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GOLNAZ EBRAHIM ZADEH, HOSSEIN BAYAT*

PEDOTRANSFER FUNCTIONS CAPABILITY TO SIMULATE BEHAVIOUR OF SMECTITIC SOILS IN ESTIMATION OF VARIOUS SOIL WATER RETENTION CURVE MODELS

Abstract. For modelling the flow transport in unsaturated conditions, we can use hydraulic properties which are expensive and time-consuming to be obtained directly because of high variability and complexity of soil systems. Few studies have been done about pedotransfer functions (PTFs) in smectitic soils. Moreover, the utility of fractal parameters in the prediction of soil water retention curve (SWRC) have not been investigated in these soils. In this study, PTFs have been made for estimating the parameters of van Genuchten (VG) and Dexter models by regression and artificial neural networks methods. Therefore, 69 soil samples were collected from Guilan Province, Iran. Fractal and non-fractal models were fitted to the particle size distribution (PSD) and micro-aggregate size distribution (ASD) and their parameters were calculated. To create PTFs, the parameters of PSD and ASD models were used as estimators. The comparison of the results of the two models of Dexter and VG shows the priority of Dexter model for the purpose of testing of smectitic soils. The results showed the superiority of Fredlund *et al.* PSD model parameters and fractal parameters of ASD, in the estimation of Dexter and VG SWRC models, respectively. This outcome may be related to the higher accuracy of Fredlund *et al.* PSD model in the description of the PSD data in the clayey soils. However, the higher number of parameters in comparison to the number of fractal model parameters may be another reason.

One of the significant hydraulic properties employed for modelling the flow transport in porous media is the soil water retention curve (SWRC) which defines the relationship between soil water content and matric potential. It is vital to simulate soil processes, such as soil erosion, soil pollutant movement, and nutrient dynamics [31]. Since, direct measurement of the SWRC is difficult, expensive, time-consuming and needs special equipment [41], pedotransfer functions (PTFs) [29] and physico-empirical methods [30], have been developed

* G.E. Zadeh, MSc., Prof. H. Bayat, DSc.; Department of Soil Science, Faculty of Agriculture, Bu Ali Sina University, Hamadan, Iran.

to estimate SWRC by using available data, such as soil particle size distribution (PSD), soil texture [34], particle density, bulk density, porosity and pore size distribution [4].

The mineral properties of clay are essential for numerous soil functions, including water and nutrient retention, contaminant (pesticides, heavy metals) attenuation, carbon storage, the stability of soil structure and filtering of both ground and surface waters. In temperate regions, 2:1 clay minerals (smectite, vermiculite, illite, chlorite and their intergrades) have been considered to a greater extent as they dominate the clay mineralogy of many soils. Smectite and 'mixed layer' clays have been reported to include an important part of the clay fraction in most areas where Vertisols have been studied [63].

The Vertisols are soils with a high clay content and smectitic type of clays [54] that exhibit high potential of swelling and shrinkage with minimal horizon differentiation due to pedoturbation [1]. Wetting Vertisols make them very plastic and sticky. On wetting the soil increases its volume by swelling, the cracks are closed, and soil level rises [43]. In soils with high clay content under field conditions, the mineral particles are likely to form soil aggregates. Consecutive swelling and drying cycles makes aggregates stronger and smaller [28].

Some researchers have employed pedotransfer functions in various soil types. Tomasella *et al.* [59] used PTFs for estimation of the SWRC in Brazilian soils. Hodnett and Tomasella [27] developed a new PTF for tropical soils. Manyam *et al.* [36] studied the modelling of hydraulic properties in sandy soils of Niger using PTFs. Patil and Rajput [44] evaluated water retention function in shrinking and swelling soils. Das and Verma [11] used PTFs in sandy to clayey soils. Kodaverdiloo *et al.* [33] used PTFs in calcareous soils, and Mosaddeghi and Mahboubi [40] used PTFs in saline soils in Western Iran. However, little research has been conducted on the application of PTFs in smectitic soils.

Estimating hydraulic properties from PSD is particularly useful. Since a detailed characterization of hydraulic properties is usually impossible, PSD may be obtained from soil databases [53]. So, the retention function can be related directly to the PSD of the soil.

Fractal mathematics is a good method to characterize PSD [19]. The introduction of physical models based on the fractal geometry of natural media [35] have provided soil scientists with the first integrated model of soil structure [50]. Various authors [25] have suggested physically based models that use the well-known relation between pore diameter and water potential expressed by Jurin's law, and deduce pore size distribution from the PSD. There are available studies which indicate that data about the structure of the soil can be interpreted by fractal geometry. These studies have proved the existence of a unique fractal dimension (usually a mass fractal dimension) within the scale range where data are available, while other investigations have modelled the SWRC as the effect of an underlying fractal surface [13].

The mass-based models assume that soil pores desaturate as predicted by the Young-Laplace equation [60], while surface-based models consider the existence of a thin layer of water [13, 58].

Bayat *et al.* [7, 8], have used the fractal parameters of particle and aggregate size distributions as predictors to estimate the SWRC using ANNs in non-smectitic soils and reported that the accuracy and reliability of the PTFs were improved. Despite the usefulness and applicability of fractal models, the utility of the fractal parameters especially the fractal parameters of the micro-aggregate size distribution in the estimation of SWRC has not so far been investigated in the smectitic soils. On the other hand, Millan *et al.* [38] have successfully used the model of Perrier and Bird [47, 48] to describe the micro-aggregate size distribution of the Vertisols and Fredlund *et al.* [21] reported that their model could estimate PSD with a high accuracy and its accuracy was improved by increasing soil clay content. Therefore, in this study these two models were used to describe the PSD and ASD and their parameters have been used as predictors to estimate the SWRC in smectitic soils.

