Pedotransfer Functions for the Estimation of Soil Water Retention in Brazilian Soils

Javier Tomasella,* Martin G. Hodnett, and Luciana Rossato

ABSTRACT

Various studies have shown that micro-aggregated, strongly weathered tropical soils have different water retention properties than temperate-region soils because of differences in mineralogy and weathering history. Hence, pedotransfer functions (PTFs), derived from data from temperate-region soils (temperate PTFs) have limitations when applied to tropical soils. In the absence of PTFs specifically for tropical soils, temperate PTFs are being applied worldwide in global climate modeling exercises, regardless of their textural validity. We derived a PTF to predict the water retention parameters of the van Genuchten (1980) equation using data from more than 500 Brazilian soil horizons. A modified approach was adopted: Multiple regression was used to derive coefficients that relate the van Genuchten parameters to basic soil data, followed by re-optimization of those coefficients by fitting the individual water content estimations to the measured data simultaneously. Pedotransfer functions were developed for four levels of availability of basic soils data and validated using independent data from 113 Brazilian soil horizons. Water retention curves were better predicted by the new PTFs than by two temperate PTFs tested: The root mean square deviation (RMSD) ranged from 3.78 to 5.84, compared with 9.08 and 10.44, respectively. The new PTFs performed better even when the comparison was restricted to the range of textural validity of the temperate PTFs. For the proposed PTF, RMSDs increased with increasing silt content, but decreased for the temperate PTFs. This reflects the differences in silt content between temperate and strongly weathered tropical soils.

In recent years there has been increased interest in understanding land surface–atmosphere interactions. The exchanges of ideas among various scientific groups during major multidisciplinary experiments have led to new perceptions of the relationships between the surface and the atmosphere, and have driven the development of conceptual and complex models known as soil–vegetation–atmosphere transfer (SVAT) schemes (e.g., Sellers et al., 1986).

The interactions between soil moisture and atmospheric processes have been explored in detail by Entekhabi et al. (1996). Based on field data and modeling results, these authors showed that these linkages can take place over a wide range of temporal and spatial scales. In another study, Betts et al. (1996, p. 7222) concluded that "the soil moisture (in conjunction with soil temperature) provides a long term memory of the surface boundary condition as does the sea surface temperature over the oceans." Cuenca et al. (1996) noted that there was a strong influence of the soil-moisture profile on atmospheric simulations, with a natural impact on the final results of climate predictions.

An accurate simulation of water transport in the unsaturated zone (with various hydrological implications) or of the exchanges of gases and vapor between the soil and the atmosphere requires a knowledge of hydraulic properties on a regional and/or continental scale. Xue et al. (1996), comparing soil moisture observations with modeling results, showed that the soil hydraulic parameters have a profound impact on the model simulations.

Since soil hydraulic properties are expensive and difficult to obtain, the data needed for more realistic simulations of the land-surface atmosphere processes are rarely available at the scale required to run SVAT models. This is particularly true in Brazil, where detailed studies of soil hydrology have been conducted only on a very limited scale. However, the whole country has been mapped on a pedological basis by EMBRAPA (1981) and the Radambrasil Project (1973–1986), and particle size and chemical data are available at a reasonable scale of resolution. Therefore, the simplest and most practical currently available means to estimate the soil hydraulic parameters required by hydrological–atmospheric–ecological models on meso- and macroscales, is to obtain them from the available pedological data through the use of pedotransfer functions (PTFs).

Various PTFs have been published for a wide range of applications, but all have been derived empirically and mostly using data from soils of temperate regions. Tomasella and Hodnett (1998) recently showed that, in many cases, the textures of many tropical soils, particularly oxisols such as those of Brazilian Amazonia, are outside the range of validity of these PTFs. As a result, the water retention estimations may also be significantly in error, or they may fail totally, for example by indicating a water content at field capacity that is higher than that at saturation. This occurs using the PTF of Mishra et al. (1989) for oxisols from Nigeria and Brazil with clay contents of 52 and 85%, respectively.

A further reason for discrepancies may be the *hybrid* behavior often observed in tropical soils, particularly oxisols. Holzhey and Kimble (1988) concluded that the water retention curve of oxisols with a well-developed, fine, granular structure is characteristic of a clay soil at the higher suctions. However, at intermediate suctions it reflects the low silt content, and at lower suctions, there is a characteristic *bulge* in the curve, reflecting the large number of pores $>$ 0.1 mm in diam. This part of the curve, according to Sharma and Uehara (1968), is similar to sandy soils. Sanchez (1976) made similar observations on the properties of oxisols.

J. Tomasella, Centro de Previsão do Tempo e Estudos Climáticos/INPE, Cx. Postal 01, Rod. Presidente Dutra Km 40, 12630-000 Cachoeira Paulista/SP, Brazil; M.G. Hodnett, Institute of Hydrology, Wallingford, Oxfordshire, OX10 8BB, UK; and L. Rossato, Centro de Previsão do Tempo e Estudos Climáticos/INPE, Cx. Postal 01, Rod. Presidente Dutra Km 40, 12630-000 Cachoeira Paulista/SP, Brazil. Received 7 Aug. 1998. *Corresponding author (javier@cptec.inpe.br).

Published in Soil Sci. Soc. Am. J. 64:327–338 (2000).

Abbreviations: AWC, available water capacity; MD, mean difference; PTF, pedotransfer function; RMSD, root mean square deviation; SSE, sum of the squared errors; SVAT, soil–vegetation–atmosphere transfer; vG, van Genuchten.

Pedotransfer functions can be developed to predict single values, for example the water content at a particular value of matric potential (e.g., −10 kPa or −1500 kPa) or the available water capacity (AWC). They may also be developed to predict the parameters of an expression to describe the water retention curve, for example those of van Genuchten (1980) or Brooks and Corey (1964). Several attempts to derive PTFs for Brazilian soils have been made. Arruda et al. (1987) produced a PTF for soils in São Paulo State and Silva et al. (1990) produced one for the soils of the semiarid Northeast. More recently, van den Berg (1996) derived a PTF for the oxisols of SE and S Brazil. All of these PTFs were developed to estimate AWC. van den Berg et al. (1997) published PTFs to estimate AWC and van Genuchten parameters for oxisols using data from various countries, including Brazil, but these require aluminium content as an input. This is generally not widely available. In another study, Tomasella and Hodnett (1998) derived and tested a PTF to estimate the Brooks and Corey (1964) retention parameters using soil data from Brazilian Amazonia.

The objective of this work was to derive and validate, for Brazilian soils, a more accurate PTF to estimate the parameters of the van Genuchten (1980) equation for the water retention curve of Brazilian soils and other similar tropical soils. This was carried out using more detailed water retention data from the whole of Brazil and an improved statistical methodology. The derived PTF was validated using Brazilian soils data that had not been included in the fitting procedure. Although the van Genuchten (1980) equation may not be the most appropriate function to describe the behavior of soils with hybrid behavior such as oxisols, it has been adopted widely by the modeling community who require the best estimates of parameters to run their models. The widespread adoption of equations that can adequately describe dual porosity will take time. Further time and effort will then be required to derive the relevant parameters on a large scale. In the meantime, use of the van Genuchten (1980) equation is the best alternative if PTFs are to be developed to predict the water retention curve of tropical soils.

