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Estimation of the van Genuchten Soil Water Retention Properties from Soil Textural Data*1

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ABSTRACT

The van Genuchten (vG) function is often used to describe the soil water retention curve (SWRC) of unsaturated soils and fractured rock. The objective of this study was to develop a method to determine the vG model parameter m from the fractal dimension. We compared two approaches previously proposed by van Genuchten and Lenhard *et al.* for estimating m from the pore size distribution index of the Brooks and Corey (BC) model. In both approaches we used a relationship between the pore size distribution index of the BC model and the fractal dimension of the SWRC. A dataset containing 75 samples from the UNSODA unsaturated soil hydraulic database was used to evaluate the two approaches. The statistical parameters showed that the approach by Lenhard *et al.* provided better estimates of the parameter m. Another dataset containing 72 samples from the literature was used to validate Lenhard's approach in which the SWRC fractal dimension was estimated from the clay content. The estimated SWRC of the second dataset was compared with those obtained with the Rosetta model using sand, silt, and clay contents. Root mean square error values of the proposed fractal approach and Rosetta were 0.081 and 0.136, respectively, indicating that the proposed fractal approach performed better than the Rosetta model.

Key Words: fractal dimension, soil water retention curve, van Genuchten parameterization

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Many soil and water management and environmental protection practices require knowledge of the evolution of water and solutes in the subsurface. During the past several decades, a large number of computer models have been developed to simulate water flow and contaminant transport in saturated and unsaturated soils and fractured rock. Their application is often restricted by a lack of hydraulic property information involving the soil water retention curve (SWRC) and the unsaturated hydraulic conductivity. Furthermore, due to inherent temporal and spatial variability of the hydraulic properties in the field, large numbers of samples are generally required to properly characterize the spatial distribution of the hydraulic properties.

Accurate characterization and estimation of the SWRC has been a major focus of research for more than 60 years. Many empirical models (Gardner, 1958; Brooks and Corey, 1964; Campbell, 1974; Clapp and Hornberger, 1978; van Genuchten, 1980; Hutson and Cass, 1987; Russo, 1988) have been developed for modeling the SWRC. Unfortunately, estimating the coefficients in these various models remains difficult and time-consuming. Several studies consequently have been carried out to predict the coefficients using pedotransfer functions (PTFs) (Cosby *et al.*, 1984; Saxton *et al.*, 1986; Vereecken *et al.*, 1989; Wösten *et al.*, 1995; Wösten, 1997; Rawls *et al.*, 2001), including neural network analyses (Schaap and Bouten, 1996; Schaap *et al.*, 1998; Minasny and McBratney, 2007), and the use of tables

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based on soil texture (Rawls *et al.*, 1982). Schaap *et al.* (2001) recently developed a computer program (Rosetta) that implements five PTFs for hierarchical estimation of the soil water retention and the saturated and unsaturated hydraulic conductivity. The hierarchy in the PTFs allows predictions of the hydraulic parameters using limited (textural classes only) to more extended (texture, bulk density, and one or two water retention points) input data. Rosetta is based on neural network analyses combined with the bootstrap method, thus allowing the program to provide uncertainty estimates of the predicted hydraulic parameters (Schaap *et al.*, 2001). As noted by Giménez *et al.* (1997) most PTFs are essentially empirical, which causes their application to be restricted by the data upon which they were based. Another approach of estimating the SWRC from the particle-size distribution is based on the premise of shape similarity between the water retention curve and the cumulative particle-size distribution. Several quasi-physical models (Arya and Paris, 1981; Haverkamp and Parlange, 1986; Fredlund *et al.*, 2002; Haverkamp *et al.*, 2005; Leij *et al.*, 2005) have been developed using this premise.

Considerable attention has been focused recently on the development of functional relationships between the water content and the matric potential using fractal geometry models. Fractal models have solid mathematical and physical bases in their description of the geometry of porous media. Three types of SWRC models have been proposed based on the fractal organization of soil structure. One type is the mass fractal (Sierpinski carpet or Menger sponge) in which the fractal dimensions of mass, pore surface and pore volume have the same value (Rieu and Sposito, 1991; Perfect, 1999). A second approach is based on the fractal surface (de Gennes, 1985; Toledo *et al.*, 1990) without considering the scaling of mass. A third approach considers the fractal pore-size distribution without any assumption about the geometry of mass and the solid-pore interface (Tyler and Wheatcraft, 1990; Pachepsky *et al.*, 1995; Perrier *et al.*, 1996).