In addition to linear and non-linear regression and artificial neural networks (ANNs), the group method of data handling (GMDH), the k-Nearest Neighbor (k-NN) and the boosted regression method are other methods that can be used to create PTFs. The k-NN algorithm is a method for classifying objects based on closest training examples in the feature space and is amongst the simplest of all machine learning algorithms [32]. The GMDH is a self-organization model (an extremely high-order polynomial in input variables) that can be used to solve prediction, identification, control synthesis, and other system problems. The GMDH algorithms are characterized by the inductive procedure that performs sorting-out of gradually complicated polynomial models and selecting the best solution by means of the so-called external criterion [18]. Regression tree modelling is an exploratory technique based on uncovering structure in data [10]. Alternative to multiple regression, rather than fitting a model to the data, a tree structure is generated by dividing the sample recursively into a number of groups, each division being chosen to maximize the difference in the predicted variable in the resulting two groups [57].

Although plenty of research has been done to estimate the SWRC by means of various estimators, the SWRC models - particularly Dexter SWRC model - have not so far been predicted by fractal and non-fractal parameters of PSD and micro-aggregate size distribution (ASD) in smectitic soils. Therefore, the objective of this study is to investigate the possibility of improving the estimation of van Genuchten and Dexter models parameters by using Perrier and Bird's [47, 48] PSD and ASD fractal parameters and Fredlund *et al's* [21] PSD model parameters as predictors in smectitic soils.

THEORY

SWRC Models

This study has been conducted to assess the performance and suitability of some PTF models in estimating the SWRC of the smectitic soils of selected soil series in a wet region of Northern Iran. Van Genuchten (VG) [62] and Dexter *et al.* [14] (hereafter referred to as Dexter model) models were used for the SWRC.

Van Genuchten SWRC Model

The van Genuchten [62] SWRC function was represented by:

$$S_e = \frac{1}{[1+(\alpha h)^n]^{1-1/n}} \quad (1)$$

where, h is matric suction (cm); α (cm^{-1}) and n are shape factors of the SWRC model. The parameter α is described as inverse of air entry value. The dimensionless van Genuchten's parameter n refers to the steepness of the water retention curve. S_e is the effective saturation and expressed as:

$$S_e = (\theta - \theta_r)/(\theta_s - \theta_r) \quad (2)$$

where θ_r (cm^{3}cm^{-3}) is residual water content, θ_s (cm^{3}cm^{-3}), is saturated water content which is a physical parameter that can be measured and θ (cm^{3}cm^{-3}) is soil water content.

Van Genuchten model, which includes three shape parameters, (two if the parameters are limited to certain values), estimates a sigmoidal shape of the SWRC [24].

Dexter SWRC Model

Another SWRC model used in this study is the Dexter *et al.* [14] model, that is based on the notion that soil porosity is comprised of four parts. The total void ratio, e_{total}, is defined as the volume of pores (or voids) per unit volume of solid (mineral) matter.

$$e_{total} = e_{residual} + e_{matrix} + e_{structural} + e_{macro} \quad (3)$$

where, $e_{residual}$ and e_{macro} are the void ratios corresponding with pores that are too small and too large, respectively, to be characterized in standard water retention experiments. Matrix porosity (e_{matrix}) is the pore space between individual soil mineral particles. Structural porosity ($e_{structural}$) is the pore space between the micro-aggregates and between primary aggregates too. In most soils, the matrix and structural pore spaces can be emptied and therefore studied in conventional SWRC studies which cover the range of soil water suctions from 10–15,000 hPa.

The Dexter *et al.* [14] SWRC function was represented by:

$$W = C + A_1 e^{(-h/h_1)} + A_2 e^{(-h/h_2)} \tag{4}$$

where C, is the asymptote of the equation, and this is the residual water content (i.e. the water content as $h \to \infty$). When $h_1 > h_2$, we identify the second term with the emptying of the matrix pore space and the third term with the emptying of the structural pore space. The amounts of matrix and structural pore spaces are proportional to A_1 and A_2, respectively. The values of h_1 and h_2 are the characteristic pore water suctions at which the matrix and structural pore spaces empty, respectively. This model is a double-exponential water retention equation with 5 adjustable parameters is introduced in order to fill the need for a user-friendly equation in which all the terms have a distinct physical meaning [14].

PSD Models
Perrier and Bird [47, 48] Model

In addition to the cumulative number-size distribution of soil units, the standard pore-solid fractal model derives cumulative mass-size distributions [49] of soil particles or aggregates which are very useful for experimental analyses. This case may be generally expressed in the following term:

$m(x \leq x_i) = (\alpha^{D-3})(L^{D-3})(x_i)^{3-D}$

where $m(x \leq xi)$ is the soil mass (or soil mass percentage) formed by units (primary particles, fragments or micro-aggregates) with characteristic diameter, x, smaller than or equal to a defined diameter, x_i, α is a similarity ratio, L is the initiator size and D is the fractal dimension. An important point is that fractal mass-size relationships are based on the assumption of a scale invariant bulk density. In this study if the above model was fitted on the PSD data, its parameters were shown with the subscript "*p*" and if it was fitted on the ASD data, its parameters were shown with the subscript "*a*".

Fredlund et al. [21] PSD Model

$$\mathrm{Pp(d)} = \frac{1}{\left\{\ln\left[\exp(1)+\left(\frac{a_{gr}}{d}\right)^{n_{gr}}\right]^{m_{gr}}\right\}}\left\{1-\left[\frac{\ln\left(1+\frac{d_{rgr}}{d}\right.}{\ln\left(1+\frac{d_{rgr}}{d_m}\right)}\right]^7\right\} \tag{5}$$

$P_p(d)$ is the percentage, by mass, of particles passing a particular size, a_{gr} is a parameter designating the inflection point on the curve, n_{gr} is related to the steepest slope on the curve, m_{gr} is a parameter related to the shape of the curve as it approaches the fines region, d_{rgr} is a parameter related to the amount of fines in a soil, d is the diameter of any particle size under consideration and d_m is the diameter of minimum allowable size particle.