MATERIALS AND METHODS

Soil water retention data were selected from numerous studies that had been carried out for various purposes throughout Brazil. Only those water retention data that had been determined following the same methodology were selected: tension tables were used for matric potentials between saturation and −10 kPa, and pressure chambers were used for matric potentials between −10 kPa and −1500 kPa, both methods using undisturbed soil cores. The core size varied depending on the study from which the data were extracted, and the minimum internal volume was 50 cm^3. For all of the data, bulk density was determined after drying the soil cores at 105°C for 24 h, and particle density (when available) was determined by volumetric flask. Porosity was derived from bulk and particle density, when both were available. The sand fractions were determined by dry sieving and the silt and clay fractions by the pipette method. Organic C, another variable used in the PTF, was estimated by wet digestion in acid dichromate and automatic titration with iron sulphate. Table 1 summarizes the available data, their source, the number of water retention curves and the number of data points. Figure 1 shows the geographic locations of the soil profiles sampled. The database

Table 1. Data used in the derivation (coded roman) and validation (coded in italics) of the pedotransfer function.

Code	Site	Number of curves	Number of data points	Reference
		Derivation data		
MG1	**Sete Lagoas**	**5**	**55**	**Andrade (1987)**
PR	**Londrina**	**3**	**24**	**Calheiros (1991).**
MG2	**Northern Minas Gerais**	**41**	**287**	**Fontes & Oliveira (1982)**
PA1	**Pará State**	**62**	**434**	**Embrapa/Fao (1991)**
AM1	**Careiro Island**	**38**	**304**	**Ferreira (1993)**
SE	**Itaporanga**	**4**	**40**	**Fontes (1984)**
MG3	**Lavras**	**7**	**119**	**Freire & Scardua (1978)**
AM2	**Manaus**	**96**	**576**	**Freitas (1981)**
RJ	**Itaguaí**	**33**	**231**	**Jaccoud & Castro (1976); Ramos et al. (1973)**
PA2	**Igarapé Açu, Capitão Poço**	**32**	**192**	**Carvalho & Costa (1997a,b)**
ES	**Aracruz**	**9**	**90**	**Mattos (1978)**
PE	**Goiana**	**5**	**65**	**Moreira & Silva (1987)**
RN	**Mossoró**	**7**	**119**	**Mota (1976)**
BA	**Rio Corrente**	**14**	**126**	**Muggler (1989)**
MG4	**Poços de Caldas**	**45**	**270**	**Rodrigues (1984)**
SP1	**Araras**	**6**	**42**	**Rosenfeld (1989)**
SP-DF	**NE São Paulo, SW Minas Gerais, SE Goiás and Brasília**	**110**	**559**	**Camargo et al. (1988)**
Total		**517**		
		Validation data		
MG4	**Viçosa**	**10**	**110**	**Azevedo (1976)**
PA2	**Rio Guamá**	**9**	**64**	**Carvalho (1994)**
SP2	**Campinas**	**18**	**234**	**Castro (1995)**
PA3	**Capitão Poço**	**8**	**48**	**Costa & Teixeira (1992)**
NE	**Eastern Alagoas, Pernambuco & Paraíba**	**42**	**294**	**Oliveira & Queiroz (1975)**
MG6	**SW Minas Gerais**	**5**	**50**	**Fernandes et al. (1978)**
SP3	**Piracicaba**	**12**	**156**	**Scardua (1972)**
RS	**Pelotas**	**9**	**81**	**Winkler & Goedert (1972)**
Total		**113**		

was divided randomly into two groups: The first group contained 517 water retention curves and was used to derive the PTF. The second group contained 113 curves and was used in the validation. The two groups are coded in normal letters and italics, respectively, in Table 1. Both sets are from a large area of northern and eastern Brazil, cover a wide range of soil textures, and are representative of the most common soils that occur in the country. Although the database was split randomly, the validation data set was inspected to ensure that it covered a wide variety of soils and geographic locations.

The soil water–retention data in Table 1 were collected for different objectives, and as a result, the number of points for each water retention curve varied from source to source, although all included a measurement at −1500 kPa. As the analytical water retention curves more commonly used have four or more parameters (e.g., Brooks & Corey, 1964; van Genuchten, 1980), only those curves defined by *at least* five pairs of soil water potential data points were included in Table 1. This was a somewhat arbitrary minimum. However, had this number been set to a minimum of six points (or even to a greater minumum), many curves that are representative of the field variability of Brazilian soils would have been eliminated from Table 1 and this would have restricted the validity of the derived PTF.

A property commonly determined by the Brazilian Soil Survey is the moisture equivalent. This is the water content remaining in a sample (fraction <2 mm) after centrifuging at 2400 rpm for 30 min, generally expressed in gravimetric units. The moisture equivalent for Brazilian soils has been shown by Richards and Weaver (1944) and by Oliveira (1982) to be highly correlated with the water content at −33 kPa. As the predictive ability of a particular PTF is often improved by introducing the moisture content at a fixed matric potential (e.g., Rawls et al., 1982), the possibility of using moisture equivalent as an additional variable to enhance the prediction capability of the PTF was investigated. For 47% of the derivation data set shown in Table 1, both moisture equivalent and water content at −33 kPa were available, and the hypothesis that both parameters are almost identical was tested. Figure 2 shows the result of this analysis. Since there was a strong similarity between the two values, where moisture equivalent was not available in Table 1, it was assumed that the gravimetric water content at −33 kPa could be substituted.