Perfect (1999) presented a SWRC function based on the capillary equation and a randomized Menger sponge algorithm with upper and lower scaling limits. The theoretical equation was fitted to water retention data of six soils collected by Campbell and Shiozawa (1992). While all of the fits were excellent, refitting the same data over restricted subsets of the matric potential caused the fractal dimension to become greater than the theoretical limit of 3.0. Perfect (2005) later presented a modification of Rieu and Sposito's (1991) prefractal water retention equation to accommodate hysteresis during monotonic drying. Model testing consisted of fitting the modified equation to previously published water retention data for different randomized Sierpinski carpets and soils. A more generalized model for the SWRC was recently developed by Bird *et al.* (2000) based on the pore-solid fractal (PSF) distribution. The PSF model displays symmetry between the solid and pore phases (Bird *et al.*, 2000) and includes as special cases several existing models, such as the Brooks and Corey (BC) model (Brooks and Corey, 1964). Theoretically, the PSF model provides a direct method to estimate the SWRC fractal dimension from the particle-size distribution. However, Bird *et al.* (2000) used only two datasets to test their model. Using data from the unsaturated soil hydraulic database (UNSODA), Huang and Zhang (2005) used the PSF model to obtain a method of estimating the fractal dimension by using either clay content or soil textural class.

As an alternative to the BC model, van Genuchten (1980) proposed an empirical SWRC model which assumes a more or less sigmoidal shape and includes three shape parameters (two if the parameters are restricted to certain values). As a special case of the PSF model, the BC model can be related to the van Genuchten (vG) model when certain relationships are assumed between the vG and BC model parameters (van Genuchten, 1980; Lenhard *et al.*, 1989; Morel-Seytoux *et al.*, 1996). Since the power of the BC model is a function of the fractal dimension of the PSF model, this implies that the vG model parameters can also be expressed as functions of the fractal dimension. However, to our knowledge no literature exists where fractal methods have been used to estimate vG model parameters. Thus, the objective of this study was to develop a fractal method for estimating the vG model parameters and the soil water retention curve, and to compare results with those obtained with the Rosetta software, which has been used widely in the literature.

THEORY

The vG model has the following form (van Genuchten, 1980):

$$S_e = \frac{1}{[1 + (\alpha h)^n]^m} \tag{1}$$

where S_e is the effective saturation and calculated by $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$, where θ is the water content ($cm^3\ cm^{-3}$), θ_r is the residual water content, and θ_s is the saturated water content, and where h is the matric potential (kPa), and α (kPa^{-1}), n and m ($m = 1 - 1/n$) are empirical parameters.

Assuming no residual water, the BC model (Brooks and Corey, 1964) has the following form:

$$\frac{\theta}{\theta_s} = \left(\frac{h}{h_{\min}}\right)^{-\lambda} \tag{2}$$

where λ is an empirical parameter often referred to as the pore size distribution index, and $h_{\min}$ is the air entry value (kPa). Assuming the fractal pore-size distribution to be that of a Sierpinski carpet, Tyler and Wheatcraft (1990) proposed a SWRC model without a lower cut-off of scale, which has a form similar to the BC model:

$$\frac{\theta}{\theta_s} = \left(\frac{h}{h_{\min}}\right)^{D-E} \tag{3}$$

where E is the Euclidian dimension, being equal to 2 or 3 for two- and three-dimensional systems, respectively, and D is the fractal dimension of the SWRC. Based on the assumptions of a Sierpinski carpet, the fractal dimension D can be defined as (Mandelbrot, 1983):

$$D = \frac{\log[(b^i)^E - z]}{\log(b^i)} \tag{4}$$

where b is a scale factor and z is the number of removed squares in each iteration i of the Sierpinski carpet.

Eq. 3 has a similar form as the BC model. The fractal dimension D could explain the empirical exponent λ (Huang *et al.*, 2006). We note that the corresponding fractal model is only a distribution model without considering the solid phase. The power-law form of the SWRC is a special case of the pore-solid fractal model (Bird *et al.*, 2000; Huang and Zhang, 2005), and has been presented also by de Gennes (1985), Hunt and Gee (2002), and Xu (2004).