MATERIALS AND METHODS

Soil Sampling and Analysis

The data set used in this study was taken from Bayat *et al.* [6]. Sixty-nine soil samples were used to obtain PTFs for estimation of parameters of VG and Dexter models. The disturbed and undisturbed soil samples were collected from Guillan province (36° 34′-38° 27′ N, 48° 53′-50° 34′ E), Iran. According to Davatgar *et al.* [12] smectite is the dominant clay mineral in Guilan province of Iran. The disturbed samples were collected by means of an auger and the undisturbed samples were collected by use of sampling cylinders of 4 cm in height and of 5.1 cm in diameter.

Particle size distribution was measured by combination of sieve and hydrometer in the range of 0–2 mm. During 24 hours, 9 readings were performed by hydrometer. Afterwards, the particles were divided into very fine sand (0.05–0.1 mm), fine sand (0.1–0.25 mm), medium sand (0.25–0.5 mm), coarse sand (0.5–1 mm) and very coarse sand (1–2 mm) by the dry sieving method [23]. Micro-aggregate size distribution in the range of 0–2 mm was measured by the method of wet sieving and a hydrometer. This method was similar to the PSD, but a dispersing agent was not used and the separation of fine aggregates which were as big as the sand was done by wet sieving. BD was measured by the sampling cylinder method.

In order to gain SWRC at suctions lower than 10 kPa, the sand box was used and at suctions higher than that, pressure plate apparatus was used. The amount of water at the suctions of 0, 1, 5, 10, 25, 50, 100, 200, 500, 1000 and 1500 kPa was determined for 69 collected soil samples. The above measurements were done up to100 kPa suction on undisturbed soil samples and above that, it was done on disturbed soil samples. Then VG and Dexter models were fitted on the experimental data by use of Solver function of Excel software [22], and their parameters were arrived at.

Perrier and Bird [47, 48] fractal model was fitted on the PSD and ASD data by use of Solver function of Excel software. Fredlund *et al.* [21] model was fitted only on the PSD data by means of Solver function of Excel software.

Development of PTFs
Artificial Neural Network

The 69 data that had been taken from Bayat *et al.* [6] were partitioned into 2 sets using a randomized approach: a training set of 46 data and a testing set of 23 data.

Artificial neural network (ANN) ensembles method was used to develop the PTFs in order to predict the parameters of the VG and Dexter SWCC models. For every PTF, 75 models were developed using two types of ANNs; feed-forward Multilayer perceptrons (MLP) and radial basis function (RBF). Performances of two types of ANNs were evaluated; each type was run with one hidden layer and different hidden neurons ranging from 3 to 12. Therefore, a combination of ANN and bootstrap method was used to develop each of 75 models for prediction of the parameters of the VG and Dexter SWRC models [17].

Several transfer functions including tanh, exponential, logistic, identity, and sine in hidden and output layers were examined. The influence of the number of ANN ensemble members is evaluated on the RMSE of the ensemble models, and behaving conservatively the 25 most successful ANN models with the least Akaike information criterion (AIC) and integral root mean square error (IRMSE) values and the highest coefficient of determination (R^2) values, were selected carefully out of 75 developed ones to make an ANN ensemble model.

Pedotransfer Functions Development

The first process was to normalize the data which resulted in the fact that only m_{gr} had a normal distribution, and then the transformation of data was conducted for other parameters. Sand - using the equation $0.0016\text{sand}^2+0.16\text{sand}$, clay - using the equation log(clay), bulk density (BD) - using the equation cosBD, the fractal parameter of PSD (α_p) - using the equation of $-14.1\alpha_p^2+33.9\alpha_p$, the fractal dimension of PSD (D_p) - using the equation of D_p-2, the fractal parameter of PSD (L_p) - using the equation $-14.2L_p^2+34.1L_p$, the fractal parameter of ASD (α_a) - using the equation of $-2.98\alpha_a^2+12.2\alpha_a$, the fractal dimension of ASD (D_a) - using the equation of D_a-2, the fractal parameter of ASD (L_a) - using the equation of $-2.91L_a^2+12.06L_a$, a_{gr} - using the equation of $1.33\ln(a_{gr})$, n_{gr} - using the equation of $3.18\ln(n_{gr})$, d_{rgr} - using the equation of $\log(d_{rgr})$, the θ_r - using the equation of $-5.73\theta_r^2+7.63\theta_r^{0.3}$, θ_s - using the equation of $\log(\theta_s)$, α - using the equation of $\log(\alpha)$, n - using the equation of $-0.24n^2+2.3n-2.92$, the C parameter of Dexter model - using the equation of $\log(C)$, A_1 - using the equation of $-7.6A_1^2+11.2A_1–2.18$, A_2 - using the equation of $1.10\ln(A_2)+3.4$, h_1 - using the equation of $10^{-8}h_1^2–0.00004h_1+0.005$ and h_2 - sing the equation of $\log(h_2)$. Then all the variables standardized to have a zero mean and unit variance.

The clay and sand contents, BD, fractal parameter of PSD and ASD as well as the parameters of Fredlund *et al.* [21] model were used as the independent variables while the parameters of the SWRC models of VG and Dexter were the dependent variables. One third of the samples (23) were randomly taken for validation process and the rest (46) were employed for training.

Linear and nonlinear regressions and ANNs were used in order to develop the PTFs. By comparing the results of the linear and nonlinear regressions, the models of the method with the better results were kept and the results of the other method were not shown. Four steps applied to develop PTFs. At the first step in order to develop PTF1 the basic soil properties of clay, sand and BD, were used as estimators and the parameters of VG and Dexter models were estimated. At the second step PTF2 used the fractal parameters of PSD ($\alpha_{p,}$ D_p, L_p) as additional inputs. At the third step input variable of the PTF3 included the fractal parameter of ASD ($\alpha_{a,}$ D_a L_a) as additional inputs. At the fourth step to develop PTF4, the parameters of Fredlund *et al.* [21] PSD model (a_{gr}, n_{gr}, m_{gr}, d_{rgr}) were used as additional inputs to estimate the parameters of VG and Dexter models. The estimated parameters of each step were used to form the SWRC models of VG and Dexter as the estimated curves for the related steps. Then, the estimated curves of each step were compared with measured SWRCs and the evaluation criteria were computed. Finally the improvement of SWRC estimations was investigated by using PSD and ASD parameters as estimators.