Figures 3 and 4 show the data used in the derivation and

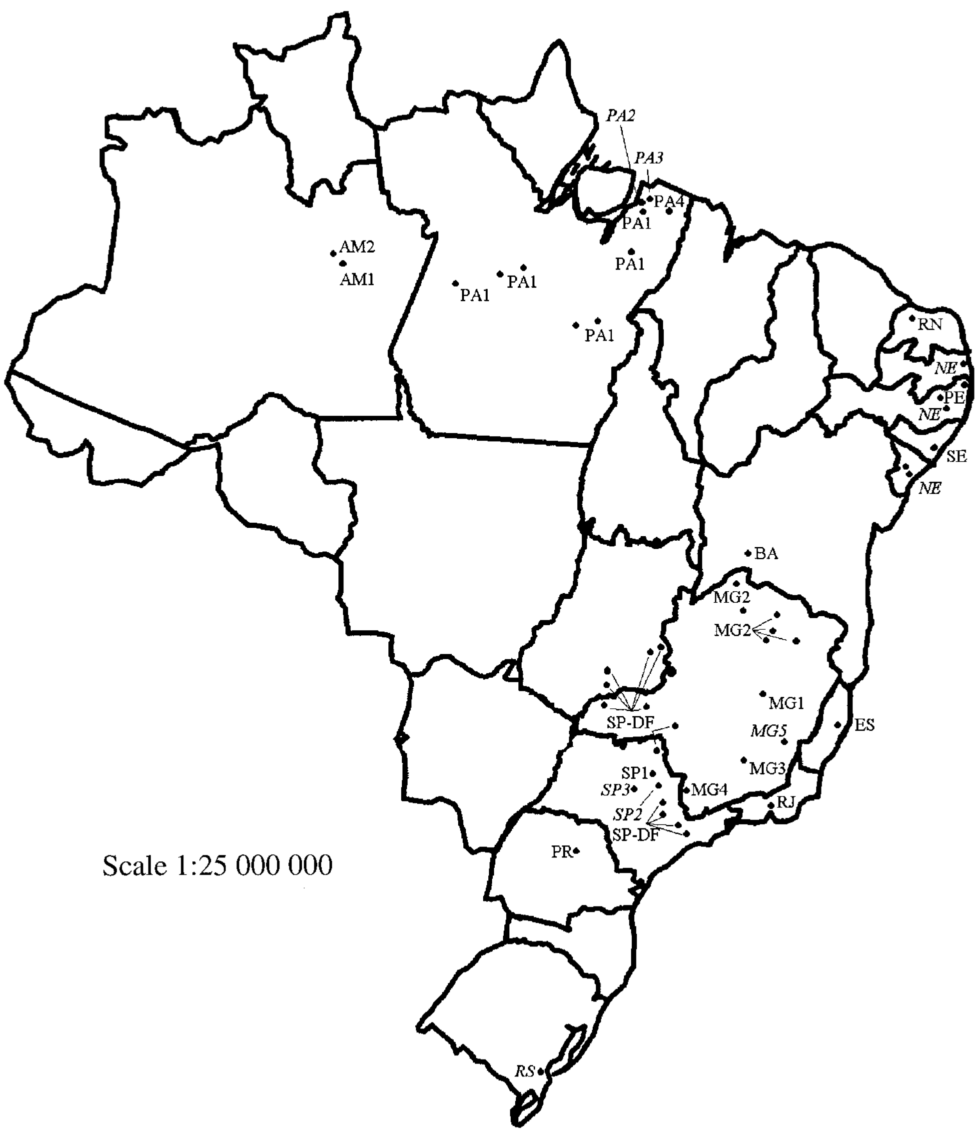

Fig. 1. Location of the soil profiles used in the derivation of the pedotransfer function. Data used for the validation are also shown, in italics. For further details refer to Table 1.

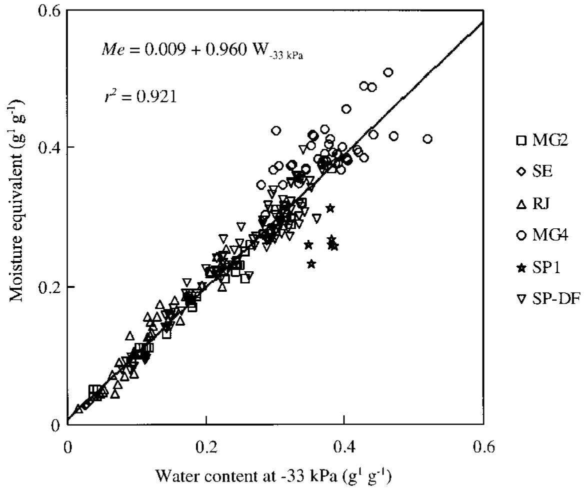

Fig. 2. Comparison between the moisture equivalent obtained by centrifuging (M_e) and the gravimetric water content at −33 kPa (W^{-33kPa}) obtained using the pressure chamber method.

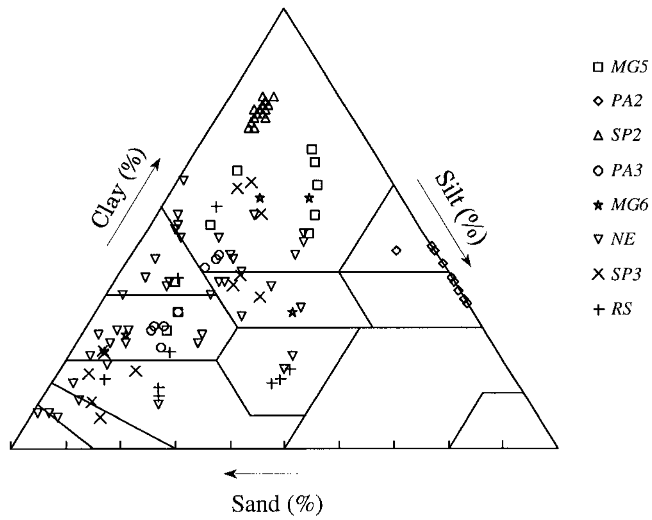

Fig. 4. Textural classification of the data set used in the validation of the pedotransfer function.

validation on the textural triangle. Tietje and Tapkenhinrichs (1993) used a data set of soils from Germany to compare a range of published PTFs, and their Fig. 1 showed these data plotted on the textural triangle. There is a very pronounced difference in the particle-size distribution between the German and Brazilian data sets, notably with regard to silt content: in the area of the textural triangle indicating clay contents >30% and silt contents <17%, there was a strong concentration of Brazilian soils, but no German soils. Oliveira (1968) noted that, in general, >60% of the Brazilian soils of the northeast and southeast had a silt content of <10%, and ≈85% had a silt content of <20%. Tomasella and Hodnett (1998) found a similar distribution in Amazonia and concluded that in this humid tropical region, only hydromorphic soils may have a silt content of >40%. This can be seen in Fig. 3. The soils coded AM are from Central Amazonia: AM1 are hydromorphic soils from Careiro Island and these contrast strongly with the soils coded AM2 from the uplands.

Table 2 summarizes, for each variable, the maximum, minimum, mean, and standard deviation for the data set used in the derivation and validation of the PTF. It can be seen that for the two soil groups, the average silt content is usually between 15 and 20%, and rarely exceeds 50%. In contrast, the clay content averages >40%, and usually ≈60%. The mean bulk density is ≈1.25 g cm^{-3}, which probably reflects the dominance of low-density kaolinitic clay soils in Brazil. Although there are differences in the maximum and minimum values of the variables, the t test showed that both data sets are statistically similar. Except for a single value for coarse sand, the maximum and minimum of the validation group are enclosed by the derivation data set.

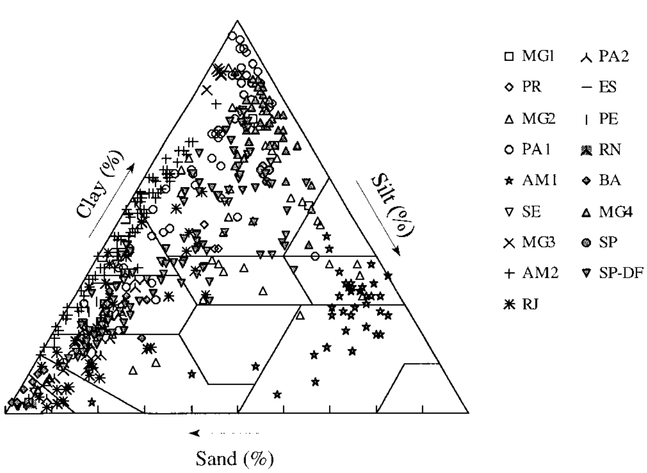

Fig. 3. Textural classification of the data set used in the derivation of the pedotransfer function.

Tietje and Tapkenhinrichs (1993) and Rawls et al. (1991) have presented excellent reviews of the most common PTFs. Pedotransfer functions can be classified into three groups according to the estimation procedure: the point regression method, the physical model method, and the functional parameter regression method. Most recent approaches (e.g., Vereecken et al., 1989) used the last of these three methods, which relates analytical water retention parameters, able to describe the whole range of matric potential variability, to textural data.

Cuenca et al. (1996) demonstrated that simulation of the atmospheric boundary layer is sensitive to different parameterization of soil water processes. They recommended incorporating the van Genuchten (1980) parameterization into the atmospheric boundary layer simulation since, of the representations available, it is the most realistic when compared with laboratory and field measurements. Therefore, the PTF developed in this paper is based on the van Genuchten (1980) water retention equation, given by

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

where θ is the volumetric soil water content (cm^3 cm^{-3}); θ_s and θ_r are the saturated and residual water content, respectively; $|\psi|$ is the absolute value of the matric potential (kPa); and α (kPa^{-1}), n, and m are shape parameters, derived by fitting Eq. [1] to observed water retention data. van Genuchten (1980) assumed that $m = 1 - 1/n$, which allows the derivation of an analytical expression for hydraulic conductivity. Vereecken et al. (1989) showed that there is more flexibility in fitting the water retention curve if m is set to 1, rather than assuming $m = 1 - 1/n$. However, fixing m to 1 will result in values of n that are not directly comparable to those of van Genuchten (1980), and the ability to predict hydraulic conductivity using the parameters of Eq. [1] will be lost. Based on our experience, the optimization of Eq. [1] for Brazilian soils

Table 2. Ranges of soil texture (according to USDA classification) and other basic information in the data base used for pedotransfer function derivation and validation.

