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Estimating the water retention curve from soil properties: comparison of linear, nonlinear and concomitant variable methods

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Abstract

The unsaturated soil hydraulic functions involving the soil–water retention curve (SWRC) and the hydraulic conductivity provide useful integrated indices of soil quality. Existing and newly devised methods were used to formulate pedotransfer functions (PTFs) that predict the SWRC from readily available soil data. The PTFs were calibrated using a large soils database from Hungary. The database contains measured soil–water retention data, the dry bulk density, sand, silt and clay percentages, and the organic matter content of 305 soil layers from some 80 soil profiles. A three-parameter van Genuchten type function was fitted to the measured retention data to obtain SWRC parameters for each soil sample in the database. Using a quasi-random procedure, the database was divided into ''evaluation'' (EVAL) and ''test'' (TEST) parts containing 225 and 80 soil samples, respectively. Linear PTFs for the SWRC parameters were calculated for the EVAL database. The PTFs used for this purpose particle-size percentages, dry bulk density, organic matter content, and the sand/silt ratio, as well as simple transforms (such as logarithms and products) of these independent variables. Of the various independent variables, the eight most significant were used to calculate the different PTFs. A nonlinear (NL) predictive method was obtained by substituting the linear PTFs directly into the SWRC equation, and subsequently adjusting the PTF parameters to all retention data of the EVAL database. The estimation error (SSQ) and efficiency (EE) were used to compare the effectiveness of the linear and nonlinearly adjusted PTFs. We found that EE of the EVAL and the TEST databases increased by 4 and 7%, respectively, using the second nonlinear optimization approach. To further increase EE, one measured retention data point was used as an additional (concomitant) variable in the PTFs. Using the 20 kPa water retention data point in the linear PTFs improved the EE by about 25% for the TEST data set. Nonlinear adjustment of the concomitant variable PTF using the 20 kPa retention data point as concomitant variable produced the best PTF. This PTF produced EE values of 93 and 88% for the EVAL and TEST soil data sets, respectively.

Keywords: Soil–water retention function; Pedotransfer functions; Unsaturated flow; Soil quality

1. Introduction

The unsaturated soil hydraulic functions are important parameters in many soil, hydrological, ecological and agricultural studies, are critical input parameters

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in models for variably-saturated flow and contaminant transport, and often serve as integrated indices for soil quality (e.g., National Research Council, 1993; Lin, 2003). Unfortunately, direct measurement of these functions is impractical for most applications in research and management, especially for relatively large-scale problems. For this reason, many applications rely on pedotransfer functions (PTFs) to indirectly estimate the hydraulic properties from more easily measured or more readily available information (e.g., soil texture and bulk density). Reviews of studies of this type are given by Tietje and Tapkenhinrichs, 1993, Bruand et al. (1997) and van Genuchten et al. (1999).

In this paper, we study how successfully the soil water retention curve (SWRC) can be predicted with PTFs that were derived using conventional and modified statistical approaches. A soil hydraulic database from Hungary will be used to demonstrate and test the proposed method. The database for our study was divided into ‘‘evaluation’’ (EVAL) and ‘‘test’’ (TEST) parts. A three-parameter van Genuchten type function (van Genuchten, 1984) will be used for the SWRC. We first use relatively standard approaches to derive PTFs for estimating the retention parameters. In attempts to improve the SWRC predictions, and following previous work by Scheinost et al. (1997), the linear PTFs are substituted directly into the SWRC, after which the parameters are further adjusted nonlinearly using all retention data of the EVAL database. Since the linear PTFs of the three SWRC parameters each contained nine unknows, this second nonlinear approach will involve 27 adjustable parameters. To further improve the accuracy of the PTFs, additionally one measured retention data point will be used as a concomitant variable in the PTF models. The retention data point that most significantly improves the SWRC predictions will be used as concomitant variable for the final PTFs.

2. The Hungarian soils database

The Hungarian database contains data from 305 soil samples. Water retention data were measured on core samples collected in 100 cm^3 cylinders having a height of 5 cm and an outer diameter of 5 cm. Retention data were obtained along the main drying curve at tensions of 0.1, 0.25, 1, 3.2, 10, 20, 50, 250 and 1500 kPa. Retention values between 1 and 50 kPa were obtained with the hanging water column method using sand- and kaolin-plate boxes (Várallyay, 1973), while the higher suction values (250 and 1500 kPa) were obtained using pressure chambers (Buzás, 1993). Particle-size fractions were measured with the conventional pipette method using 0.5 N $Na_2P_2O_5$ to facilitate dispersion. Particle-size limits were set at 0.002, 0.005, 0.01, 0.02, 0.05 and 0.25 mm. The coarsest particle fraction between 0.25 and 2 mm was determined by wet sieving. The dry bulk density of the soils was measured on core samples, while the soil organic matter content was obtained using conventional oxidation methods (Buzás, 1989).