Table1 shows the statistical characteristics of variables that are used to develop PTFs. The clay and sand contents show the heavy to moderate texture of the soils in this research. The mean percentage of sand in both train and test data was lower than the mean percentage of clay. The used samples in this study cover soil textural classes except, five classes of sandy, silty, sandy loam, sandy clay loam and sandy clay (Fig. 1). The range of variables in this study was high which shows high applicability of developed PTFs. Ungaro *et al.* [61] have proven that under these circumstances, employing the developed PTFs within the range of applied data entail greater accuracy. Because data for test and train steps is selected randomly, the range of changes and the average of the variables is similar in the testing and training data sets. The t-test comparison between the average of the variables in the testing and training data sets did not reveal a significant difference between them (the data are not shown).

TABLE 1: STATISTICAL CHARACTERISTICS OF TRAINING AND TESTING DATA SETS

	S (%)	C (%)	BD (g^{cm-3})	α_p	D_p	L_p	α_a	D_a	L_a	a_{gr}	n_{gr}	m_{gr}	d_{rgr}	Θ_r	Θ_s	α (cm^{-1})	n	C	A_1	h_1	A_2	h_2
									Training													
Mean	16.7	32.8	1.28	0.79	2.86	0.79	1.17	2.81	1.17	0.04	1.36	0.84	134	0.07	0.57	0.007	37.98	0.067	2388	0.28	0.16	1.83
Standard deviation	10.8	11.4	0.23	0.09	0.04	0.09	0.21	0.06	0.21	0.06	0.44	0.27	176	0.1	0.15	0.009	1.31	0.06	0.15	1171	0.08	44
Minimum	1	13	0.86	0.63	2.73	0.62	0.65	2.68	0.65	0.01	0.8	0.31	8.83	0	0.3	0.0007	1.004	0.002	1194	0.005	0.05	1.06
Maximum	59	56	1.7	1.22	2.93	1.22	2.09	2.95	2.09	0.43	2.89	1.81	752	0.44	0.93	0.05	197	0.529	6378	0.66	0.39	6.79
									Testing													
Mean	15.2	32.9	1.27	0.78	2.86	2.86	1.16	2.84	1.16	0.03	1.44	0.81	93	0.05	0.55	0.021	45.94	0.06	198	0.18	0.21	1.32
Standard deviation	8.9	1161	0.28	0.07	0.04	0.04	0.17	0.08	1.18	0.02	0.46	0.28	117	0.09	0.1	0.032	31.33	0.036	980	0.1	0.09	0.034
Minimum	1	14	0.73	0.73	2.77	2.77	0.96	2.68	0.92	0.01	0.81	0.32	7.77	0	0.25	0.0008	8.6	0.005	728	0.029	0.1	1.04
Maximum	36	58	1.7	1.7	2.93	2.93	1.6	2.93	1.6	0.08	2.47	1.48	546	0.34	0.7	0.13	108	0.174	4781	0.46	0.5	2.33

S – percentage of sand, C – percentage of clay, BD – bulk density, α_p – similarity ratio of PSD, D_p – fractal dimension of PSD, L_p – empirical constant of PSD, α_a – similarity ratio of ASD, D_a – fractal dimension of ASD, L_a – empirical constant of ASD, a_{gr} – a parameter designating the inflection point on the PSD curve, n_{gr} – a related to the steepest slop on the PSD curve, m_{gr} – a parameter related to the shape of the PSD curve as it approaches the fines region, d_{rgr} – a parameter related to the amount of fine particles in a soil, θ_r – residual water content, θ_s – saturated water content, α and n are shape parameters of SWRC, C – the asymptote of the equation, A_1 – the amounts of matrix pore space, A_2 – the amounts of the structural pore space, The values of h_1 and h_2 are the characteristic pores water suctions at which the matrix and structural pores spaces empty, respectively.

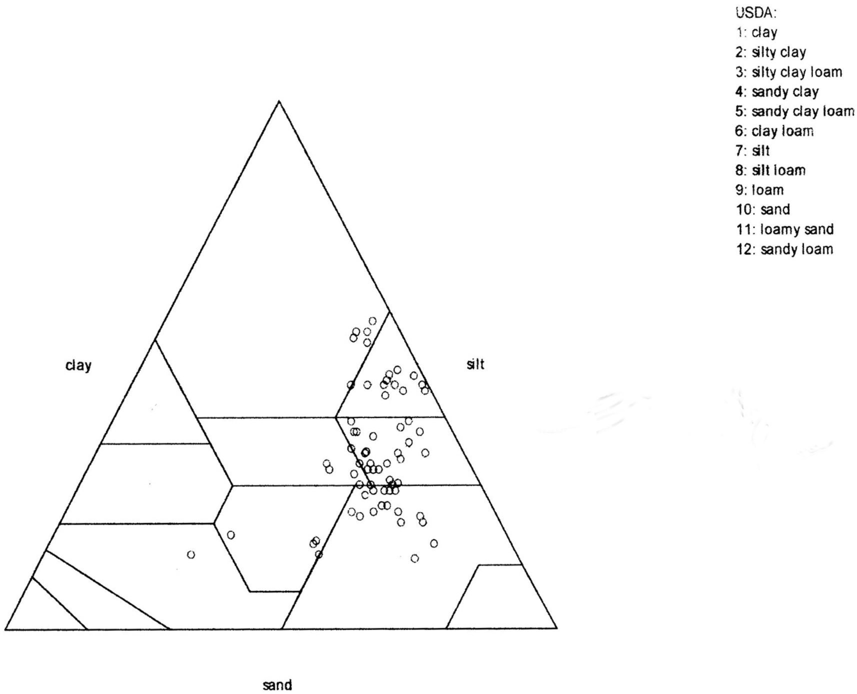

Fig 1: Distribution of soil samples in soil textural triangle.

Evaluation Criteria

Akaike information criterion (AIC), coefficient of determination (R^2), relative improvement (RI), integral root mean square error (IRMSE) and integral mean error (IME) were used for investigating the accuracy and reliability.

