Pedotransfer functions for point and parametric estimations of soil water retention curve

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ABSTRACT

A water retention curve is required for the simulation studies of water and solute transport in unsaturated or vadose zone. Unlike the direct measurement of water retention data, pedotransfer functions (PTFs) have attracted the attention of researchers for determining water retention curves from basic soil properties. The objective of this study was to develop and validate point and parametric PTFs for the estimation of water retention curve from basic soil properties such as particle-size distribution, bulk density, and porosity using multiple-linear regression technique and comparing the performances of point and two parametric methods using some evaluation criteria. 140 soil samples were collected from three different databases and divided as 100 and 40 for the derivation and validation of the PTFs. All three methods predicted water contents at selected water potentials and combined water retention curves pretty well, but van Genuchten's model performed the best in prediction. However, the differences among the methods in point and water retention curve predictions were not statistically significant ($P > 0.05$). Prediction accuracies were evaluated by the coefficient of determination (R^2) and the root mean square error (*RMSE*) between the measured and predicted values. The R^2 and *RMSE* were 0.962 and 0.036, 0.994 and 0.067, and 0.946 and 0.082 for point and parametric (van Genuchten, and Brooks and Corey) methods, respectively, in predicting combined water retention curve. The three methods can be alternatively used in the estimation of water retention curves, but parametric methods are preferred for yielding continuous water retention functions used in flow and transport modeling.

Keywords: comparison; regression; soil properties; validation

The quality of soil and water is under threat due to agricultural and industrial applications on the earth. Modeling of water and solute transport in vadose zone helps to understand the complex nature of transport phenomena. The movement of water and solute in this zone is so complicated because of nonlinearity and spatial variability of soil hydraulic characteristics. One-dimensional water flow requires the numerical solution of the Richards equation given as:

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

where: θ is the water content (cm^3/cm^3), K is the unsaturated hydraulic conductivity (cm/h), h is the soil water pressure (cm), t is the time (h), z is the vertical distance (cm), and S is the source-sink term.

The solution of the Richards equation (Eq. 1) requires nonlinear soil water retention curves, water content as a function of soil water potential $\theta(h)$, with depth in a soil profile. The water retention curves can be represented by the Eq. 2 (the van Genuchten 1980) or the Eq. 3 (Brooks and Corey 1964) as:

$$\theta(h) = \frac{\theta_s - \theta_r}{\left(1 + |\alpha h|^n\right)^{1-1/n}} + \theta_r \qquad (2)$$

$$\theta(h) = \theta_r + (\theta_s - \theta_r)(\alpha h)^{-n} \qquad (3)$$

where: θ_s and θ_r are the saturated and residual soil water contents (cm^3/cm^3), respectively, and α (per cm) and n are the shape factors of the water retention curve.

One-dimensional solute transport is described by the convection-dispersion equation (CDE) for non-reactive tracers as:

$$\frac{\partial(\theta c)}{\partial t} = \frac{\partial}{\partial z}\left(D\theta\frac{\partial c}{\partial z} - qc\right) \pm U \qquad (4)$$

where: c is the solute concentration, D is the dispersion coefficient, q is the Darcy water flux density, and U is the mass exchange between flow domains.

The solution of the Eq. 1 is prerequisite for the solution of the Eq. 4. Measuring water retention data is time-consuming, labor-intensive, and thereby expensive. Indirect estimation of water retention curves from basic soil properties such as sand (S), silt (Si) and clay (C) fractions, bulk density (BD), and porosity (P) using pedotransfer functions (PTFs) has received considerable attention (Pachepsky et al. 1996, Koekkoek and Booltink 1999, Tomasella et al. 2000, Minasny et al. 2004).

Water retention curves can be constructed by mainly two approaches: point and parametric estimation. In point estimation, soil water contents are estimated at selected water potentials (Batjes 1996, Pachepsky et al. 1996, Minasny et al. 1999). The parameterization method estimates the parameters of soil water retention models (Vereecken et al. 1992, Wösten et al. 1995, Schaap et al. 1998, Minasny and McBratney 2002). Two of the most commonly used water retention models are van Genuchten (1980) and Brooks and Corey (1964). Parametric PTFs are developed by estimating the parameters of a retention model by fitting it to data and then relating the parameters to basic soil properties.

PTFs for point and parametric estimation of water retention curve from basic soil properties can be developed using multiple-linear regression (Lin et al. 1999, Mayr and Jarvis 1999, Tomasella et al. 2000). An advantage of regression techniques is that most fundamental input parameters can be determined using stepwise regression. Site-specific data is required in order to develop an accurate water retention curve compared to large and general data. In addition, even though the van Genuchten's water retention model is commonly used in PTF studies, its comparison with the Brooks and Corey (1964) model is absent in the literature. Moreover, the comparison of point estimation with the parametric estimation using both retention models (Eq. 2 and 3) is very limited.

