−0.0326	0.0053	−0.0398	−0.0227	*−0.0279*	–
H2m	−0.0018	−0.0168	−0.0278	0.0014	−0.0352	−0.0197	*−0.0240*	–
H3m	−0.0131	−0.0158	−0.0334	−0.0144	−0.0408	−0.0209	*−0.0275*	–
H4m	0.0076	0.0047	−0.0110	0.0068	−0.0303	−0.0173	*−0.0141*	–
H5m	0.0118	0.0116	−0.0045	0.0077	−0.0231	−0.0133	*−0.0086*	–
RBC	−0.0036	−0.0228	−0.0385	−0.0246	−0.0298	−0.0074	*−0.0233*	–
RVG	−0.0235	−0.0339	−0.0421	−0.0251	−0.0301	−0.0074	*−0.0258*	–
COS1	0.0023	−0.0181	−0.0207	0.0035	−0.0060	0.0043	*−0.0084*	–
COS2	0.0090	−0.0118	−0.0153	0.0102	−0.0021	0.0069	*−0.0043*	–
VER	−0.0071	−0.0090	−0.0220	−0.0145	−0.0127	0.0107	*−0.0065*	–
WOE	−0.0154	−0.0153	−0.0233	−0.0077	−0.0137	−0.0025	*−0.0131*	–
				URMSE				RMSE
				cm³ cm⁻³				
H1m	0.0713	0.0809	0.0706	0.0557	0.0611	0.0493	*0.0625*	*0.0687*
H2m	0.0693	0.0776	0.0666	0.0503	0.0561	0.0452	*0.0585*	*0.0635*
H3m	0.0696	0.0789	0.0609	0.0519	0.0617	0.0477	*0.0574*	*0.0641*
H4m	0.0497	0.0485	0.0219	0.0559	0.0599	0.0452	*0.0396*	*0.0427*
H5m	0.0519	0.0516	0.0207	0.0496	0.0469	0.0252	*0.0292*	*0.0315*
RBC	0.0737	0.0824	0.0674	0.0376	0.0494	0.0398	*0.0571*	*0.0634*
RVG	0.0687	0.0798	0.0662	0.0379	0.0495	0.0398	*0.0562*	*0.0639*
COS1	0.0758	0.0832	0.0709	0.0344	0.0485	0.0433	*0.0599*	*0.0616*
COS2	0.0754	0.0829	0.0719	0.0381	0.0522	0.0464	*0.0616*	*0.0626*
VER	0.0699	0.0867	0.0730	0.0332	0.0575	0.0491	*0.0636*	*0.0657*
WOE	0.07	0.0795	0.0610	0.0367	0.0522	0.0437	*0.0551*	*0.0575*

than those found by Kern (1995) while the results for the VER model are somewhat worse. Tietje and Tapkenhinrichs (1993) also found underestimated water contents in their evaluation of the COS2, RBC, and VER models on a German dataset.

Models that did not include water retention points showed weighted URMSE values ranging from 0.0551 (WOE) to 0.0636 cm³ cm⁻³ (VER). Corresponding (biased) RMSE values ranged from 0.0575 to 0.0657 cm³ cm⁻³, respectively; however, in this case PTF H1m had a slightly higher error (0.0687 cm³ cm⁻³) than the VER PTF. Excluding H4m and H5m, all models produced the largest URMSE values at 100 cm. This pressure head is located near the steepest decrease in water contents for most water retention curves. Relatively small errors in estimated α or h_b can therefore cause large URMSE errors. The weighted URMSE errors decreased to 0.0396 and 0.0292 cm³ cm⁻³ when one (H4m) or two (H5m) retention points were included, respectively. Of course, much of this decrease is realized at the included retention points (at 330 and 15 000 cm), but the URMSE values at most other pressures also decreased significantly. RMSE errors for the (modified) Models H1m through H5m were generally comparable to those for Rosetta's calibration database, presented in Table 2.