Variable	Coarse sand	Fine sand	Silt	Clay	Organic C	Moist. Eq.	Bulk density
	%				g kg^{-1}	g g^{-1}	g cm^{-1}
				Derivation			
Mean	**21.82**	**18.78**	**15.70**	**43.73**	**9.133**	**0.2374**	**1.2742**
Maximum	**74.60**	**93.00**	**71.00**	**96.00**	**59.500**	**0.5319**	**1.9100**
Minimum	**0.00**	**0.00**	**0.00**	**1.70**	**0.063**	**0.0150**	**0.7800**
SD	**19.46**	**17.67**	**16.03**	**23.37**	**7.851**	**0.1207**	**0.2097**
				Validation			
Mean	**23.08**	**17.49**	**18.21**	**41.22**	**8.663**	**0.1967**	**1.3298**
Maximum	**76.00**	**62.65**	**67.00**	**80.00**	**47.600**	**0.5133**	**1.6540**
Minimum	**0.00**	**0.00**	**1.00**	**7.00**	**0.638**	**0.0295**	**0.7800**
SD	**17.11**	**13.53**	**15.59**	**20.60**	**7.640**	**0.1053**	**0.1829**

rarely produces values of θ_r lower than 0, which seems to be the main reason for loss of flexibility of Eq. [1] for fitting the water retention curve of some soils (Vereecken et al., 1989). For this reason, we used the assumption that $m = 1 - 1/n$.

Deriving the pedotransfer function

To derive the PTF, the following steps were followed:

Step 1

The van Genuchten (vG) parameters θ_s, θ_r, α, and n of Eq. [1] were all estimated fitting the water retention curves of Table 1 to Eq. [1], producing 517 sets of values for the parameters, using the Rosenbrock (1960) algorithm. In the data set, porosity (when available) was assumed to be equal to a measured volumetric water content at saturation and was used as a starting value of θ_s in the optimization. The initial value of θ_r in the optimization was set to the minimum measured water content (at −1500 KPa).

Step 2

Multiple linear-regression techniques were used to relate each of the parameters of Eq. [1] to texture, organic C, moisture equivalent, and bulk density, using a second-order polynomial with linear coefficients with the following form:

$$X_i = a_{i,1} + a_{i,2}\mathrm{CS} + a_{i,3}\mathrm{FS} + a_{1,4}S + a_{i,5}C + a_{i,6}\mathrm{OC} + a_{i,7}M_e + a_{i,8}D_b + a_{i,9}\mathrm{CS}\cdot\mathrm{FS} + \ldots + a_{i,j}S\cdot C + a_{i,j+1}\mathrm{CS}^2 + \ldots + a_{i,n}S^2 \qquad [2]$$

where x_i is the value of the parameter of Eq. [1] ($i = 1, 4$ corresponds to α, n, θ_s, and θ_r, respectively) or its natural logarithm (only for α and n , as suggested by Vereecken et al., 1989); CS, FS, S, and C are, respectively, the percentages of coarse sand (2–0.2 mm), fine sand (0.2–0.05 mm), silt (0.05–0.002 mm), and clay (<0.002 mm); OC is the percentage of organic C; M_e is the moisture equivalent (g g^{-1}); D_b is the bulk density (g cm^{-3}); and $a_{i,j}$ ($j = 1..n$) are coefficients derived by multiple linear regression.

Equation [2] provided the most accurate estimations to our measured data. Saxton et al. (1986) used a similar expression (with texture combinations until the third order), while Vereecken et al. (1989) used the square of sand content for log n. In another study, Wösten et al. (1995) derived a PTF that included first- and second-order terms and the reciprocal and logarithm of the independent variables. Both the reciprocal and the logarithm of independent variables could be approximated by a second-order polynomial similar to Eq. [2] in the range of variability of the independent variable, without the restriction of singularity whenever the variable is zero.

Unlike texture, the square of moisture equivalent and the square of bulk density did not explain a significant part of the variability of the vG parameters in the data set. Therefore, and for the sake of simplicity, we did not use combinations of M_e and D_b with texture.

The reason why expressions analogous to Eq. [2] give reasonable estimations of water-release parameters might be related to the logistic distribution of the cumulative particle-size distribution curve. Scheinost et al. (1997), who used the Arya and Paris (1981) assumptions of connections between pore-size and particle-size distribution, suggested that the geometric mean diameter of the cumulative particle-size distribution curve should be linearly related to α and its standard deviation to the reciprocal of n. The same principle was invoked by Rajkai et al. (1996), who used the mean particle-size diameter and its standard deviation as independent variables to estimate vG retention parameters. Mathematical manipulation will show that the geometric mean diameter (see, for instance, Eq. [1] of Scheinost et al., 1997) could be approximated by second-order polynomials, which will result in a combination of particle sizes similar to Eq. [2], and will therefore be related to the water retention parameters. Since a widely accepted theory that relates the particle-size and water retention properties for all soil types is not available, it was felt that empirical relationships such as Eq. [2] are useful and convenient.

Step 3

For the sake of parsimony, the number of parameters in Eq. [2] was reduced using step-wise techniques (probability level 0.01), leaving in the final equation only those variables that explained a significant proportion of the parameter variability. This was also to avoid the problem that some terms of Eq. [2] are linear combinations of others (for instance, $\mathrm{CS} = 100 - \mathrm{FS} - S - C$) that do not introduce additional information into the regression equation and cause multicollinearity. The final correlation matrix of independent variables was also inspected to avoid this problem, as suggested by Wösten (1997). Since basic data from soil surveys do not always provide information such as bulk density and moisture equivalent, four equations were derived for each vG parameter, depending on the amount of information available: Level 1 included all basic information (coarse sand, fine sand, silt, clay, organic C, bulk density, and moisture equivalent); Level 2 excluded bulk density; Level 3 excluded moisture equivalent; and Level 4, excluded both bulk density and moisture equivalent.

Step 4

The coefficient of determinations derived in Step 3 indicated that the estimated values for the parameters α and n were not as good as those for θ_s and θ_r. Poor estimation of vG parameters has consequences for the quality of the water retention curve predicted by the PTF. To improve the quality

Table 3. Mean, minimum, and maximum values resulting from the fitting of van Genuchten (1980) model, and mean difference (MD), root mean square difference (RMSD), and sum of the square errors (SSE) for each water-release curve.