The majority of soil samples in the Hungarian database (225 of 305) are representative of the main soil types of the Hungarian lowland (Rajkai et al., 1981), while 75 samples are from hill slope areas. About 75% of the soils are medium, 15% fine, and 10% coarse textured. The medium-textured soils formed mostly on loess parent materials. The finer-textured soils are mostly from the Trans–Tisza area where loess materials settled into a wet alluvial basin, and from hill slope areas where clay formation was an important part of the soil genesis process. The coarse-textured soils were collected from sandy areas of the Hungarian Lowland. Table 1 summarizes the main soil characteristics of the EVAL and TEST subsets of the Hungarian soils database.

3. Soil–water retention model

The following three-parameter van Genuchten function was used to the describe water retention data (van Genuchten, 1984):

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

Table 1
Selected properties of the evaluation (EVAL) and test (TEST) arts of the Hungarian soils database

Case	Sand	Silt	Clay	OM (%)	ρ (mg/m^3)	Pressure head (kPa)			
						1	20	1500	N
EVAL	25.4	47.1	27.5	1.4	1.44	46.6	35.6	17.0	225
TEST	26.8	47.8	26.8	1.6	1.43	47.0	36.9	17.9	80

where θ is the soil moisture content (m^3/m^3), h is the soil water tension (cm), and θ_s, α, and n are model parameters. Eq. (1) was fitted to the measured data of each soil sample using a nonlinear least-squares optimisation approach (Marquardt, 1963) that minimized the sum of squared deviations (SSQ) between observed and fitted water contents.

4. Pedotransfer functions

The fitted SWRC parameters were correlated with soil properties in the Hungarian database, as well as several derived soil properties. For the original properties we used the bulk density, ρ, the organic matter content,OM, the sand fraction, S, the silt fraction, S_i, and the clay fraction, C. As derived soil properties we selected the logarithm of the clay fraction, ln (C), the sand/silt ratio, S/S_i, the squares of the original properties (e.g., ρ^2 and C^2), and several simple products (e.g., $(\rho C)^2$ and $\rho^2 C^2$) as shown in Table 2 listing the different pedotransfer functions. Linear regression techniques were subsequently used to correlate the SWRC parameters with the most significant soil properties as predictors (Rajkai and Várallyay, 1992). As dependent variables for the linear PTF regressions we used θ_s and the log transforms of α and n.

To make the linear regression approach more flexible, all eight independent explanatory variables were entered and maintained in the PTF; this approach is further referred to as the LR8 predictive model. Next, the goodness of prediction of the LR8 model was improved by adding one measured water retention data point to the PTFs. Rawls and Brakensiek (1989) among others suggested that the wilting point should be used for this purpose. We also investigated the effect of using other measured retention data, and found that using retention data close to the SWRC inflection point (at about 20 kPa for most of our soils)

Table 2
Linear and nonlinearly adjusted pedotransfer functions obtained for the evaluation (EVAL) data base