Estimation of Available Water Content

Knowledge of the available water content is useful in applications that involve plants, such as regional or global change soil–vegetation–atmosphere coupling studies, or for agricultural purposes. The available water content is loosely defined as the difference between the water content at the pressure head where gravity drainage becomes negligible (known as field capacity) and the permanent wilting point. The latter value is often defined at 15 000-cm pressure. Since different pressure heads for field capacity are commonly used, we evaluated the models for three available water contents: 60–15 000 cm (AWC1, 1288 pairs of points), 100–15 000 cm (AWC2, 7309 pairs), and 330–15 000 cm (AWC3, 47 162 pairs).

The results in Table 4 show that, in general, most

Table 4. Available water content (AWC) for three pressure differences; negative mean errors (MEs) indicate underestimated available water contents.

	AWC1 60–15 000 cm	AWC2 100–15 000 cm	AWC3 330–15 000 cm
		ME	
		cm³ cm⁻³	
H1m	0.0086	−0.0089	−0.0103
H2m	0.0102	−0.0067	−0.0084
H3m	0.0011	−0.0053	−0.0127
H4m	0.0173	0.0110	0.0063
H5m	0.0197	0.0175	0.0085
RBC	0.0009	−0.0198	−0.0313
RVG	−0.0189	−0.0310	−0.0349
COS1	−0.0043	−0.0218	−0.0253
COS2	−0.0007	−0.0177	−0.0226
VER	−0.0114	−0.0181	−0.0328
WOE	−0.0105	−0.0115	−0.0210
		RMSE	
		cm³ cm⁻³	
H1m	0.0746	0.0765	0.0626
H2m	0.0745	0.0751	0.0612
H3m	0.0731	0.0761	0.0578
H4m	0.0637	0.0617	0.0393
H5m	0.0531	0.0512	0.0174
RBC	0.0728	0.0779	0.0663
RVG	0.0692	0.0785	0.0671
COS1	0.0689	0.0764	0.0650
COS2	0.0668	0.0739	0.0629
VER	0.0677	0.0798	0.0680
WOE	0.0656	0.0735	0.0575

PTFs underestimated available water content values. Although Models H4m and H5m overestimate field capacity only slightly, these models are not likely to be practical for estimating of available water contents since in those situations the available water content can be calculated directly from the water content data used as input to these models. Models H3m, RBC, and COS2 provided the lowest ME values for AWC1. Models H1m through H5m generally gave the best ME values for AWC2 and AWC3. Root mean square residuals, however, are considerable. Except for H4m and H5m, the RMSE for AWC1 ranged from 0.0575 to 0.0798 cm^3 cm^{-3}. It appears that Models H1m through H3m perform slightly worse for AWC1; for AWC2 and AWC3 little difference exists among the models. The WOE model seems to slightly outperform the other PTFs for applications involving available water.

SUMMARY AND CONCLUSION

In this study, we improved a sequence of hierarchical PTFs by modifying parameter estimates from an optimum in terms of variance between fitted and estimated parameters to an optimum in terms of variance between estimated and observed water contents. The modification was accomplished by using simple linear equations that modified the original estimates with an offset and a slope. The largest change was found for parameter *n*, whereas smaller changes were necessary for the other retention parameters. The procedure resulted in substantial reductions in the systematic errors. An average underestimation of about 0.02 cm^3 cm^{-3} was reduced to less than 0.0015 cm^3 cm^{-3}. The error in terms of root-mean-square residuals was reduced by about 0.005 to 0.008 cm^3 cm^{-3}. The modification procedure was found to be simple, flexible, and can potentially be used for other models.

As we noted in a previous study (Schaap and Leij, 1998), the performance of a PTF depends strongly on the databases being used for PTF calibration and testing. The heuristic procedure outlined here makes it possible to modify existing PTFs toward characteristics of particular datasets. A potential application is to take a calibrated PTF (e.g., any of the 11 models used in this study) and modify its output using a smaller database of site-specific local data. This would be beneficial in two ways. First, it is not necessary to invoke the complete PTF development procedure for site-specific data. Pedotransfer function development for small data sets is often problematic because the size of the available database may limit the statistical reliability of the PTFs. Second, insight obtained in the calibration of the original PTFs is largely retained since the parameter modification procedure makes only minor changes to the estimated parameters. Within this context we also mention Bayesian modeling of PTFs (e.g., Meyer et al., 1999), which offers a more formal way to accomplish the use of prior information (the existing PTFs) with new or site-specific data.