Parameter	Mean	Minimum	Maximum	SE†
α (kPa^{-1})	1.0631	0.0150	10.6045	1.1483
n	1.5710	1.1534	6.6018	0.1838
θ_s (cm^3 cm^{-3})	0.5020	0.2575	0.7305	0.0131
θ_r (cm^3 cm^{-3})	0.1866	0.0001	0.4838	0.0275
MD (100 cm^3 cm^{-3})	0.0132	−0.6346	0.5687	
RMSD (100 cm^3 cm^{-3})	0.6576	0.0021	3.5802	
SSE (100 cm^3 cm^{-3})	0.0510	0.0000	0.8058	

† SE indicates the mean standard error of the estimation.

of the prediction of the matric potential–soil moisture measured values, a new optimization was run: the simplified equations (from Step 3), used to predict the vG parameters from readily available data, were introduced into the van Genuchten equation, Eq. [1]. The coefficients of the equations (i.e., $a_{1,1}$, ...$a_{4,n4}$) were then fitted to minimize the deviations between estimations and observations for all pairs of soil water content–matric potential data simultaneously, using the Rosenbrock (1960) algorithm. Since substituting the equations derived in Step 3 into Eq. [1] leads to an estimation equation with a very large number of parameters, the optimization was carried out in stages: first the linear coefficients corresponding to α ($a_{1,1}$,$a_{1,2}$, ...$a_{1,n1}$) were optimized, followed by those of n ($a_{2,1}$, $a_{2,2}$, ...$a_{2,n2}$), θ_s ($a_{3,1}$, $a_{3,2}$, ...$a_{3,n3}$), and finally those of θ_r ($a_{4,1}$, $a_{4,2}$, ...$a_{4,n4}$). This procedure was repeated until no significant improvement in the sum of the squared errors was observed.

This methodology gives more weight to those curves defined by a greater number of observations, and for the water retention curves with the most frequently occurring particle-size distributions. An important aspect of this procedure relates to the sensitivity of the van Genuchten (1980) equation: Vereecken et al. (1989) showed that the van Genuchten (1980) water retention curve is not equally sensitive to a percentage change of any of the four parameters. Therefore, errors in the estimation (and the sign of the error) of one particular parameter have more impact on the shape of the water retention curve than the others. The methodology proposed here implicitly takes into account these characteristics.

The quality of the fittings of the water retention curves resulting from Steps 3 and 4 were evaluated calculating the sum of squared errors (and testing the difference by the F test), and using the mean difference (MD) and the root mean square difference (RMSD), calculated from the following integrals (Tietje and Tapkenhinrichs, 1993):

$$\mathrm{MD} = \frac{1}{d-c}\int_c^d (\theta_p - \theta_m)\,d\psi \qquad [3]$$

$$\mathrm{RMSD} = \sqrt{\frac{1}{d-c}\int_c^d (\theta_p - \theta_m)^2\,d\psi} \qquad [4]$$

where the subscripts p and m indicate predicted and measured soil-moisture values, respectively, and c and d define the integration interval. As suggested by Tietje and Tapkenhinrichs (1993), the integrals were calculated using log10(ψ), and for this reason porosity was assumed to correspond to the water content at a matric potential of −0.01 kPa. The integration boundaries were therefore set to c = log10(0.01 kPa) and d = log10(1500 kPa).

It should be noted that the objective of Step 4 is to provide a fine tuning of PTF parameters, not to derive a new set of equations. For this reason, this step was applied after selecting the most significant variables through the stepwise procedure in Step 3. To check whether independent variables that were not significant in Step 3 might have become significant in Step 4 after the re-optimization, a thorough analysis was carried out. Steps 2 and 4 were repeated including the maximum number of variables of Eq. [2] for each vG parameter, avoiding linear combinations of independent variables by forward inclusion. The difference in the sum of the squared errors was then checked using the F test (Rajkai et al., 1996). A simplified form of Eq. [2] that included only squared and single terms of particle sizes was also tried, to verify if the quality of the estimations were as good as in the case of the inclusion of combinations of particle sizes.

Step 5

Finally, the proposed PTF was validated using data not included in the fitting procedure. These data are coded in

Table 4. Derivation data. Coefficients of Eq. [2], selected in Step 3 by the stepwise procedure at 0.01 probability level, degrees of freedom (DF), and coefficient of determination (r^2).

	Level 1†				Level 2†			
Variable‡	ln α	n	θ_s	θ_r	ln α	n	θ_s	θ_r
	100 kPa^{-1}	× 100	100 cm^3 cm^{-3}		100 kPa^{-1}	× 100	100 cm^3 cm^{-3}	
$a_{i,1}$	248.3130	232.1787	83.2778	−10.3977	−235.2564	232.1787	41.6485	−1.6722
FS								
S			−0.0556	0.2494				0.2823
C	2.1614			0.2898	1.4370			0.2563
M_e	−377.1065	−168.9308	23.5536	54.7640	216.1505	−168.9308	57.4345	49.0371
D_b	−355.0657		−28.1694	5.8190				
OC							1.9329	−0.8201
CS · FS	0.1196				0.0630		−0.0035	
CS · S	0.1537	−0.0546	0.0079		0.1397	−0.0546	0.0053	
CS · C			−0.0050				−0.0054	
FS · S								
FS · C	0.0745	−0.0535	0.0021		0.0357	−0.0535		0.0017
S · C					−0.0531		−0.0037	
CS^2	0.0279	−0.0091	−0.0010		0.0334	−0.0091		
FS^2		0.0169				0.0169		
S^2				−0.0082				−0.0085
C^2				−0.0015				−12
DF	509	511	509	510	509	511	510	509
r^2	0.4124	0.3703	0.8402	0.8262	0.2874	0.3703	0.7350	0.8257

† Level 1 includes all basic information; Level 2 excludes bulk density.
‡ Size fractions and its combinations are in percentage; D_b, (g cm^{-3}); M_e, (g^1 g^{-1}); and OC in percentage.

Table 5. Derivation data. Coefficients of Eq. [2], selected in Step 3 by the stepwise procedure at 0.01 probability level, degrees of freedom (DF), and coefficient of determination (r^2).

	Level 3†				Level 4†			
Variable‡	ln α	n	θ_s	θ_r	ln α	n	θ_s	θ_r
	100 kPa^{-1}	× 100	100 cm^3 cm^{-3}		100 kPa^{-1}	× 100	100 cm^3 cm^{-3}	
$a_{i,1}$	183.2601	176.9160	91.9015	23.7919	−226.5823	176.9160	38.3774	16.0791
CS					4.6172			
FS								
S	−2.0403						0.3697	
C	0.7677			0.1032				0.135
M_e								
D_b	−289.7127		−29.4141	−4.5938				
OC			0.7976				3.2360	
CS · FS	0.0909							
CS · S	0.1651	−0.0397	0.0053		0.0976	−0.0397		
CS · C			−0.0051		−0.0483		−0.0032	
FS · S								
FS · C	0.0650	−0.0448			0.0708	−0.0448	0.0024	
$S \cdot C$				0.0041			−0.0030	0.0040
CS^2	0.0289		−0.0021	−0.0031				−0.0030
FS^2		0.0231	−0.0007	−0.0020		0.0231		−0.0019
S^2		−0.0079		−0.0050		−0.0079		−0.0043
C^2					0.0199		0.0025	
DF	509	512	510	510	511	512	510	511
r^2	0.4001	0.3470	0.8318	0.7716	0.2745	0.3470	0.6631	0.7661

† Level 3 excludes moisture equivalent; Level 2 excludes both moisture equivalent and bulk density.
‡ Size fractions and its combinations are in percentage; D_b, (g cm^{-3}); M_e, (g^1 g^{-1}); and OC in percentage.

italics in Table 1. Comparisons of the performance of the newly derived PTF with those of Saxton et al. (1986) and Vereecken et al. (1989) were carried out using Eq. [3] and [4].