Therefore, in this study, point and parametric PTFs for estimation of water retention curve from basic soil properties such as particle-size distribution, bulk density, and porosity were developed and validated using multiple-linear regression. The performances of point and two parametric methods were compared in predicting water retention curve. In order to satisfy the objectives, 140 soil samples, which include basic soil properties and water retention data, were collected from three different sources. The water retention models of van Genuchten (1980) and Brooks and Corey (1964) were fitted to water retention data to estimate the parameters of these models. PTFs were developed for point and parametric estimations of water retention curve and the results were compared.

MATERIAL AND METHODS

The data was taken from three different sources. Hatfield (1988) determined particle-size distribution, bulk density, porosity, and water retention data as a function of depth (5, 10, 15, 20, 30, 45, 60, 75, 90, and 105 cm) on 6 plots of Cecil loamy sand (clayey, kaolinitic, thermic Typic Hapludults) in the Clemson Experimental Forest near Clemson, South Carolina. Dane et al. (1983) measured the same soil physical and hydraulic characteristics at 10 depths in 3 plots of Lakeland sandy soil in South Carolina. The remaining data was taken from Elliot and Brown (1998).

Both hydraulic models (Eq. 2 and 3) were fitted to the water retention data using the nonlinear least-squares optimization program RETC (van Genuchten et al. 1991) to estimate the parameters (θ_r, θ_s, α, and n) of both models.

Each of the water contents at selected water potentials of 10, 50, 100, 200, 330, and 500 cm H_2O and estimated parameters of both models were related to basic soil properties (S, Si, C, BD, and P) using multiple-linear regression techniques in order to develop PTFs. The most significant input variables were determined using backwards-stepwise method, and then linear, quadratic, and possible interaction terms of these basic soil properties were investigated using the Statistical Analysis System (SAS Institute Inc., Cary, NC). The general form of the resulted regression equations can be expressed as:

$$Y = b_0 + b_1X_1 + \dots + b_5X_5 + b_6X_1^2 + \dots + b_{10}X_5^2 + b_{11}X_1X_2 + \dots + b_nX_4X_5 \quad (5)$$

where: Y represents the dependent variable such as water content at selected water potential or one of the parameters of the retention models, b_0 is the intercept, $b_1, \dots, b_n$ are the regression coefficients, and X_1 to X_5 refer to the independent variables representing the basic soil properties.

Approximately two third of the data ($N = 100$) were used in the derivation and the remaining data ($N = 40$) were used in the validation of PTFs.

The performances of point and parametric PTFs in predicting the measured or fitted data were evaluated using R^2, *RMSE*, and mean error (*ME*) and expressed as:

$$R^2 = 1 - \frac{\sum_{1}^{N}\left(y_i - \hat{y}_i\right)^2}{\sum_{1}^{N}\left(y_i - \bar{y}_i\right)^2} \quad (6)$$

$$RMSE = \sqrt{\frac{\sum_{1}^{N}\left(y_i - \hat{y}_i\right)^2}{N}} \quad (7)$$

$$ME = \frac{\sum_{1}^{N}\left(y_i - \hat{y}_i\right)}{N} \quad (8)$$

where: y_i denotes the measured value, $\hat{y}_i$ refers to the predicted value, $\bar{y}_i$ represents the average of the measured value y, and N is the total number of observations.

Under- and over-prediction of PTFs for a given parameter are represented by positive and negative values of *ME*, respectively. Moreover, the analysis of variance (ANOVA) was performed using SAS (SAS Institute Inc., Cary, NC) to determine if there were differences among the methods (point and parametric) in prediction of soil water content on water retention curve at a given water potential and combined water retention curves.

RESULTS AND DISCUSSION

Some basic statistics (minimum, maximum, mean, and standard deviation) of soil physical and hydraulic properties used in the derivation and validation of PTFs is summarized in Table 1. Hydraulic properties mainly include soil water contents θ (cm^3/cm^3) at water potentials of 10, 50, 100, 200, 330, and 500 cm water, respectively, and parameters of both water retention models. Soils used in this study had wide ranges of physical properties. The ranges and means (in parenthesis) of sand, silt, and clay fractions (kg/kg), bulk density, and porosity were 0.054–0.962 (0.559), 0.003–0.660 (0.191), 0.010–0.680 (0.251), 0.88–1.69 (1.50 g/cm^3), 0.308–0.675 (0.443), respectively, for derivation data set. The collection of data from three states (South Carolina, Oklahoma, and Kansas), which have relatively large area, in the USA may lead to such large ranges in soil properties. The data used in the validation of the developed PTFs had similar properties. The soils can be assumed as coarse-textured based on the mean sand fraction, bulk density, and porosity, where the mean bulk density and porosity are relatively high and low, respectively. The water contents at different potentials correspond to the physical properties of soils, where the mean water retention capacity of soils is relatively low with the range of (0.380–0.231 cm^3/cm^3). The data used for the validation have similar physical and hydraulic properties.