Akaike information criterion (AIC) [2]:

$$AIC = N\ln\left[\sum_{i=1}^{N}\frac{(\theta_m-\theta_p)^2}{N}\right] + 2n_p \tag{6}$$

where n_p is the number of parameters of the model that should be estimated, N is the number of the observations of the SWRC, θ_m and θ_p are the measured and estimated volumetric water contents, respectively. The more negative the AIC values, the more accurate the estimations.

To evaluate the error of PTFs in each step after the estimation of the parameters of VG and Dexter models, they are used to simulate SWRC. Then the simulated curves were compared with the measured curves using the IRMSE (m^3 m^{-3}) and IME (m^3 m^{-3}) criteria.

$$IME = \frac{1}{b-a}\int_a^b (\theta_p - \theta_m) \, d \log |h| \tag{7}$$

$$IRMSE = \left[\frac{1}{b-a}\int_a^b (\theta_p - \theta_m)^2 \, d \log |h|\right]^{1/2} \tag{8}$$

where h is the matric potential (kPa), θ_m and θ_p are the measured and the estimated volumetric water contents, respectively. IME can also have positive and negative values but, IRMSE can only have positive values. If the value of IME and IRMSE were close to zero, estimated accuracy increases.

Relative improvement:

$$RI = \frac{IRMSE_1 - IRMSE_i}{IRMSE_1} \times 100 \quad i=2, 3 \text{ or } 4 \tag{9}$$

where $IRMSE_1$ is IRMSE of the first step; $IRMSE_i$ is IRMSE of the second to fourth steps.

RESULTS AND DISCUSSION

Correlation between Fractal Parameters and Soil Texture

The correlation of fractal dimension of PSD with clay and sand contents was positively and negatively significant, respectively (Table 2). According to the previous studies, by increasing the sand content and decreasing clay content, fractal dimension [37] and water retention [26] decreases. So there is a direct relationship between the fractal dimension and water retention.

Correlation between the Parameters of the PSD and SWRC Models

The simple linear correlation between the parameters of the VG and Dexter SWRC models and the PSD fractal parameters and the parameters of Fredlund *et al.* [21] model were significant, in some cases (Table 2). One of the reasons for the correlation between the fractal parameters of PSD and the shape parameters of the SWRC was the similarity of the PSD curve and the SWRC [29]. Zoo and Dong [65] reported that PSD had the same fractal dimension as the pore size distribution. There is no linear correlation between the parameters of the VG and Dexter SWRC models and the ASD fractal parameters. However, in the VG model PTF3 was the superior PTF in comparison with the other PTFs.

TABLE 2: THE CORRELATION BETWEEN PARAMETERS

	S	C	BD	α_p	D_p	L_p	α_a	D_a	L_a	a_{gr}	n_{gr}	m_{gr}	d_{rgr}
C	-0.76**	1											
BD	0.13	-0.02	1										
α_p	0.95**	-0.76**	0.19	1									
D_p	-0.84**	0.96**	-0.12	-0.85**	1								
L_p	0.95**	-0.74**	0.20	0.99**	-0.83**	1							
α_a	-0.24	0.32*	-0.24	-0.17	0.34*	-0.17	1						
D_a	-0.46**	0.37*	0.18	-0.44**	0.40**	-0.42**	0.04	1					
L_a	-0.26	0.34*	-0.25	-0.18	0.36*	-0.18	0.99**	0.05	1				
a_{gr}	0.77**	-0.65**	0.19	0.80**	-0.78**	0.79**	-0.44**	-0.35*	-0.45**	1			
n_{gr}	-0.045	-0.32**	0.05	-0.025	-0.35**	-0.04	-0.18	0.13	-0.19	0.35**	1		
m_{gr}	0.36**	-0.46**	-0.06	0.32**	-0.32**	0.33**	-0.11	-0.22	-0.12	-0.11	-0.47**	1	
d_{rgr}	0.26*	-0.17	-0.10	0.21	-0.20	0.20	-0.09	0.02	-0.10	0.15	0.007	-0.02	1
θ_r	-0.14	0.13	-0.15	-0.15	0.11	-0.15	0.006	0.29*	0.03	-0.02	0.05	-0.09	-0.01
θ_s	-0.08	-0.01	0.13	-0.04	0.01	-0.05	-0.03	-0.13	-0.01	-0.03	0.06	-0.02	-0.34**
α	0.09	0.01	0.02	0.11	-0.05	0.10	0.15	0.04	0.14	0.07	-0.06	-0.06	0.11
n	-0.08	0.01	-0.23	-0.11	0.05	-0.10	-0.09	-0.03	-0.07	-0.02	-0.005	0.03	0.01
c	-0.13	0.07	-0.28*	-0.13	0.07	-0.14	0.28	0.07	0.28	-0.12	0.11	-0.13	-0.09
A_1	-0.01	-0.11	-0.17	-0.06	-0.03	-0.05	-0.10	-0.28	-0.09	-0.09	-0.12	0.24*	-0.14
h_1	-0.06	0.18	0.25*	-0.15	0.18	-0.13	-0.12	-0.11	-0.12	-0.15	-0.12	0.02	0.01
A_2	0.01	0.07	-0.13	-0.04	0.07	-0.04	0.12	-0.19	0.11	-0.02	-0.07	-0.008	0.05
h_2	-0.036	0.05	0.05	0.01	0.03	0.005	0.05	*0.29	0.06	-0.009	0.09	-0.08	-0.01

S – percentage of sand, C – percentage of clay, BD – bulk density, α_p – similarity ratio of PSD, D_p – fractal dimension of PSD, L_p – empirical constant of PSD, α_a – similarity ratio of ASD, D_a – fractal dimension of ASD, L_a – empirical constant of ASD, a_{gr} – a parameter designating the inflection point on the PSD curve, n_{gr} – a related to the steepest slop on the PSD curve, m_{gr} – a parameter related to the shape of the PSD curve as it approaches the fines region, d_{rgr} – a parameter related to the amount of fine particles in a soil, θ_r – residual water content, θ_s – saturated water content, α and n are shape parameters of SWRC, C – the asymptote of the equation, A_1 – the amounts of matrix pore space, A_2 – the amounts of the structural pore space, The values of h_1 and h_2 are the characteristic pores water suctions at which the matrix and structural pores spaces empty, respectively.