Lenhard *et al.* (1989) related the BC and vG models by equating the differential fluid saturation capacities, dS_e/dh, of the two models to obtain the following relationship between the BC model pore size distribution index λ and the vG model parameter m:

$$\lambda = \frac{m}{1-m}(1 - S_e^{1/m}) \tag{5}$$

To define a single "effective" λ, the authors proposed using S_e equal to 0.5 in accordance with the suggestion by van Genuchten (1980) that the best location for evaluating dS_e/dh is midway between the saturated and residual water contents. Employing this approach, Eq. 5 becomes:

$$\lambda = \frac{m}{1-m}(1 - 0.5^{1/m}) \tag{6}$$

Comparing Eqs. 2 and 3 and considering a three-dimensional Euclidian domain, one has:

$$\lambda = 3 - D \tag{7}$$

Substituting Eq. 7 in Eq. 6 leads to:

$$D = 3 - \frac{m}{1-m}(1 - 0.5^{1/m}) \tag{8}$$

Based on Eq. 8, the value of m can be estimated from the fractal dimension D of the SWRC. Another way to estimate m from D is using one of the van Genuchten (1980) restrictions on the value of m. When assuming $m = 1 - 1/n$, we have:

$$\lambda = n - 1 \tag{9}$$

which results from equating the BC and vG models at large values of h such that $(\alpha h)^n \gg 1$ in Eq. 1, and hence $\lambda = mn$. The equation alternatively follows from Eq. 5 by setting $S_e = 0$. Eq. 9 was used by Ma *et al.* (1999). Substituting Eq. 9 into 7 and using $m = 1 - 1/n$, one has:

$$m = \frac{3-D}{4-D} \tag{10}$$

A relationship between $h_{\min}$ (kPa) and the vG model parameter α (kPa^{-1}) was suggested by Lenhard *et al.* (1989) as follows:

$$\alpha = \frac{S_x^{1/\lambda}}{h_{\min}}(S_x^{-1/m} - 1)^{1-m} \tag{11}$$

where S_x is a match-point effective wetting phase saturation and is given by the empirical equation:

$$S_x = 0.72 - 0.35\exp(-n^4) \tag{12}$$

Based on an analysis of 24 compacted clay samples, Tinjum *et al.* (1997) presented another empirical relationship between $h_{\min}$ (kPa) and α (kPa^{-1}):

$$\alpha = 0.078(h_{\min})^{-1.26} \tag{13}$$

MATERIALS AND METHODS

The measured SWRC data of 75 soil samples (*i.e.*, dataset 1) with a wide range of textures (as shown in Table I) were taken from the UNSODA database of Leij *et al.* (1996) to analyze the relationships between the fractal dimension and the soil hydraulic parameters, especially m in Eqs. 8 and 10.

TABLE I

Soil properties of the 75 samples from the unsaturated soil hydraulic database (Leij *et al.*, 1996) and the fitted van Genuchten model (1980) parameters m and α

Texture	No. of samples	D[a]		$h_{\min}$[b]		m		α	
		Max	Min	Max	Min	Max	Min	Max	Min
				kPa				kPa^{-1}	
Sand	6	2.668	2.245	1.73	0.36	0.85	0.47	1.28	0.20
Loamy sand	8	2.817	2.493	1.21	0.29	0.68	0.16	1.30	0.30
Sandy loam	6	2.915	2.667	1.61	0.12	0.73	0.11	5.61	0.09
Sandy clay loam	5	2.946	2.877	2.03	0.28	0.39	0.07	1.60	0.20
Sandy clay	3	2.965	2.922	19.05	1.49	0.26	0.11	0.24	0.01
Loam	8	2.920	2.861	2.68	0.24	0.34	0.08	1.97	0.09
Silt loam	7	2.907	2.744	2.37	0.39	0.29	0.09	1.47	0.13
Silty clay loam	10	2.947	2.819	4.42	0.49	0.48	0.09	1.51	0.01
Clay loam	5	2.967	2.851	1.24	0.32	0.26	0.05	2.46	0.21
Silt	1	2.802	-	0.92	-	0.25	-	0.10	-
Silty clay	8	2.960	2.832	4.07	0.02	0.50	0.05	16.30	0.04
Clay	8	2.969	2.941	3.74	0.02	0.13	0.02	50.30	0.01

[a] D is the fractal dimension of soil water retention curve; [b] $h_{\min}$ is the air entry value.