The PTFs developed for the estimation of water contents at selected water potentials and parameters of water retention models are summarized in Table 2. Overall, PTFs performed better in estimation of water contents at selected water potentials than in estimation of parameters of both water retention models based on the R^2 and *RMSE*. PTF for estimation of water content at 10 cm potential had worst performance compared to the other points possibly due to the fact that this was the division point between macropores and micropores. Activation of macropores around this potential may affect retention of water significantly. Similarly, PTFs in estimation of shape parameters of both models had worse performance than in estimation of residual and saturated water contents.

Derivation and validation accuracies of PTFs between measured or fitted and predicted water contents and model parameters are tabulated in Table 3. Even though derivation accuracies of PTF are slightly better than validation accuracies, they are comparable based on the R^2 and *RMSE.* For the validation data set, PTFs performed better in point prediction than in parameter prediction, but the results of both retention models were similar. PTFs over-predicted all water contents and most of model parameters, where *ME* was < 0.

Accuracies of point and parametric (by van Genuchten and Brooks and Corey models) predictions of water contents at selected water potentials on water retention curve and combined water retention curves are presented in Table 4. Water contents at selected water potentials on water retention curve and combined water retention curves were predicted in decreasing accuracy in the order of van Genuchten and Brooks and Corey models, and point prediction method. However, these differences among the three methods in predictions were statistically not significant ($P > 0.05$).

In several studies, PTFs were developed for estimation of water contents at selected water potentials and van Genuchten parameters using regression techniques. Pachepsky et al. (1996) reported relatively high prediction accuracies, R^2 = 0.738–0.984 (range) and 0.915 (mean), between measured and predicted water contents at 8 selected water potentials. Similarly, Batjes (1996)

Table 1. Descriptive statistics for soil physical and hydraulic properties used in derivation and validation of PTFs

Variables	Derivation data set				Validation data set			
	min	max	mean	*SD*	min	max	mean	*SD*
Physical properties								
Sand (kg/kg)	0.054	0.962	0.559	0.283	0.110	0.957	0.612	0.294
Silt (kg/kg)	0.003	0.660	0.191	0.186	0.020	0.604	0.184	0.189
Clay (kg/kg)	0.010	0.680	0.251	0.207	0.000	0.612	0.205	0.188
Bulk density (g/cm^3)	0.88	1.69	1.50	0.13	1.08	1.77	1.51	0.13
Porosity (cm^3/cm^3)	0.308	0.675	0.443	0.053	0.329	0.600	0.443	0.059
Hydraulic properties								
θ_{10}	0.210	0.643	0.380	0.079	0.200	0.570	0.356	0.090
θ_{50}	0.076	0.482	0.295	0.125	0.082	0.500	0.261	0.125
θ_{100}	0.042	0.469	0.265	0.129	0.042	0.427	0.231	0.125
θ_{200}	0.030	0.456	0.246	0.129	0.036	0.407	0.212	0.123
θ_{330}	0.022	0.450	0.235	0.130	0.028	0.400	0.201	0.122
θ_{500}	0.020	0.445	0.231	0.131	0.025	0.396	0.195	0.122
van Genuchten parameters								
θ_r	0.000	0.404	0.128	0.112	0.000	0.313	0.111	0.1000
θ_s	0.307	0.668	0.433	0.060	0.318	0.589	0.429	0.059
α	0.01446	1.63744	0.14751	0.22800	0.02024	1.68728	0.26511	0.34706
n	1.03931	6.04210	1.62514	0.64017	1.03529	2.70076	1.65085	0.55405
Brooks-Corey parameters								
θ_r	0.000	0.426	0.142	0.130	0.000	0.335	0.116	0.115
θ_s	0.284	0.664	0.425	0.061	0.313	0.568	0.423	0.059
α	0.02026	1.75348	0.18178	0.26331	0.01690	1.84552	0.28558	0.36002
n	0.04510	2.81535	0.45516	0.35135	0.05025	1.31021	0.49605	0.32081