Estimation of VG and Dexter Models by Regression and ANN Methods
Comparison of Regression and ANN Methods

To estimate the VG and Dexter models, three methods of linear and non-linear regression and ANNs were employed. The results obtained from these methods (Table 3) demonstrated that the ANNs created the best results for the VG and Dexter models. The comparisons of measured and predicted values by the SWRC models for two soils were shown in Fig. 2 and 3. As it was depicted in Fig. 2 and 3 ANN models performed better than the regression models.

TABLE 3: THE RESULTS OF THE ESTIMATION OF VG AND DEXTER SWRC MODELS BY USING REGRESSION AND ANNs METHODS

	IME	IRMSE	R^2	AIC	RI
VG			**Train (regression)**		
PTF1	-0.322	0.307	0.860	-1166	
PTF2	-0.055	0.150	0.908	-1740*	50.9
PTF3	-0.074	0.155	0.878	-1364*	49.4
PTF4	-0.072	0.151	0.896	-1823*	50.6
			Test (regression)		
PTF1	-0.347	0.334	0.924	-501	
PTF2	-0.015	0.120	0.949	-911*	64
PTF3	-0.010	0.087	0.933	-544*	73.8
PTF4	-0.012	0.128	0.951	-850*	61.7
VG			**Train(ANN)**		
PTF1	-0.011	0.110	0.919	-1069	
PTF2	-0.036	0.105	0.936	-2011*	4.6
PTF3	-0.023	0.108	0.910	-1392*	1.7
PTF4	-0.028	0.092	0.935	-2266*	16.1
			Test(ANN)		
PTF1	0.012	0.110	0.897	-1015	
PTF2	-0.017	0.108	0.953	-1073*	2.2
PTF3	0.028	0.062	0.961	-1103*	43.6
PTF4	0.021	0.076	0.946	-993	31.2
Dexter			**Train (regression)**		
PTF1	0.062	0.235	0.639	-1330	
PTF2	-0.018	0.126	0.961	-1833*	46.2
PTF3	0.085	0.162	0.963	-1468*	30.7
PTF4	0.001	0.109	0.883	-2221*	53.4

TABLE 3. CONTINUATION

			Test (regression)		
PTF1	0.125	0.2399	0.551	-567	
PTF2	0.052	0.094	0.966	-1125*	60.8
PTF3	0.066	0.105	0.906	-782*	56.6
PTF4	0.049	0.079	0.918	-978*	67
Dexter			**Train(ANN)**		
PTF1	-0.031	0.107	0.968	-2255	
PTF2	-0.041	0.121	0.968	-1846	-13.5
PTF3	-0.032	0.117	0.970	-1447	-9.1
PTF4	-0.034	0.117	0.970	-2049	-9.5
			Test(ANN)		
PTF1	0.006	0.075	0.975	-1117	
PTF2	0.003	0.084	0.963	-834	-12.7
PTF3	0.037	0.0602	0.981	-895	19.6
PTF4	0.011	0.073	0.972	-1038	1.6

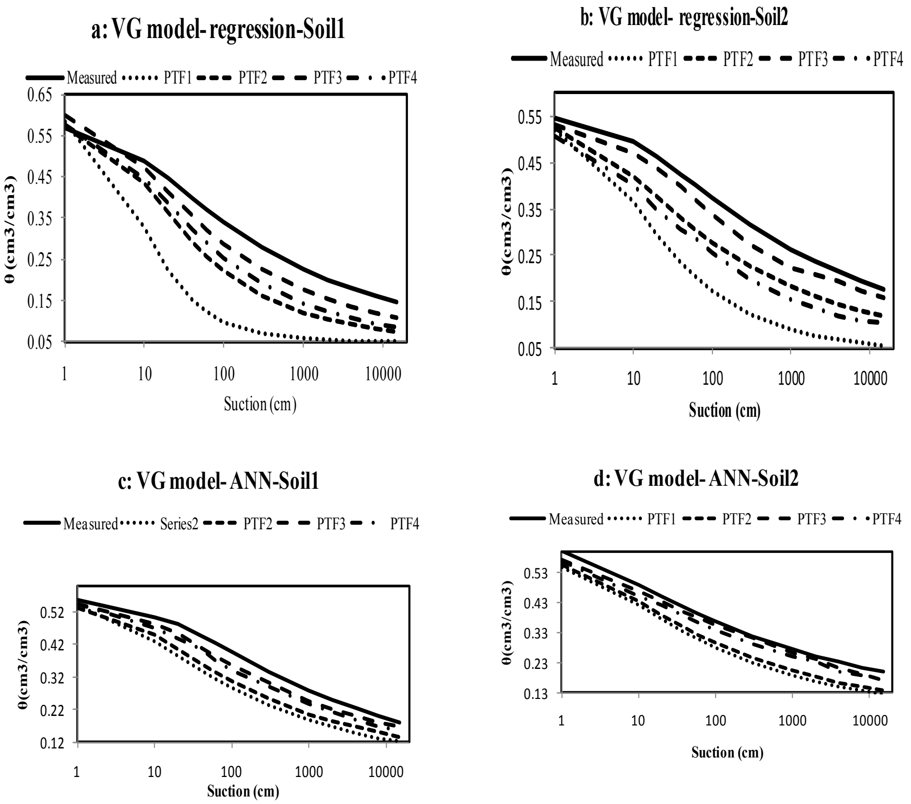

Fig. 2. Measured and predicted SWRCs by regression (a – soil 1 and b – soil 2) and ANNs (c – soil1 and d – soil 2) methods for VG model.