The vG model parameters m, α and θ_r were calculated directly by fitting the vG model to the measured data using the RETC (RETention Curve) program (van Genuchten *et al.*, 1991), given the condition that $m = 1 - 1/n$. The fractal dimension and air entry value were determined directly by fitting the Tyler and Wheatcraft's (1990) model (*i.e.*, Eq. 3) to the measured data by nonlinear least-squares optimization method using the MATLAB software (MathWorks, 2005). The calculated fractal dimension was subsequently used to estimate the values of m of the 75 soil samples using Eqs. 8 and 10. Values for α were estimated by Eqs. 11 and 13, in which m and $h_{\min}$ were the directly determined values. The estimated m and α values were subsequently compared with the directly calculated m and α values.

Another 72 soil samples (referred to as dataset 2) representing 11 different soil textures, collected from the literature (Puckett *et al.*, 1985; Leij *et al.*, 1996; Huang *et al.*, 2006), were used to further test the various methods for estimating m and α. Selected properties of these samples are presented in Table II.

TABLE II

Soil properties of 72 samples collected from the literature and the fitted van Genuchten model (1980) parameters m and α

Texture	No. of samples	Clay content		m		α	
		Max	Min	Max	Min	Max	Min
		g kg^{-1}				kPa^{-1}	
Sand	2	18	14	0.61	0.55	0.28	0.27
Loamy sand	10	108	23	0.61	0.25	0.45	0.24
Sandy loam	11	178	70	0.58	0.11	0.50	0.13
Sandy clay loam	15	349	208	0.46	0.06	0.40	0.15
Loam	7	260	122	0.49	0.19	0.50	0.18
Silt loam	5	270	120	0.20	0.12	0.98	0.15
Silty clay loam	8	390	280	0.30	0.12	0.90	0.10
Clay loam	6	348	304	0.39	0.05	0.50	0.08
Sandy clay	5	421	352	0.33	0.09	0.50	0.18
Silty clay	2	460	420	0.09	0.08	0.65	0.55
Clay	1	452	-	0.34	-	0.09	-

We evaluated two methods for estimating m when $m = 1 - 1/n$. One approach (method 1) was based on Eq. 8 with known D values estimated by a relationship proposed by Huang and Zhang (2005):

$$D = a_0 + \frac{1 - e^{a_1 C_p}}{a_2(1 + e^{a_1 C_p}) + a_3(1 - e^{a_1 C_p})} \quad (14)$$

where C_p is the soil clay percentage, and a_0, a_1, a_2 and a_3 are constant coefficients equal to 2.35, 0.0822, −0.497 and 1.238, respectively. Eq. 14 was based on data from 148 disturbed and undisturbed soil samples. Method 2 used the Rosetta software assuming known clay, silt and sand percentages. The methods used for estimating α were: (1) Eq. 11 with $h_{\min}$ determined from the literature (Rawls *et al.*, 1982) for different soil textures, and λ and m from Eqs. 7 and 8, respectively, while the fractal dimension was estimated from the clay content using Eq. 14; and (2) the Rosetta software using sand, silt and clay contents. Consequently, the estimated vG model parameters using methods 1 and 2 as well as the measured saturated water content were used to estimate the soil water retention curve.

For the estimation and validation procedures, the following statistical measures were used to evaluate the results: mean of residuals (MR), root mean square error (RMSE), and Akaike's information criterion (AIC), which are calculated as follows:

$$\mathrm{MR} = \frac{\sum_{i=1}^{j}(P_i - O_i)}{j} \quad (15)$$

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{j}(P_i - O_i)^2}{j}} \tag{16}$$

$$\mathrm{AIC} = j\ln\left(\frac{\sum_{i=1}^{j}(P_i - O_i)^2}{j}\right) + 2q \tag{17}$$

where O_i and P_i are the observed and predicted values, respectively; j is the number of observations; and q is the number of model parameters.

RESULTS AND DISCUSSION

For dataset 1 (Leij *et al.*, 1996), the estimated m values were obtained with Eqs. 8 and 10. A comparison of the estimated m values with the directly calculated values as obtained with RETC is shown in Fig. 1. The two equations both underestimated m as evidenced by the negative MR values listed in Table III. Predictions of m using Eq. 8 were slightly better than those obtained with Eq. 10. This result is further confirmed by the relatively low RMSE and AIC values obtained with Eq. 8 as shown in Table III. Similar results were also found by Ma *et al.* (1999).