θ_{10}, θ_{50}, θ_{100}, θ_{200}, θ_{330}, and θ_{500} = soil water contents θ (cm^3/cm^3) at water potentials of 10, 50, 100, 200, 330, and 500 cm water, respectively; θ_r and θ_s = residual and saturated soil water contents (cm^3/cm^3), respectively; α and n = water retention curve parameters; *SD* = standard deviation

developed PTFs for water contents at 10 different water potential with the equation accuracies between R^2 = 0.880 and 0.940. Vereecken et al. (1992) found that estimation accuracies of PTFs for van Genuchten parameters ranged between 0.560 and 0.848 (R^2). Wösten et al. (1995) derived PTFs for estimation of these parameters in sandy soils with the accuracy of R^2 = 0.71, 0.53, and 0.63 for θ_s, α, and n, respectively. Wösten et al. (2001) reported that the equation accuracies were 0.76, 0.20, and 0.54 for the same parameters. Tomasella et al. (2000) also developed regression PTFs for Brazilian soils with the equation accuracy of 0.83, 0.84, 0.41, and 0.37 for θ_r, θ_s, α, and n, respectively. These results indicate that the prediction accuracies of parametric PTFs are generally lower, as in this case, than that of the point predictions, possibly due to the collection of data from relatively large area where spatial variability exists in soil properties.

Even though point estimation method needs less input variables in predicting water retention curve with relatively high accuracy (high R^2 and low *RMSE*), parametric estimation of water retention curve using either of water retention models with better accuracy is preferred for especially producing continuous functions of water retention used in water and solute transport modeling studies.

Table 2. PTFs developed for estimation of water contents at selected water potentials and parameters of water retention models

Pedotransfer functions derived for		R^2	*RMSE*
prediction of soil water content at selected water potentials	$\theta_{10} = 0.127 - 0.125S - 0.212Si + 0.626P + 0.032S^2 + 0.219Si^2 + 0.498P^2 + 0.367SSi - 0.213SP - 0.184SiP$	0.865	0.0307
	$\theta_{50} = 0.699 - 0.712S - 0.876Si + 0.0828S^2 + 0.558Si^2 + 1.256SSi$	0.919	0.0364
	$\theta_{100} = 0.715 - 0.820S - 0.898Si + 0.140S^2 + 0.465Si^2 + 1.303SSi$	0.937	0.0332
	$\theta_{200} = 0.697 - 0.814S - 0.836Si + 0.141S^2 + 0.409Si^2 + 1.118SSi$	0.940	0.0324
	$\theta_{330} = 0.677 - 0.775S - 0.757Si + 0.116S^2 + 0.340Si^2 + 0.918SSi$	0.934	0.0342
	$\theta_{500} = 0.644 - 0.687S - 0.658Si + 0.0626S^2 + 0.253Si^2 + 0.761SSi$	0.880	0.0467
van Genuchten water retention curve parameters	$\theta_r = -0.558 + 0.284S + 0.520C + 2.057P - 0.054S^2 - 1.750C^2 - 1.511P^2 - 0.794SC - 0.547SP + 1.732CP$	0.565	0.0781
	$\theta_s = -0.178 + 0.331C + 1.538P - 0.105C^2 - 0.409P^2 - 0.530CP$	0.969	0.0108
	$\alpha = 70.72 - 9.060Si - 54.73BD - 123.7P - 0.988Si^2 + 10.36BD^2 + 50.86P^2 + 3.273SiBD + 10.27SiP + 49.65BDP$	0.179	0.2178
	$\ln(n) = -21.79 + 2.893C + 8.474BD + 67.08P - 0.605C^2 + 0.579BD^2 - 41.10P^2 - 3.103CBD + 2.498CP - 19.96BDP$	0.615	0.2040
Brooks-Corey water retention curve parameters	$\theta_r = -0.152 + 0.300Si + 2.509C + 0.164BD + 0.0346Si^2 - 0.306C^2 - 0.032BD^2 + 0.0463SiC - 0.157SiBD - 1.348CBD$	0.474	0.0994
	$\theta_s = 0.159 - 0.189S + 0.472P - 0.037S^2 + 0.329P^2 + 0.464SP$	0.946	0.0144
	$-\ln(\alpha) = -208.5 - 23.58C + 172.2BD + 373.8P + 8.045C^2 - 34.50BD^2 - 157.6P^2 + 6.650CBD + 22.30CP - 157.2BDP$	0.286	0.8401
	$-\ln(n) = -0.250 + 8.380Si + 5.208C + 0.541P - 1.433Si^2 - 3.704C^2 + 0.375P^2 - 8.319SiC - 11.81SiP + 0.556CP$	0.426	0.6740