Linear and nonlinearly adjusted PTFs	Predictive		
	R^2	method	N
$\theta_s = 118.76 - 60.02 \times \rho - 0.25 \times OM - 0.0007 \times C^2 - 1.99 \times \ln(C) + 9.78 \times \rho^2 - 0.04 \times \rho S + 0.116 \times S/S_i + 0.00078 \times \rho^2 C^2$	0.84	LR8	225
$\theta_s = 123.76 - 65.37 \times \rho - 0.28 \times OM - 0.000048 \times C^2 - 1.99 \times \ln(C) + 12.46 \times \rho^2 - 0.054 \times \rho S + 0.14 \times S/S_i + 0.00049 \times \rho^2 C^2$		NLR8	2025
$\theta_s = 134.88 - 0.127 \times FC - 74.4 \times \rho - 0.19 \times OM - 0.00027 \times C^2 - 2.83 \times \ln(C) + 14.37 \times \rho^2 - 0.053 \times \rho S - 0.0074 \times S/S_i - 0.00087 \times \rho^2 C^2$	0.85	LR8FC	225
$\theta_s = 107.95 - 51.5 \times FC - 0.00008 \times \rho - 0.086 \times OM - 0.042 \times C^2 + 0.0003 \times \ln(C) - 0.38 \times \rho^2 - 2.07 \times \rho S + 7.9 \times S/S_i + 0.067 \times \rho^2 C^2$		NLR8FC	2025
$\ln(\alpha) = 27.18 + 0.15 \times \rho S_i + 0.18 \times C - 13.32 \times \ln(S_i) - 0.024 \times \rho^2 C + 0.314 \times S_i - 0.0027 \times C^2 - 0.75 \times S/S_i - 0.0013 \times \rho^2 S_i^2$	0.23	LR8	225
$\ln(\alpha) = 16.97 + 0.12 \times \rho S_i + 0.22 \times C - 9.34 \times \ln(S_i) - 0.039 \times \rho^2 C + 0.21 \times S_i - 0.0029 \times C^2 - 0.435 \times S/S_i - 0.00093 \times \rho^2 S_i^2$		NLR8	2025
$\ln(\alpha) = -31.74 - 0.26 \times FC - 0.37 \times \rho S_i + 0.81 \times S/S_i + 0.157 \times C + 0.01 \times \rho^2 C + 13.52 \times \ln(S_i) - 0.01 \times S_i - 0.0016 \times C^2 + 0.0014 \times \rho^2 S_i^2$	0.64	LR8FC	225
$\ln(\alpha) = -13.89 + 4.67 \times FC - 0.0085 \times \rho S_i + 0.81 \times S/S_i + 0.213 \times C - 0.033 \times \rho^2 C - 0.002 \times \ln(S_i) - 0.12 \times S_i + 0.00048 \times C^2 + 0.294 \times \rho^2 S_i^2$		NLR8FC	2025
$\ln(n) = -0.287 + 0.47 \times \rho - 0.008 \times OM - 0.00007 \times C^2 + 0.06 \times \ln(C) - 0.00046 \times \rho S - 0.01 \times \rho^2 C - 0.0068 \times S/S_i + 0.00015 \times \rho^2 C^2$	0.61	LR8	225
$\ln(n) = -0.069 + 0.32 \times \rho - 0.007 \times OM - 0.000009 \times C^2 + 0.00147 \times \ln(C) - 0.00011 \times \rho S - 0.0064 \times \rho^2 C + 0.0015 \times S/S_i + 0.000081 \times \rho^2 C^2$		NLR8	2025
$\ln(n) = -0.67 + 0.0039 \times FC + 0.59 \times \rho - 0.01 \times OM - 0.0001 \times C^2 - 0.0005 \times \rho S + 0.11 \times \ln(C) - 0.012 \times \rho^2 C + 0.013 \times S/S_i + 0.00018 \times \rho^2 C^2$	0.64	LR8FC	225
$\ln(n) = 0.36 + 0.000045 \times FC + 0.0116 \times \rho - 0.002 \times OM + 0.16 \times C^2 - 0.0737 \times \rho S + 0.0000105 \times \ln(C) - 0.00046 \times \rho^2 C - 0.0055 \times S/S_i - 0.0035 \times \rho^2 C^2$		NLR8FC	2025

ρ = bulk density (mg/m^3); OM = organic matter (%); S = sand fraction (>50 μm S_i = silt fraction (50–2 μm); C = clay fraction (<2 μm); ln (S_i) = logarithm of silt fraction; ln (C) = logarithm of clay fraction; S/S_i = sand–silt ratio; FC = field capacity retention data.

produced the best predictions (results not further shown here). The predictive model using an independently measured retention point at this 20 kPa tension (approximately field capacity, FC) will be referred to as LR8FC.

To further improve the LR8, and LR8FC methods, we carried out an additional nonlinear adjustment procedure as outlined by Scheinost et al. (1997) and Minasny et al. (1999). For this purpose we generalized the estimated linear PTFs as listed in Table 2 (i.e., those for LR8 and LR8FC) by allowing the fitted coefficients to become unknowns in a new set of regressions. For example, the LR8 PTF for θ_s was generalized to (Table 2):

$$\theta_s = a_1 + a_2\rho + a_3\mathrm{OM} + a_4C^2 + a_5\ln(C) + a_6\rho^2 + a_7\rho S + a_8(S/S_i) + a_9\rho^2C^2 \tag{3}$$