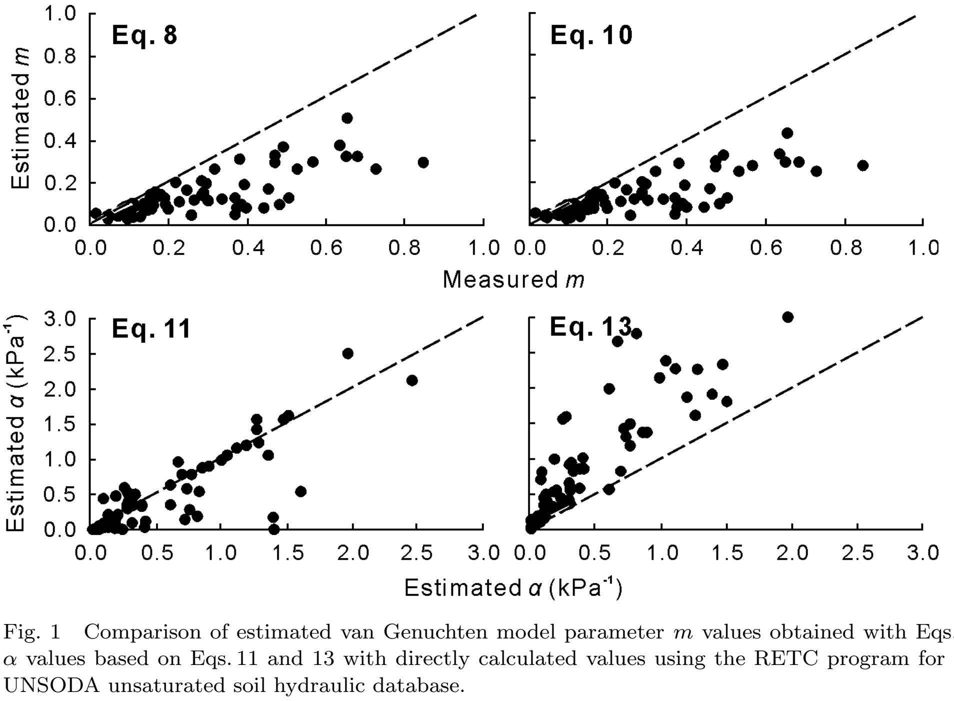

Fig. 1 Comparison of estimated van Genuchten model parameter m values obtained with Eqs. 8 and 10 and estimated α values based on Eqs. 11 and 13 with directly calculated values using the RETC program for 75 soil samples from the UNSODA unsaturated soil hydraulic database.

TABLE III

Statistical parameters for different methods used to estimate the van Genuchten (1980) model parameters m and α (kPa^{-1}) for the 75 soil samples from the unsaturated soil hydraulic database

Parameter	Model	Mean of residuals	Root mean square error	Akaike's information criterion
m	Eq. 8	−0.120	0.176	−258.7
	Eq. 10	−0.125	0.183	−252.9
α	Eq. 11	0.100	3.266	174.4
	Eq. 13	3.666	14.760	391.6

In Eq. 8, the only parameter for estimating m is the fractal dimension D ($0 < D < 3$). We found that when D ranged from 0 to 3, the value of m ranged from 0.84 to 0.0001. The value of m hence did not cover the entire range of m values ($0 < m < 1$). The values of m were found to be underestimated using Eq. 8. Also, the van Genuchten approximation, Eq. 9, assumed that the value of $(\alpha h)^n$ was much higher than 1 so that it was possible to ignore the term 1 in the vG model. By ignoring this factor in Eq. 1, to achieve a constant value for effective saturation, the value of m or n was underestimated. Therefore, Eq. 9 inherently underestimated the m values. The α values were also estimated with Eqs. 11 and 13 for dataset 1. A comparison of estimated α values with directly calculated results using RETC is shown in Fig. 1. Eq. 11 with $\lambda = 3 - D$ was found to give a more reasonable estimation for the α values. As shown in Table III, the RMSE values for Eq. 11 were significantly lower than those of Eq. 13. This confirmed that Eq. 11 with the given $h_{\min}$ and m values estimated α values better than Eq. 13.