θ_{10}, θ_{50}, θ_{100}, θ_{200}, θ_{330}, and θ_{500} = soil water contents θ (cm^3/cm^3) at water potentials of 10, 50, 100, 200, 330, and 500 cm water, respectively; S, Si, C = sand, silt, and clay fractions (kg/kg); BD = bulk density (g/cm^3); P = porosity (cm^3/cm^3); θ_r and θ_s = residual and saturated soil water contents (cm^3/cm^3), respectively; α and n = water retention curve parameters; R^2 = coefficient of determination; *RMSE* = root mean square error

This paper presented the development and validation of point and parametric PTFs for the estimation of water retention curve from basic soil properties using regression technique and comparison of the performances of point and two parametric methods using some evaluation criteria. There was statistically no significant difference among the three methods in predicting water retention curves, but van Genuchten's model predicted somewhat better than the other two.

In point estimation, limited discrete points on water retention curves are estimated; otherwise, it is time-consuming and needs intensive efforts especially for large and spatially variable lands. However, parametric estimation methods yield continuous water retention functions in less time and effort. Since the soils used in this study are relatively sandy-textured, PTFs developed in this study should be cautiously applied to other soils with wide range of textures. Therefore, similar

Table 3. Derivation and validation accuracies of PTFs between measured or fitted and predicted water contents and model parameters

Variables	Derivation			Validation		
	R^2	*RMSE*	*ME*	R^2	*RMSE*	*ME*
θ_{10}	0.930	0.029	0.000	0.863	0.048	–0.015
θ_{50}	0.959	0.035	0.000	0.945	0.041	–0.006
θ_{100}	0.968	0.032	–0.001	0.962	0.034	–0.005
θ_{200}	0.970	0.031	0.000	0.971	0.029	–0.005
θ_{330}	0.967	0.033	0.000	0.971	0.029	–0.004
θ_{500}	0.938	0.045	0.000	0.969	0.031	–0.008
van Genuchten parameters						
θ_r	0.752	0.074	0.000	0.545	0.094	–0.015
θ_s	0.985	0.010	0.000	0.929	0.024	–0.002
α	0.423	0.207	0.021	0.430	0.331	0.121
n	0.783	0.193	0.002	0.661	0.243	–0.021
Brooks-Corey parameters						
θ_r	0.688	0.094	0.001	0.538	0.100	–0.006
θ_s	0.973	0.014	0.001	0.931	0.023	0.000
α	0.535	0.796	–0.071	0.213	1.234	–0.406
n	0.654	0.638	–0.004	0.668	0.641	0.051

θ_{10}, θ_{50}, θ_{100}, θ_{200}, θ_{330}, and θ_{500} = soil water contents θ (cm^3/cm^3) at water potentials of 10, 50, 100, 200, 330, and 500 cm water, respectively; θ_r and θ_s = residual and saturated soil water contents (cm^3/cm^3), respectively; α and *n* = water retention curve parameters; R^2 = coefficient of determination; *RMSE* = root mean square error; *ME* = mean error

Table 4. Accuracies of point and parametric (by van Genuchten and Brooks and Corey models) predictions of soil water retention curves

	R^2			*RMSE*			*ME*		
	point	VG	BC	point	VG	BC	point	VG	BC
θ_{10}	0.863	0.950	0.689	0.048	0.076	0.136	–0.015	0.006	–0.044
θ_{50}	0.945	0.996	0.994	0.041	0.070	0.070	–0.006	0.013	0.010
θ_{100}	0.962	0.999	0.998	0.034	0.068	0.068	–0.005	0.011	0.009
θ_{200}	0.971	0.999	0.999	0.029	0.064	0.065	–0.005	0.010	0.010
θ_{330}	0.971	0.999	0.999	0.029	0.063	0.063	–0.004	0.009	0.010
θ_{500}	0.969	0.999	0.999	0.031	0.063	0.063	–0.008	0.010	0.011
θ_{10-500}	0.962	0.994	0.946	0.036	0.067	0.082	–0.007	0.010	0.001

θ_{10}, θ_{50}, θ_{100}, θ_{200}, θ_{330}, and θ_{500} = soil water contents θ (cm^3/cm^3) at water potentials of 10, 50, 100, 200, 330, and 500 cm water, respectively; θ_{10-500} = the water retention curve between 10 and 500 cm soil water potential; point = point prediction; VG = van Genuchten model; BC = Brooks and Corey model; R^2 = coefficient of determination; *RMSE* = root mean square error; *ME* = mean error studies need to be conducted on soils having wide ranges of physical properties.

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