The modified models were evaluated on selected records from the NRCS soil characterization database and compared with six previously published PTFs (see Table 1). Given the range in complexity of the models that were evaluated in this study, we were somewhat surprised to find relatively small differences in performance among the models. It is therefore difficult to identify a superior PTF. Model complexity, required input variables, and overall model precision all play a role. The COS1, COS2, and VER models are by far the most simple in terms of model complexity, yet these models do not necessarily perform much worse than other models. In terms of input data, Model H1m may be the most attractive since it requires only the USDA textural class, which is readily available or may be estimated in the field by experienced soil surveyors. Next are Models H2m, COS1, and COS2, which require sand, silt, and clay percentages. For this group of PTFs, Model H2m provides the lowest URMSE, but a higher ME. Models H3m, RVG, RBC, VER, and WOE additionally require bulk density and, in the case of VER and WOE, also organic C or organic matter content. With the possible exception of the WOE model, this group does not necessarily provide smaller errors than the PTFs based on only sand, silt, and clay. We previously showed (Schaap et al., 2001) that PTFs that use bulk density probably perform better near saturation. Unfortunately, no water retention points below a pressure head of 60 cm were available in the NRCS database to test this assertion. Models H4m and H5m require measured water contents and, although more accurate, they may generally be the most difficult to implement in practice. However, the relatively good performance of these models indicates that they can be used to generate complete water retention curves for a large part of the NRCS database. Other PTFs may be used for records where the required input water contents at pressure heads of 330 and 15 000 cm are missing. In addition, the hierarchical Models H1m through H5m are also able to estimate saturated and unsaturated conductivities (Schaap and Leij, 2000; Schaap et al., 2001). The modified models can thus be used to populate the NRCS database with a complete set of hydraulic parameters, and consequently increase the usefulness of this database for a large number of applications.

ACKNOWLEDGMENTS

The authors gratefully acknowledge the support by NSF and NASA (EAR-9804902), the ARO (39153-EV), and the SAHRA science and technology center under a grant from NSF (EAR-9876800).

REFERENCES

Brooks, R.H., and A.T. Corey. 1964. Hydraulic properties of porous media. Hydrol. Paper 3. Colorado State Univ., Fort Collins, CO.

Campbell, G.S. 1974. A simple method for determining unsaturated hydraulic conductivity from moisture retention data. Soil Sci. 117: 311–314.

Carsel, R.F., and R.S. Parrish. 1988. Developing joint probability distributions of soil water retention characteristics. Water Resour. Res. 24:755–769.

Cosby, B.J., G.M. Hornberger, R.B. Clapp, and T.R. Ginn. 1984. A statistical exploration of the relationships of soil moisture charac-