Dataset 2 was used for further validation of the proposed methods for estimation of m and α. A comparison of m values estimated with the two methods against the directly calculated m values is shown in Fig. 2. We found that Rosetta (method 2) provided better estimates of the m values than Eq. 8 (method 1). As shown in Table IV, method 2 had lower AIC values than method 1. This implies that the neural network approach of Schaap *et al.* (2001) is more appropriate for estimating the vG model parameter m than the developed fractal approach. As shown in Fig. 2 and by the MR values in

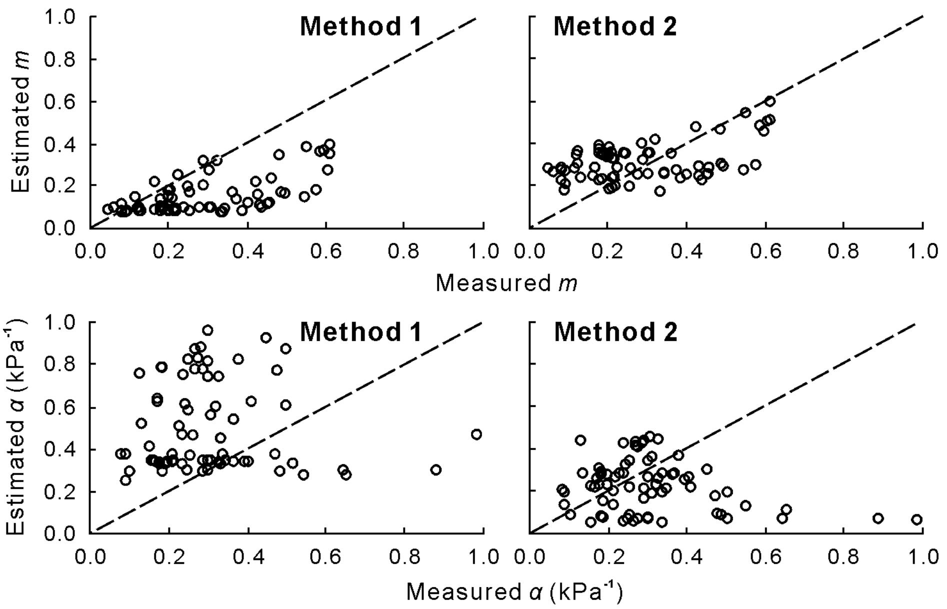

Fig. 2 Comparison of estimated van Genuchten model parameter m values obtained with method 1 based on Eq. 8 and method 2 using the Rosetta software, and estimated α values obtained by method 1 based on Eq. 11 and method 2 using the Rosetta software with directly calculated values using the RETC program for 72 soil samples collected from the literature.

TABLE IV

Statistical parameters for different methods used to estimate the van Genuchten model parameters m and α (kPa^{-1}) and the soil water retention curve (SWRC) for 72 soil samples collected from the literature

Parameter	Method	Mean of residual	Root mean square error	Akaike's information criterion
m	Method 1 (Eq. 8)	−0.130	0.179	−245.7
	Method 2 (Rosetta)	0.028	0.141	−275.7
α	Method 1 (Eq. 11)	0.202	0.337	−150.4
	Method 2 (Rosetta)	−0.078	0.236	−201.7
SWRC	Method 1 (Eqs. 8 and 11)	−0.041	0.081	−3 099.3
	Method 2 (Rosetta)	−0.111	0.136	−2 456.1

Table IV, the Rosetta software (method 2) overestimated the m values. An overestimation of m was also noted by Schaap *et al.* (2001). They found that Rosetta often underestimates the water content. A sensitivity analysis of the vG model showed that the water content was underestimated when the shape parameter n was overestimated. Overestimation or underestimation of the m values with Eq. 8 may be attributed to underestimation or overestimation of the fractal dimension when using Eq. 14.