Linear regression equations of this type for each of the three unknown retention parameters were substituted directly into Eq. (1) to yield the following general equation

$$\theta = \frac{a_1 + a_2\rho + a_3\mathrm{OM} + a_4C^2 + a_5\ln(C) + a_6\rho^2 + a_7\rho S + a_8(S/Si) + a_9\rho^2C^2}{\{1 + [h\exp(b_1 + b_2\rho S_i + b_3C + b_4\ln(S_i) + b_5\rho^2C + b_6S_i + b_7C^2 + b_8(S/Si) + b_9\rho^2S_i^2)]^{\lambda}\}^{\delta}} \tag{4a}$$

where

$$\lambda = \exp[c_1 + c_2\rho + c_3\mathrm{OM} + c_4C^2 + c_5\ln(C) + c_6\rho S + c_7\rho^2C + c_8(S/S_i) + c_9\rho^2C^2] \tag{4b}$$

and $\delta = 1 - 1/\lambda$. The exponential functions in Eq. (4a) and Eq. (4b) arise because ln (α) rather than α and ln (n) rather n were used in the regressions. Application of Eq. (4) to the EVAL retention data sets leads to 2025 nonlinear equations (225 data sets each having nine retention points) involving $3 \times 9 = 27$ or $3 \times (9 + 1) = 30$ unknowns (the latter when a concomitant variable is added). The resulting multivariate nonlinear optimization (inverse) problem may in general present severe uniqueness and convergence problems. However, our objective was not to find a unique inverse solution, but rather to improve (lower) the sum-of-squares error, SSQ, from the case when the three unknown retention parameters were regressed separately (i.e., only the PTF end result is important, not the individual PTF calibration parameters). SSQ values decreased substantially when Eq. (4) was used rather separate linear regressions. We will use the prefix NL to refer to this improved nonlinear global optimization approach. The NL-adjusted PTFs for the LR8 and LR8FC methods are given in Table 2. The effects of NL global optimization of the different PTFs are clearly demonstrated in Fig. 1. The mean prediction errors (ME) for the SWRCs of the EVAL and TEST soil data sets are given in Table 3.

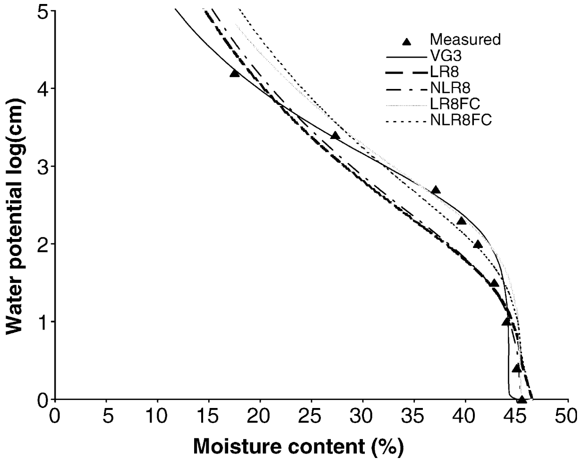

Fig. 1. Fitted (VG3) and predicted 3-parameter van Genuchten functions and measured water retention values at various pressure heads of a soil sample of the TEST data set.

5. Goodness of the model predictions

Following Rajkai et al. (1996), we consider a SWRC prediction 'good' if the mean estimation error (ME) for all measured retention data is less than 2.5%. This means that the mean absolute difference between the estimated and measured retention data values is less than 2.5%. The residuals are expressed in terms of volumetric water content percentages. The estimation efficiency (EE) of the different PTF models is defined as the percentage of soils for which the predictions are 'good'.

The accuracy of a prediction can also be expressed using the mean prediction error PE_h at a particular tension h for the databases as a whole:

$$\mathrm{PE}_h = \sqrt{(\mathrm{SSQ}/N)} \tag{4}$$

Table 3
Model selection criteria and statistical data of the predictive water retention models

Statistical Factors	Predictive models									
	Fitted model		LR8		LR8FC		NLR8		NLR8FC	
	EVAL	TEST	EVAL	TEST	EVAL	TEST	EVAL	TEST	EVAL	TEST
Residual SSQ	2814	1062	21893	11453	14601	6190	19540	10186	9284	4348
Model DF	675	240	27	27	30	30	27	27	30	30
N	2025	720	2025	720	2025	720	1810	720	1810	720
ME	0.39	0.40	1.10	1.33	0.90	0.98	1.04	1.25	0.71	0.82
AIC	2016	760	4875	2046	3839	1609	4644	1962	3019	1355
SBC	5805	1859	5026	2170	4004	1746	4796	2085	3184	1492

SSQ: the sum of square error; model DF: the total number of degrees of freedom of the optimization (number of models or equations × number of model parameters); N: the total number of water retention data (number of soil samples × number of retention data per sample); AIC: the Akaike information criteria and SBC: the Schwartz and Bayes information criteria.

where SSQ is the sum of square error and N the number of data sets in the database. In addition we calculated the mean prediction error, ME, for a retention curve as follows

$$\mathrm{ME} = \sum \frac{\mathrm{PE}_h}{n} \tag{5}$$

where n is now the number of retention data points.