RESULTS AND DISCUSSION

Table 3 shows the results of fitting Eq. [1] (Step 1) to 517 water retention curves in the data set. The total sum of the squared errors, SSE, was 0.26367 cm^3 cm^{-3}, resulting in an average value of 0.00051 cm^3 cm^{-3} in each curve. Only seven individual curves had SSE higher than 0.005 cm^3 cm^{-3}, and those curves were inspected to detect possible measurement errors. Higher values of SSE were generally due to scatter in the measurements (inconsistent data). There were occasional curves that had very small changes of water content from saturation to −100 kPA and then an abrupt drop in water content; these tended to have poorer fits. For those curves where the optimization produced unusual values of vG parameters (see maximum and minimum of Table 3), inspection of the data and the fitted curve did not suggest errors in the measured data or problems in the optimization. Although these curves might affect the quality of the derived PTF, it was decided to keep them in the dateset since they represent field variability. It was noted that occasional values of θ_r appeared to be very high, however, they were not inconsistent with the raw data. M.G. Hodnett (personal communication, 1999) has noted that 2% (mainly montmorillonitic and kaolinitic clay soils) of a data set of 750 tropical soils had θ_r values >0.4 cm^3 cm^{-3}.

The final form of the equations resulting from Step 3 are given in Tables 4 and 5, where the quality of the fitting is expressed by the coefficient of determination r^2. Table 4 shows that the r^2 is very significant for θ_s and θ_r. The relationships for α and n, although statistically significant, are not as good, especially for Levels 3 and 4.

There are various reasons for the scatter observed in the estimations of α and n. Parameters are likely to be poorly defined and fits may be poor for the curves with fewer measured data points, particularly in the range where the soil moisture is most sensitive to variations of matric potential. As a result, the parameters resulting from the optimization may not fully reflect the influence of particle size. Measurement errors could also lead to unexpected values of the parameters. In addition, there are methodological problems in deriving the water retention curve using pressure chambers and these may influence the results coming from different laboratories (Moraes et al., 1993). However, this problem is probably common to all large data sets of soil water retention data.

To increase the quality of the predictions and to avoid the problems discussed earlier, the estimation equations of Table 4 were substituted for the parameters of Eq.

Table 6. Sum of squared errors (SSE), average mean difference (MD), and root mean squared difference (RMSD) resulting from the optimization on Steps 3 and 4.

Parameter	Level 1		Level 2		Level 3		Level 4	
100 cm^3 cm^{-3}	Step 3	Step 4	Step 3	Step 4	Step 3	Step 4	Step 3	Step 4
SSE	765.13	470.40**	804.69	544.34**	906.37	724.95**	917.12	805.60†
MD	−0.7815	−0.0939	−0.6782	−0.0515	−0.8200	−0.1380	−0.7825	−0.1694
RMSD	3.7442	3.2989	4.1760	3.7153	4.0588	3.8365	4.4533	4.2711

** Significant at 0.01 probability level.
† Significant at 0.1 probability level.

Table 7. Derivation data. Coefficients of Eq. [2], obtained by optimization, fitting all the observed data simultaneously (Step 4).

	Level 1†				Level 2†			
Variable‡	ln α	n	θ_s	θ_r	ln α	n	θ_s	θ_r
	100 kPa^{-1}	× 100	100 cm^3 cm^{-3}		100 kPa^{-1}	× 100	100 cm^3 cm^{-3}	
$a_{i,1}$	264.4658	219.0951	82.1929	−13.3652	−200.8303	217.4984	42.1253	−1.0223
CS								
FS								
S			−0.0177	0.2497				0.1754
C	1.2123			0.3379	1.0190			0.2770
M_e	−378.6112	−152.9655	23.2383	39.9141	184.9474	−147.4518	57.9073	48.3545
D_b	−328.3456		−28.6741	7.6764				
OC							1.5587	−1.5731
CS · FS	0.0052				−0.0284		−0.0039	
CS · S	0.0775	−0.0299	0.0049		0.0378	−0.0295	0.0033	
CS · C			−0.0029				−0.0041	
FS · S								
FS · C	0.0963	−0.0345	0.0027		0.0634	−0.0375		0.0014
S · C					−0.0625		−0.0042	
CS^2	0.0616	−0.0105	−0.0008		0.0657	−0.0099		
FS^2		0.0025				0.0070		
S^2				−0.0048				−0.0046
C^2				−0.0013				−0.0013

† Level 1 includes all basic information; Level 2 excludes bulk density.
‡ Size fractions and its combinations are in percentage; D_b, (g cm^{-3}); M_e, (g^1 g^{-1}); and OC in percentage.

[1] and the optimization was then re-run to minimize differences between predictions and observations. Table 6 shows that the new optimization produced a significant improvement of the fitting, as reflected by the sum of squared errors (SSE) and by the average values of the MD and RMSD. The difference between the SSE resulting from Steps 3 and 4 are significant (0.01 probability level) for Levels 1 to 3, and less significant (0.1 probability level) for Level 4. It was observed that there was a reduction of minimum and maximum deviations, indicated by the reduction of RMSD and by an almost complete elimination of bias as reflected by the value of MD. The improvement was more evident for information of Level 2. Tables 7 and 8 summarize the coefficients resulting from this procedure. From the comparison of the coefficients in Table 4 and 5 and Table 7 and 8, it is clear that all of the coefficients underwent changes, and in many cases these changes were significant.

To check whether variables, not significant according to the stepwise procedure (Step 3), became significant in Step 4 after the re-optimization, we repeated Steps 2 and 4 and included all possible independent variables for each parameter in Eq. [2]. The sum of squared errors resulting from this analysis was compared using the sequential F test against (i) an alternative form of Eq. [2] that includes linear and squared terms of independent variables and (ii) the model coded Level 1 in Table 7. Table 9 provides a summary of this analysis, where the codes *complete*, *squared*, and *Level* 1 indicate, respectively, all possible variables, only linear and squared terms, and the proposed Level 1 model of Table 7. The sequential F test showed that the hypothesis of equal SSE between the complete and Level 1 models is accepted, and rejected in case of the squared model, suggesting that this model is not adequate.

A validation was carried out, using data not used in

Table 8. Derivation data. Coefficients of Eq. [2], obtained by optimization, fitting all the observed data simultaneously (Step 4).

	Level 3†				Level 4†			
Variable‡	ln α	n	θ_s	θ_r	ln α	n	θ_s	θ_r
	100 kPa^{-1}	× 100	100 cm^3 cm^{-3}		100 kPa^{-1}	× 100	100 cm^3 cm^{-3}	
$a_{i,1}$	205.6546	168.8617	91.6203	23.3867	−237.0105	170.9352	36.9797	15.7568
CS					3.6242			
FS								
S	−2.5560						0.3762	
C	−0.1329			0.1103				0.1358
M_e								
D_b	−247.4904		−30.0046	−4.7949				
OC			1.5925				3.2576	
CS · FS	−0.0189							
CS · S	0.1177	−0.0258	0.0022		0.0043	−0.0179		
CS · C			−0.0036		0.0014		−0.0026	
FS · S								
FS · C	0.0517	−0.0261			0.0898	−0.0310	0.0034	
S · C				0.0047			−0.0032	0.0052
CS^2	0.0617		−0.0018	−0.0027				−0.0028
FS^2		0.0093	−0.0010	−0.0022		0.0094		−0.0021
S^2		−0.0077		−0.0048		−0.0081		−0.0045
C^2					0.0178		0.0028	

† Level 3 excludes moisture equivalent; Level 4 excludes both moisture equivalent and bulk density.
‡ Size fractions and its combinations are in percentage; D_b, (g cm^{-3}); M_e, (g^1 g^{-1}); and OC in percentage.

Table 9. Comparison of the performance of different forms of Eq. [2] using the sequential F test after Step 4. The model coded *all* includes all possible terms of Eq. [2], *quadratic* includes linear and squared terms, and Level 1 is the model of Table 6a.