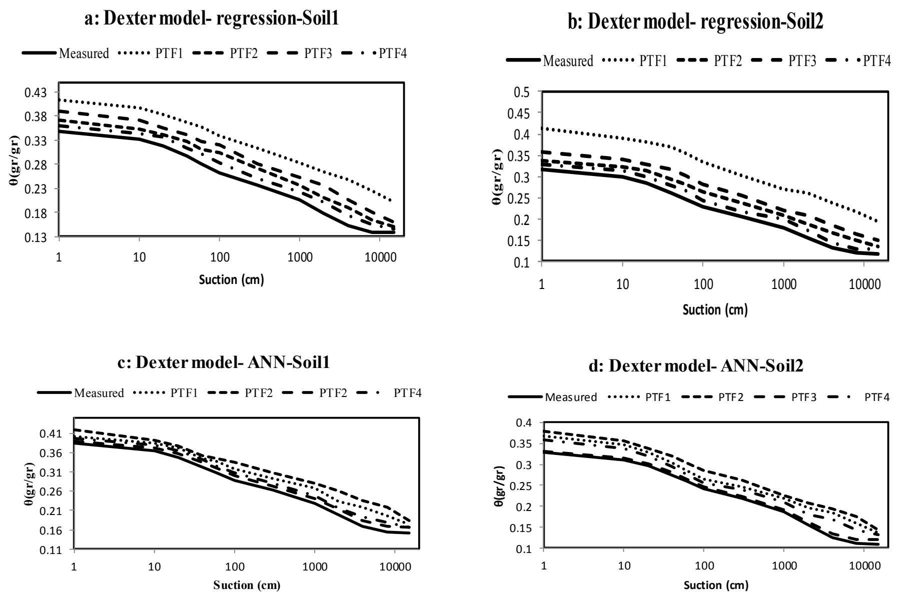

Fig. 3. Measured and predicted SWRCs by regression (a – soil 1 and b – soil 2) and ANNs (c – soil1 and d – soil 2) methods for Dexter model.

First of all, the comparison between the regression and ANNs methods was performed based on IRMSE of all PTFs in both training and testing stages. All eight PTFs were created in both the Dexter and Van Genuchten models. With the exception of PTF4 in Dexter model that had better result by using regression method, ANNs got the best result in other PTFs in the training stage (Table 3). ANNs had the better results than the regression in testing stages of all PTFs, however the value of IRMSE was equal in both methods in PTF4 of the Dexter model. Comparing these two methods regarding the AIC shows the relative superiority of ANNs. ANNs was found to be the most adequate for parametric PTFs in this study. The *t-test* comparison between the regression and ANNs methods was done based on the average of the IRMSE. The *t-test* results showed significant difference between the two methods in both the testing and the training stages. This is in accord with some reported results such as Pachepsky *et al.* [42] and Schaap *et al.* [51]. Therefore the performance of the regression and ANN PTFs in the smectitic soils are the same as in the case of the other soils. The fitted models of linear and nonlinear regressions and their coefficients were shown in Table 4.

TABLE 4: FITTED MODELS OF LINEAR AND NONLINEAR REGRESSION AND THEIR COEFFICIENTS

		Model
		VG model
PTF1	θ_r	$=-0.1444\times sand+0.1323\times clay+0.1314\times BD+0.0657$
	θ_s	$=-0.3271\times sand+1.1424\times clay+0.2478\times BD-3.5378$
	α	$=-0.1752\times sand+-0.0523\times clay+0.02109\times BD-2.0074$
	n	$=-0.4091\times sand+0.9264\times clay+0.1763\times BD+0.9447$
PTF2	θ_r	$=-0.3271\times sand+1.1424\times clay+0.2478\times BD-3.5378\times \alpha p-1.584\times Dp+3.2438\times Lp+0.1193$
	θ_s	$=-0.7424\times sand-0.7101\times clay-0.0853\times BD+0.833\times \alpha p+1.08977\times Dp+0.2987\times Lp+0.0987$
	α	$=0.4811\times sand+0.5503\times clay+0.157\times BD+4.3929\times \alpha p-0.0436\times Dp-4.4679\times Lp-0.2672$
	n	$=-0.7718\times sand+0.2358\times clay+0.2677\times BD-4.9789\times \alpha p-0.7883\times Dp+5.1977\times Lp+0.308$
PTF3	θ_r	$=-0.1752\times sand-0.0523\times clay0.021\times BD-2.0074\times \alpha a+0.1963\times Da+\times 1.9896La+0.1261$
	θ_s	$=0.2474\times sand+0.1544\times clay-0.1122\times BD-3.4581\times \alpha a-0.1972\times Da+3.4904\times La+0.1794$
	α	$=0.0058\times sand+0.5618\times clay+0.2468\times BD+1.997\times \alpha a-0.1264\times Da\times --2.0711La-0.5215$
	n	$=-0.18\times sand-0.3745\times clay+0.0183\times BD-2.4851\times \alpha a+0.0415\times Da+2.4616\times La+0.378$
PTF4	θ_r	$=-0.4091\times sand+0.9264\times clay+0.1763\times BD+0.9447\times a_{rg}+0.3855\times n_{rg}+0.7366\times m_{rg}+0.1251\times d_{rgr}+0.1165$
	θ_s	$=-0.3655\times sand-0.4156\times clay-0.02\times BD+0.2184\times a_{rg}-0.4184\times n_{rg}-0.2616\times m_{rg}-0.3256\times d_{rgr}+0.0594$
	α	$=0.4643\times sand+0.1032\times clay+0.1836\times BD-0.3992\times a_{rg}-0.1376\times n_{rg}-0.2949m_{rg}+0.0028\times d_{rgr}-0.3345$
	n	$=-0.8542\times sand+0.7048\times clay+0.3143\times BD+1.3587\times a_{rg}+0.1379\times n_{rg}+0.8212\times m_{rg}+0.1361\times d_{rgr}+0.2138$
		Dexter model
PTF1	C	$=-0.1403\times sand+0.1701\times clay+0.1955\times BD+-0.235$
	A_1	$=\exp(0.724\times sand-0.3348\times clay+6.7842\times BD-10.712)$
	h_1	$=\exp(1.7318\times sand+1.6622\times clay-1.5082\times BD-3.5208)$
	A_2	$=\exp(3.1387\times sand+2.5168\times clay+4.7121\times BD-7.4244)$
	h_2	$=\exp(15.8877\times sand+16.8381\times clay+2.6244\times BD-17.7425)$