The form of the regression model is

$$y_i = f(x_i, \beta) + e_i, \qquad i = 1, \ldots, N \tag{6}$$

where y_i and x_i are known measured values of the independent and dependent variables, respectively, β is the unknown parameter vector, and e_i is an independent zero-mean Gaussian error term. The log-likelihood function for this model (without the negligible constants, e_i) is

$$-2\ln L(\beta) = N \ln\left(\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2\right) \tag{7}$$

where $L(\beta)$ is the Gaussian likelihood function and $\hat{y}_i = f(x_i$, ML-estimator of $\beta)$.

The usual goodness-of-fit measure, R^2, and the F-test of significance have a drawback in that they are relatively insensitive to the number of parameters (i.e., the dimension of the parameter vector β) involved in the regression equation. While numerous criteria have been proposed to remedy this drawback, we use in this study Akaike's information criterion (AIC) and the Schwarz and Bayesian criterion (SBC) as follows (Kass and Raftery, 1995)

$$\mathrm{AIC} = N\ln\left[\frac{1}{N}\sum_{i=1}^{N}(y_i\hat{y}_i)^2\right] + 2P \tag{8}$$

and

$$\mathrm{SBC} = N\ln\left[\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2\right] + P\ln(N) \tag{9}$$

where P is the number of parameters used. According to Akaike (1973) the AIC is based on a predictive point of view, which makes the predictive distribution conditional on a model and its estimated parameters using the maximum likelihood method (Linhart and Zucchini, 1986). The SBC model-selection criterion above is that of Schwarz and Bayes (Schwarz, 1976) which places more emphasis on the number of parameters in a model. Schwarz (1976) introduced this criterion to select the model with the highest posterior probability using the asymptotic normality of the estimator of β with the maximum likelihood estimator as its mean, and using Fisher-information as inverse of the variance. When models are compared in terms of their AIC and SBC, the better model is that model which has a smaller value of the invoked criterion. Values for AIC and SBC were calculated using the SPSS statistical software package (SPSS, 1998).

6. Results and discussion

Fig. 1 shows that the nonlinear (NL) global optimization approach did not improve the predicted

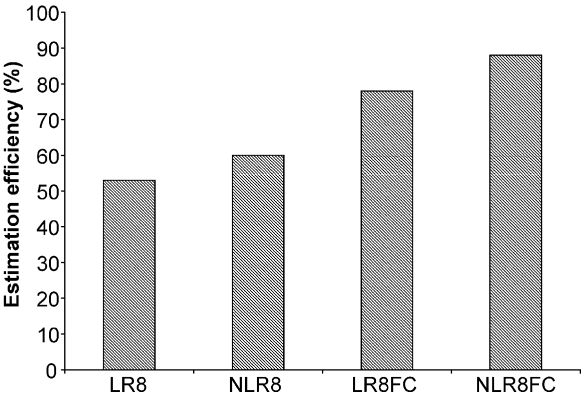

Fig. 2. Estimation efficiency (EE) of the SWRC predictive methods for the TEST data set.

SWRC close to the measured retention value at h = 1500 kPa in case of the NLR8FC PTF, but that the predictions are close to the other retention data. Fig. 1 also shows the performance of the individually fitted SWRCs.

Fig. 2 shows that the estimation efficiency, EE, is between 53 and 78% for the TEST soils for the LR8 and the LR8FC PTFs. Results indicate that the NLR8 and NLR8FC PTFs for the TEST soils have a 7–10% higher EE than their linear versions (LR8 and LR8FC).