Model	Number of curves predicted	Sum of squared errors	Degrees of freedom	F	F_{crit} ($P < 0.01$)
		100 cm^3 cm^{-3}			
All	517	442.9578	465		
Quadratic	517	507.2123	473	8.4315	2.5496
Level 1	517	470.3360	488	1.2496	1.8507

the fitting procedure (see Table 1), and the performance of the proposed PTF was compared with that of the PTFs of Saxton et al. (1986) and Vereecken et al. (1989). Although van den Berg et al. (1997) have produced a PTF to predict vG parameters for ferralsols and related soils, the basic soil data required include Fe and Al contents, which were not available for the data set used in this study. As a result, it was not possible to make a comparison with the van den Berg (1997) PTF.

Table 10 shows clearly that for the validation data set, the performance of the proposed PTF was much better than the Saxton et al. (1986) and Vereecken et al. (1989) PTFs, in terms of the SSE, MD, and RMSD. However, the ranges of validity of the latter PTFs do not cover the whole range of texture commonly encountered in soils of the tropics. Although the comparison of PTFs outside their range of validity is questionable, the lack of a specific PTF for tropical soils has resulted in applying PTFs derived from temperate regions. The results shown in Table 10 clearly show the risks of using PTFs outside the range of texture from which they were derived and for which they are valid.

The comparison was also carried out for soils whose texture was within the given ranges of validity of the Saxton et al. (1986) and Vereecken et al. (1989) PTFs, according to Table 2 of Tietje and Tapkenhinrichs (1993). The results of these comparisons are summarized in Table 11, together with the range of applicability of each PTF. It is notable that the performance of both temperate PTFs (as shown by SSE, MD, and RMSD) improved considerably when they were used within their range of textural validity. However, the proposed Brazilian soil PTF was still more accurate than the other two PTFs, even though its performance decreased. This shows that even when used within their range of validity, PTFs derived using the soils of temperate regions are less accurate than a PTF derived specifically for tropical soils.

The reason for the lack of accuracy of the Vereecken et al. (1989) and Saxton et al. (1986) PTFs in Brazilian soils was analyzed, plotting the MD and RMSD against silt content. As mentioned in the introduction, one of the distinctive features of Brazilian soils is the generally low silt content when compared with the soils of temperate regions. Figure 5 indicates that for the proposed PTF, the error in terms of MD increases gradually with the silt content, from negative values at <10% silt to a maximum at ≈40%, and then diminishes slowly. In contrast, the Vereecken et al. (1989) PTF shows a gradual decrease in MD from a high value at low silt contents to lower values of MD than those of the proposed PTF at ≈60% silt. Although these high silt contents are outside the range of validity of the Vereecken et al. (1989) PTF, as indicated by the filled symbols in Fig. 5, the values of MD continue to show the same trend as the values within the range of validity. The Saxton et al. (1986) PTF shows a large amount of scatter for low silt contents, with a larger proportion of positive values, and then a decrease from positive values of MD to negative values at a silt content of ≈60%. For low silt contents, it is clear from Fig. 5 that the Saxton et al. (1986) PTF produces the highest errors in terms of MD for those soils outside its range of validity. It is also notable that for both the Saxton et al. (1986) and Vereecken et al. (1989) PTFs, the values of MD are lowest for silt contents >50%, although this is outside the range of validity of both PTFs. This trend suggests that for high silt content Brazilian soils, the errors of the proposed PTF will be greater and the temperate soil PTFs may be more accurate.

Figure 6 shows the values of RMSD plotted against silt content. For clarity, Fig. 7 shows the data from Fig. 6 for average values of RMSD for each 10% increment of silt content. For the proposed PTF, RMSD showed a slight increase with silt content, but a rapid decrease for the other two PTFs. Silt contents outside the range of validity of these PTFs tended to produce high values of RMSD and more scatter. For silt contents >60%, it is difficult to compare the performance of the proposed PTF with those of Saxton et al. (1986) and Vereecken et al. (1989), since the values of texture are outside the range of validity of these PTFs. A direct comparison, disregarding the range of validity, reveals a similar per-

Table 10. Comparison of the average mean difference (MD), root mean square difference (RMSD), and sum of the squares error (SSE) for the proposed pedotransfer function and for those of Vereecken et al. (1989) and Saxton et al. (1986).

Parameter	Level 1	Level 2	Level 3	Level 4	Vereecken	Saxton
100 cm^3 cm^{-3}						
SSE	137.30	182.18	343.18	365.45	1272.13	1527.64
MD	0.9864	1.0894	2.8603	3.3024	5.9134	7.4870
RMSD	3.7825	4.5438	5.3376	5.8437	9.0841	10.4400

Table 11. Comparison of the average mean difference (MD), root mean square difference (RMSD), and sum of the squares error (SSE) for the proposed pedotransfer function (PTF; Level 1) and for those of Vereecken et al. (1989) and Saxton et al. (1986) for the range of applicability of the latter two PTFs.

Parameter	Proposed	Vereecken	Proposed	Saxton
SSE (100 cm^3 cm^{-3})	73.2200	479.3200	89.5400	577.1000
MD (100 cm^3 cm^{-3})	1.2938	6.2355	1.5056	7.6326
RMSD (100 cm^3 cm^{-3})	3.5813	8.8618	3.6766	9.9274
Applicability (%)		66		73

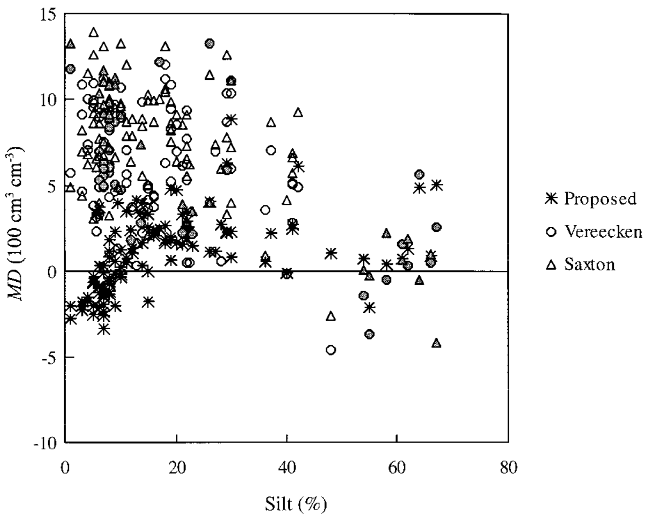

Fig. 5. Comparison of the mean difference (MD) resulting from applying various pedotransfer functions (PTF) to the validation data set. Shaded symbols indicate that the points are outside the textural range of the data from which the corresponding PTF was derived.

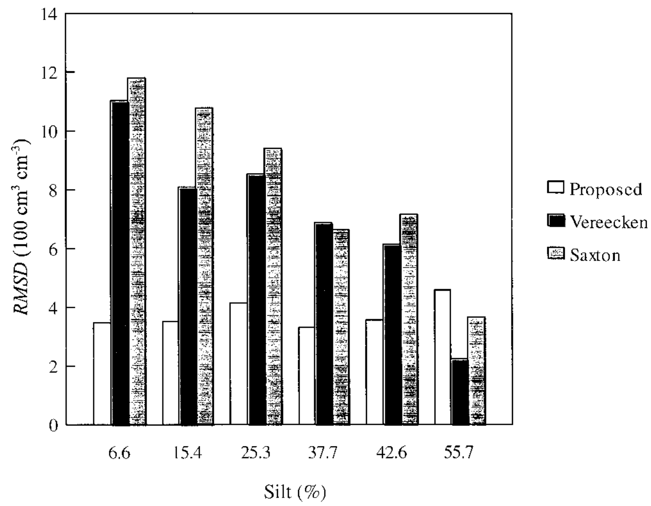

Fig. 7. Root mean square difference (RMSD) data from Fig. 6 calculated for 10% intervals of silt content.

formance for the three PTFs, although the proposed PTF shows less scatter than the other two.