Dataset 2 was also used to validate different methods for estimating α. Fig. 2 compares α values estimated by methods 1 and 2, with the directly calculated RETC values. We found that the α values estimated with Rosetta (method 2) were in a more restricted range compared with values estimated with method 1. However, both methods were unable to estimate α accurately. As shown by the MR values in Table IV, methods 1 and 2 overestimated and underestimated the α value, respectively. Judging from the AIC values, method 2 estimated the α values better than method 1. To estimate α using method 1, the values of m, λ and $h_{\min}$ should be estimated. The poor results obtained with method 1 may be due to errors in estimating these parameters. The values of $h_{\min}$ were determined using soil textural class PTFs developed by Rawls *et al.* (1982). These PTFs may introduce additional uncertainty since $h_{\min}$ is more related to soil structure and the pore size distribution. It may be better to estimate the maximum pore size from the maximum particle size. Using the relationship between the pore-size and particle-size distributions as proposed by Arya and Dierolf (1992), $h_{\min}$ could be estimated using the Young-Laplace equation and the maximum pore size.

We also found that the fitted α (kPa^{-1}) and $h_{\min}$ (kPa) were closely related. For dataset 1, we established the relationship:

$$\alpha = 0.3126 h_{\min}^{-1.2366} \qquad (R^2 = 0.88,\ m = 1 - 1/n) \tag{18}$$

Eq. 18 is similar to Eq. 13, with only a small difference in the coefficients. However, Eq. 18 was based on 75 soil samples, whereas Eq. 13 was established using only 24 compacted clay specimens.

The estimated vG model parameters m and α obtained with the different methods, in conjunction with measured saturated water contents, were next used to estimate water contents at different matric potentials and compared with measured values. Fig. 3 shows the estimated soil water contents using different methods *versus* the measured values. The MR values in Table IV show that the Rosetta software underestimated the water contents. Similar results were obtained by Schaap *et al.* (2001). The other calculated statistical parameters presented in Table IV (*i.e.*, the RMSE and AIC values) showed that method 1 based on Eqs. 8 and 11 performed better than method 2, in which the Rosetta software was used to estimate the soil water contents. The RMSE value of method 2 was 68% larger than that of method 1, thus indicating that the proposed fractal approach provided better predictions of the soil water retention curve than the Rosetta software using only soil textural properties such as sand, silt, and clay contents.

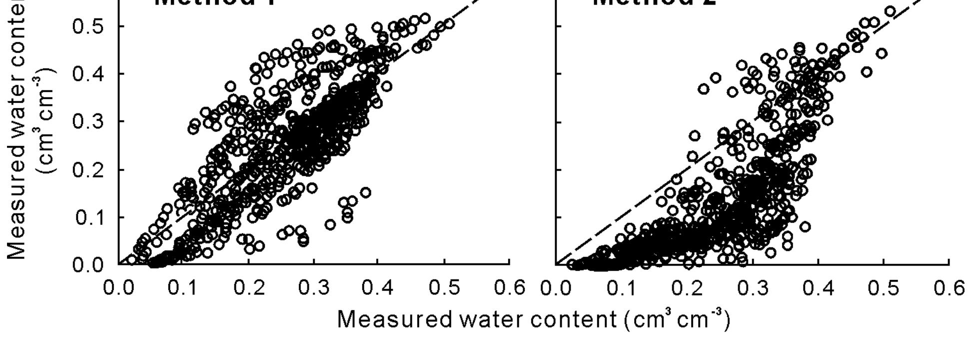

Fig. 3 Comparison of estimated soil water content obtained with method 1 based on Eqs. 8 and 11 and method 2 using the Rosetta software, with measured values of 72 soil samples taken from the literature.

It should be pointed out that the Rosetta software can lead to better estimates of the vG model parameters than the developed fractal approach (Table IV), even though the RMSE and AIC values showed that predictions of the water content using Rosetta were not as good as those obtained with method 1 (Table IV). This is due to the fact that estimation of the water content is a result of an interaction between the estimated vG model parameters, such as between α and m.

CONCLUSIONS

We used a method proposed by Lenhard *et al.* based on relationships between the vG and BC models, and relationships between the BC hydraulic parameters and the pore-solid fractal dimension, to estimate the vG model parameters and subsequently the soil water retention curve. Two datasets, one from the UNSODA database and one from the literature, were used to evaluate and validate the proposed methods. The approach allowed us to establish physical relationships that predict the vG model parameters from the fractal dimension and air entry value. The proposed method was found to perform better than the Rosetta software for the predictions of the soil water retention curve. However, none of the methods we investigated was able to obtain reasonable predictions for the vG model parameter α.

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