The mean SWRC prediction error, ME, is plotted in Fig. 3 for the different predictive models. Notice that the LR8FC model performed better for the TEST soil

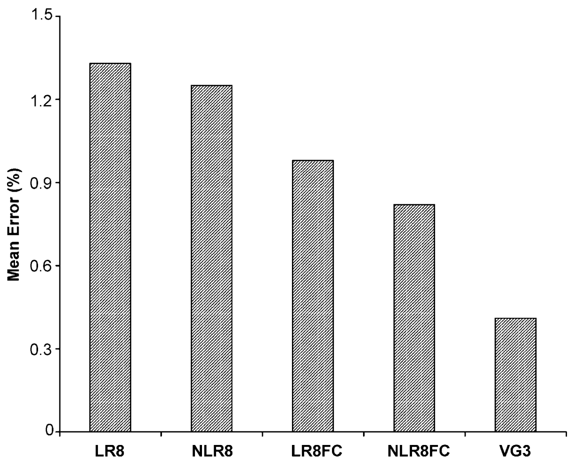

Fig. 3. Mean errors of the SWRC predictive methods and the fitted van Genuchten function (VG3).

database, and that NL optimization did improve the results somewhat further for the TEST data set as well. Using field capacity as a concomitant variable significantly improved the results; furthermore, NL adjustment did lead to substantial reductions in the Mean Error, ME.

The two model selection criteria (AIC and SBC) for the different predictive methods are listed in Table 3. As expected, the individually fitted retention data sets produced the smallest AIC values. However, while the AIC values suggest that all PTFs generate results that are worse than the individually fitted models, the SBC criterion qualifies almost all PTFs as being more effective than the individually fitted SWRCs in terms of Akaike's statistical stability criterion. The biggest difference between the AIC and SBC criteria is their sensitivity to the degrees of freedom (DF) of the PTF. When the SBCs of the predicted SWRCs are compared to each other, a rank from weak to good can be established. This shows that the nonlinearly (NL) adjusted models performed better than their linear versions.

The NL adjusted PTFs in Table 3, using FC as concomitant variable, for the EVAL and TEST data sets suggest that the predictive PTFs are fairly general. The best predictive model (NLR8FC) produces very reasonable results, giving ME values for the TEST soils that are only about two times higher than those for the individually fitted SWRCs (VG3) in Fig. 3.

The prediction efficiency (EE) represents the ratio of "good" predictions to the total number of data sets in the database. ME, together with EE, demonstrates the power of a particular PTF (Fig. 2). The relatively high ME and low EE values associated with the LR8 model indicate limited flexibility and accuracy of this model. The use of one measured retention data point (FC) in the PTF significantly decreased ME and increased EE. Using the field capacity in the LR8 model increased the EE by about 20% as compared to the LR8 (Fig. 2). Nonlinear adjustment of the LR8FC model improved the EE up to 95% for the EVAL soils, and 88% for the TEST database. This means that nonlinear adjustment leads to almost identical performance of the predictive model for the EVAL and TEST data sets. We conclude from this that the water retention data of the Hungarian soils are best predicted using the LR8FC PTF. However, the ME of the best PTF is still two times larger than the ME of the fitted SWRC model. It seems that this is probably the best result that can be achieved using the traditional statistical methods we have used. Recently several neural-network based methods have been used to derive pedotransfer functions (Pachepskij et al., 1996; Schaap et al., 1998). It would be interesting to make a detailed comparison of the prediction accuracy of those neural networks with the PTFs derived in this study.

7. Summary and conclusions

A three-parameter van Genuchten type model was used to describe the water retention curves of Hungarian soils. Fitted SWRC parameters were regressed linearly with a large number of soil physical properties in the database. To increase the flexibility of the linear PTFs we used not only the statistically most significant original soil properties, but also several derived properties (e.g., the logarithms, squares, and products of the original soil properties). Altogether we used eight measured and transformed soil properties, as well as one measured retention point to construct PTF's for the three retention parameters.

The linear PTFs were substituted into the SWRC and further adjusted nonlinearly using all measured retention data of the EVAL soil database. The estimation efficiency (EE), being the number of good estimations as a percentage of all data sets in the entire database, improved with this nonlinear adjustment from 4 to 7%. The EE further improved when one retention data point was added as a concomitant variable in the PTF analysis. Using the 20 kPa (near field capacity) retention point for this purpose in the nonlinear analysis increased the EE up to 88% of the independent TEST data set, and produced a mean estimation error of less than 1% for the TEST database. The applied techniques significantly improved the PTF prediction accuracies, and should be applicable to a much wider array of soils than only the Hungarian database. The PTFs derived in this paper provide improved relationships for estimating the soil water retention curve from soil texture and related properties, and as such may prove useful in studies dealing with assessments of physical soil quality, as well as for application to many other larger-scale soil, hydrological and agricultural problems.

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