A possible explanation for the success of the proposed PTF compared with the PTFs of temperate soils, even in the range of validity of the latter, might be related to the hybrid character of oxisols. Sharma and Uehara (1968), Sanchez (1976), and Holzhey and Kimble (1988) showed that strongly weathered tropical soils have water retention properties typical of a clay at low matric potentials and resemble sands at high matric potentials. Chauvel et al. (1991), working on Amazonian oxisols, noted that the pore-size distribution of these soils is bimodal, with a large proportion of total porosity concentrated in very fine pores of microaggregates of kaolinite particles, and a further large proportion of meso- and macro-pores of biological origin or caused by fine fissures. The very fine pores are only emptied at potentials >-3000 kPa, beyond the conventionally assumed wilting point value of -1500 kPa, resulting in high values of θ_r. Obviously, the hybrid behavior of these low-density, heavily weathered soils, which do not occur in temperate regions, cannot be captured by PTFs derived for the soils of these regions. Indeed, their unusual behavior might explain the trend observed in Fig. 7. As was shown in Fig. 3 and 4, only recent alluvial, organic, and hydromorphic Brazilian soils, which have not suffered much weathering and leaching, tend to have silt contents of >20%, whereas strongly weathered, kaolinite-rich soils such as oxisols usually have a silt content of 10% or less. The water retention properties of the recent alluvial deposits in the tropics are more similar to those of the

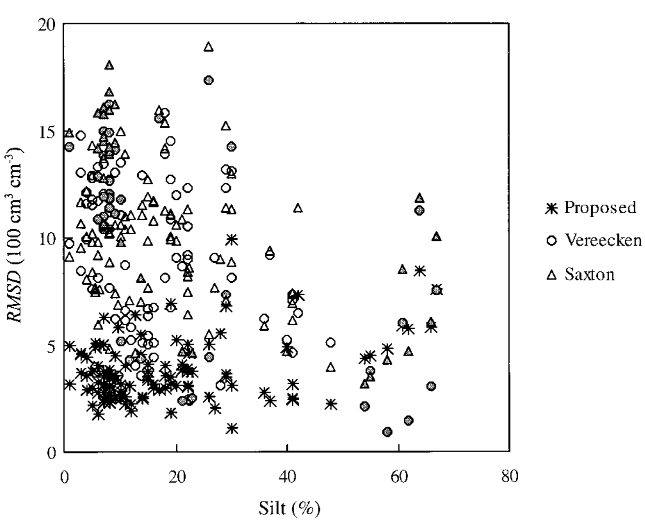

Fig. 6. Comparison of the root mean square difference (RMSD) resulting from the application of various pedotransfer functions (PTF) to the validation data set. Shaded symbols indicate that the points are outside the textural range of the data from which the corresponding PTF was derived.

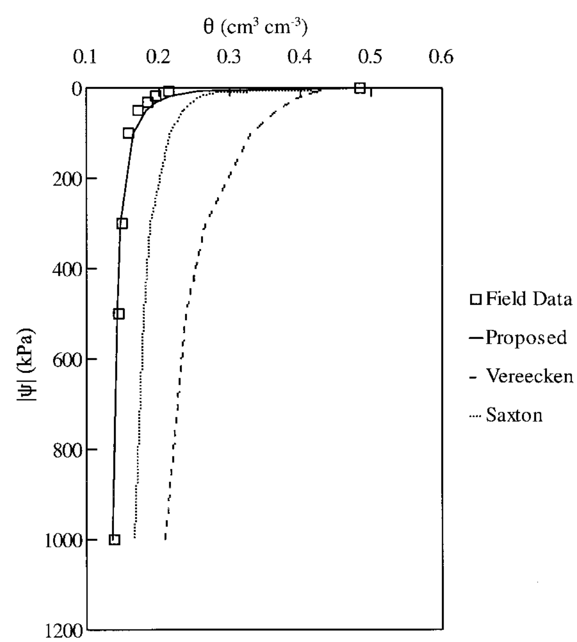

Fig. 8. Comparison of the performance of the proposed pedotransfer function and that of Vereecken et al. (1989) and Saxton et al. (1986) for an example water retention curve.

soils of temperate regions. In addition, a major source of silt in the latter is previous glacial activity, the grinding action of which produces silt-size particles. In addition, deposits of loess are rarely found in the humid tropics.

Figure 8 presents an example of the fitting of the proposed PTF and those of Vereecken et al. (1989) and Saxton et al. (1986) for an individual water retention curve. The soil type is a Latossolo Vermelho Escuro (Oxisol) and the data is within the range of validity of all three PTFs. The silt content is 8%, where, as shown in Fig. 6 and 7, the proposed PTF is the most accurate. It is quite clear the abrupt change of water content between saturation and −100 kPa, typical of oxisols, cannot be reproduced by the temperate soil PTFs. In this particular case, the Saxton et al. (1986) PTF performed better than that of Vereecken et al. (1989), but neither was able to capture the rapid decrease in water content between saturation and −100 kPa.

Although data from other tropical soils will need to be taken into account, Fig. 6 and 7 suggest that it may be possible to derive *universal* PTFs, applicable to all soils by establishing class PTFs according to silt intervals, where the lowest ranges will correspond to strongly weathered, well-drained tropical soils and the higher silt contents to hydromorphic, alluvial, or loess soils of temperate climates.

CONCLUSIONS

Relationships were established between van Genuchten water retention parameters and basic soil properties such as texture, organic C, moisture equivalent, and bulk density. Multiple linear regression analysis was used to derive the best relationship between the fitted vG parameters and the basic soil properties. A significant improvement in the estimation of the parameters describing the water retention curve can be achieved if the equations resulting from the linear regression are substituted into the van Genuchten (1980) equation, and a further optimization is carried out, this time fitting predictions to all measured points simultaneously.

The validation procedure, using an independent data set, demonstrated the ability of the proposed PTF to accurately predict the water retention curve of Brazilian soils, and also revealed the shortcomings of PTFs derived using soils data from temperate regions in predicting the water retention curves of tropical soils. The limitations of the Vereecken et al. (1989) and Saxton et al. (1986) PTFs when applied to Brazilian soils were evident, even within the range of validity (textures) for which they had been derived.

Since current SVAT model simulations have used parameters derived using temperate PTFs, it is expected that there may be significant impacts on the simulations made using these models. Considering that ecological models use water-holding capacity–soil moisture as an input variable (e.g., CASA model; Potter and Klooster, 1997), the current and future scenarios predicted by these models for regions such as Amazonia may be in doubt. The results presented in this paper refer to PTFs used to derive parameters for the van Genuchten (1980) equation. The formulation of Clapp and Hornberger (1978), with its associated ability to predict soil water–retention parameters, is also widely used in GCM modeling. Although this formulation was not specifically tested, the general conclusions from this study are also appropriate: that PTFs derived specifically for tropical soils give better predictions for tropical soils than PTFs derived using soils data from temperate regions.

Because the data set used in deriving and validating the PTF does not cover homogeneously the whole of Brazil (and probably does not include all the soil types), further tests will be necessary to assess the validity of the estimation equations. Additional field data will ultimately prove if changes to the proposed PTF are necessary.

ACKNOWLEDGMENTS

The first and third authors received support from the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq – Brazil). The second author received support from the Natural Environment Research Council of the UK.

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