teristics to the physical properties of soils. Water Resour. Res. 20: 683–690.
Hastie, T., R. Tibshirani, and J. Friedmann. 2001. The elements of statistical learning. Springer, New York.
Holtan, H.N., C.B. England, G.P. Lawless, and G.A. Schumaker. 1968. Moisture-tension data for selected soils on experimental watersheds. Rep. ARS 41-144. USDA-ARS, Beltsville, MD.
Kern, J.S. 1995. Evaluation of soil water retention models based on basic soil physical properties. Soil Sci. Soc. Am. J. 59:1134–1141.
Meyer, P.D., G.W. Gee, M.L. Rockhold, and M.G. Schaap. 1999. Characterization of soil hydraulic parameter uncertainty. p. 1439–1451. *In* M.Th. van Genuchten et al. (ed.) Proc. Int. Workshop, Characterization and Measurements of the Hydraulic Properties of Unsaturated Porous Media. University of California, Riverside.
Minasny, B., A.B. McBratney, and K. Bristow. 1999. Comparison of different approaches to the development of pedotransfer functions for water-retention curves. Geoderma 93:225–253.
Minasny, B., and A.B. McBratney. 2002. The Neuro-m method for fitting neural network parametric pedotransfer functions. Soil Sci. Soc. Am. J. 66:352–361.
Nelson, D.W., and L.E. Sommers. 1982. Total carbon, organic carbon, and organic matter. p. 539–579. *In* A.L. Page et al. (ed.) Methods of soil analysis. Part 2. 2nd ed. ASA and SSSA, Madison, WI.
Pachepsky, Ya., D. Timlin, and G. Varallyay. 1996. Artificial neural networks to estimate soil water retention from easily measurable data. Soil Sci. Soc. Am. J. 60:727–733.
Rawls, W.J., P. Yates, and L. Asmussen, 1976. Calibration of selected infiltration equations for the Georgia Coastal Plain. Rep. USDA-ARS-S-113. USDA-ARS, Beltsville, MD.
Rawls, W.J., and D.L. Brakensiek. 1985. Prediction of soil water properties for hydrologic modeling. p. 293–299. *In* E.B. Jones and T.J. Ward (ed.) Watershed Management in the Eighties. Proc. Irrig. Drain. Div., ASCE, Denver, CO. 30 Apr.–1 May 1985. ASCE, New York.
Rawls, W.J., T.J. Gish, and D.L Brakensiek. 1991. Estimating soil water retention from soil physical properties and characteristics. p. 213–233. *In* B.A. Stewart (ed.) Advances in soil science. Springer-Verlag, New York.
Schaap, M.G., and W. Bouten. 1996. Modeling water retention curves of sandy soils using neural networks. Water Resour. Res. 32:3033–3040.
Schaap, M.G., F.J. Leij, and M.Th. van Genuchten. 1998. Neural network analysis for hierarchical prediction of soil water retention and saturated hydraulic conductivity. Soil Sci. Soc. Am. J. 62:847–855.
Schaap, M.G., and F.J. Leij. 1998. Database related accuracy and uncertainty of pedotransfer functions. Soil Sci. 163:765–779.
Schaap, M.G., and F.J. Leij. 2000. Improved prediction of unsaturated hydraulic conductivity with the Mualem-van Genuchten model. Soil Sci. Soc. Am. J. 64:843–851.
Schaap, M.G., F.J. Leij, and M.Th. van Genuchten. 2001. Rosetta: A computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions. J. Hydrol. 251:163–176.
Scheinost, A.C., W. Sinowski, and K. Auerswald. 1997. Regionalization of soil water retention curves in a highly variable landscape. I. Developing a new pedotransfer function. Geoderma 78:129–143.
Soil Survey Staff. 1995. Soil survey laboratory information manual. Soil Surv. Invest. Rep. 45. Version 1.0. Natl. Soil Surv. Center, Lincoln, NE.
Soil Survey Staff. 1996. Soil survey laboratory methods manual. Soil Surv. Invest. Rep. 42. Version 3.0. Natl. Soil Surv. Center, Lincoln, NE.
Tietje, O., and V. Hennings. 1996. Accuracy of the saturated hydraulic conductivity prediction by pedo-transfer functions compared to the variability within FAO textural classes. Geoderma 69:71–84.
Tietje, O., and M. Tapkenhinrichs. 1993. Evaluation of pedotransfer functions. Soil Sci. Soc. Am. J. 57:1088–1095.
van Genuchten, M.Th. 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. J. 44:892–898.
Vereecken, H., J. Maes, J. Feyen, and P. Darius. 1989. Estimating the soil moisture retention characteristic from texture, bulk density, and carbon content. Soil Sci. 148:389–403.
Wösten, J.H.M., A. Lilly, A. Nemes, and C. Le Bas. 1999. Development and use of a database of hydraulic properties of European soils. Geoderma 90:169–185.
Wösten, J.H.M., Y.A. Pachepsky, and W.J. Rawls. 2001. Pedotransfer functions: Bridging the gap between available basic soil data and missing soil hydraulic characteristics. J. Hydrol. (Amsterdam) 251:123–150.