TABLE 4: CONTINUATION

PTF2	C	$=-0.1396\times sand+0.5106\times clay+0.2971\times BD+3.7247\times \alpha p-0.2069\times Dp-3.5274\times Lp+-0.1193$
	A_1	$=-0.4397\times sand-1.4315\times clay+0.0598\times BD-6.1549\times \alpha p+0.7353\times Dp+6.0763\times Lp+0.3576$
	h_1	$=0.8902\times sand-0.616\times clay-0.4513\times BD-0.4103\times \alpha p+0.828\times Dp-0.2711\times Lp+0.1361$
	A_2	$=0.9801\times sand-0.7216\times clay+0.1715\times BD-0.5587\times \alpha p+1.31\times Dp+0.3121\times Lp+0.0355$
	h_2	$=0.145\times sand-0.7288\times clay-0.2515\times BD+3.7309\times \alpha p+1.4123\times Dp-3.1608\times Lp-0.1838$
PTF3	C	$=-0.0912\times sand+0.5913\times clay+0.5004\times BD+1.6294\times \alpha a-0.1542\times Da-1.709\times La-0.2879$
	A_1	$=-0.0401\times sand-0.2897\times clay+0.0656\times BD-1.9987\times \alpha a-0.1055\times Da+1.8719\times La+0.4889$
	h_1	$=0.0561\times sand-0.2618\times clay-0.3953\times BD-0.6796\times \alpha a+0.0407\times Da+0.8471\times La+0.2002$
	A_2	$=0.0759\times sand+0.1551\times clay+0.2393\times BD+0.8999\times \alpha a-0.2908\times Da-0.9034\times La-0.2099$
	h_2	$=\exp(0.4974\times sand+0.3178\times clay+0.0938\times BD-0.5849\times \alpha a+0.2489\times Da+0.5936\times La-0.1965)$
PTF4	C	$=0.4336\times sand-0.3728\times clay+0.2104\times BD-0.9136\times a_{rg}-0.0748\times n_{rg}-0.6474\times m_{rg}-0.082\times d_{rgr}-0.1025$
	A_1	$=\exp(-0.9128\times sand-1.0847\times clay+0.763\times BD+1.97778\times a_{rg}-1.6031\times n_{rg}+0.24934\times m_{rg}-0.6161\times d_{rgr}-2.5064)$
	h_1	$=\exp(4.3018\times sand+4.1875\times clay-1.0801\times BD-2.1976\times a_{rg}+2.4073\times n_{rg}+1.7683\times m_{rg}-0.0639\times d_{rgr}-3.1369)$
	A_2	$=0.2851\times sand+0.4156\times clay+0.3203\times BD+0.0813\times a_{rg}+0.0204\times n_{rg}+0.118\times m_{rg}+0.0855\times d_{rgr}+-0.0868$
	h_2	$=0.7684\times sand+0.32973\times clay-0.2271\times BD-0.6845\times a_{rg}+0.3492\times n_{rg}+0.0997\times m_{rg}-0.0596\times d_{rgr}-0.1848$

Impact of PSD and ASD Parameters on Improvement of PTFs VG Model

The addition of α_p, D_p and L_p along with sand, clay and bulk density (SCBD) as estimators in PTF2 improved the accuracy and reliability of the VG model estimate and decreased AIC and IRMSE and increased R^2 in both the training and testing stages (Table 3). Scientists have extensively used particle-size distribution data as predictors of soil hydraulic properties [64]. Millan *et al.* [37] showed that the fractal dimension of PSD is significantly positively correlated with clay content following a linear trend. Fractal geometry has been used as a tool to describe both the soil structure and the soil hydraulic properties [5]. Xu and Dong [65] tried to use fractal dimension of the PSD to determine the SWRC. Therefore, fractal parameters are closely related to the SWRC and can be suitable predictors of the above, even in smectitic soils.

As α_a, D_a and L_a were added to the list of inputs, a high level of accuracy and reliability of PTF3 was noticed, as a result, a decrease in AIC and IRMSE occurred. Micro-aggregate size distribution has rarely been used as predictors of soil hydraulic properties, especially in smectitic soils. In these soils, smectite has an incredible impact on the development of micro-aggregates [66]. Fractal geometry has been used to describe aggregate size distributions [46]. Perfect and Kay [45], used fractal theory in the characterization of soil structure. Therefore, using the parameters of the fractal model of micro-aggregate size distribution to predict the VG model help us improve the performances of the PTFs in smectitic soils.

To develop PTF4, the parameters of Fredlund *et al.* [21] PSD model were used to estimate the VG model. Using these as predictors, the accuracy and reliability of the estimation of the VG model significantly improved. However, their impact was not significant in the testing stage of the ANN method. The use of Fredlund *et al.* [21] PSD model parameters showed a relative improvement in comparison with the use of fractal parameters in PTF2 for the training stage according to the amount of the AIC. The PTF3 performed better than the PTF4, in which the parameters of Fredlund *et al.* [21] PSD model are used as inputs, in testing stage. So the ASD fractal parameters were better predictors than the fractal parameters for the testing stage in the estimation of VG model (Fig. 2 a, b, c and d). Despite the high number of parameters of the Fredlund *et al.* [21] PSD model, the ASD fractal parameters had a great effect on the estimation of the SWRC for testing stage. Therefore, it could be suggested that the fractal theory is a valuable tool for the study of these soils.

Dexter Model

Using α_p, D_p and L_p along with the SCBD as estimators in PTF2 the accuracy and reliability of the Dexter model estimate significantly improved and the AIC and IRMSE decreased in both the training and testing stages of the regression method (Table 3). This indicates that the fractal parameters of the PSD can improve the estimation of the Dexter model by this method. Arya and Paris [4] and Arya and Dierolf [3] presented models to predict water retention by using information on the PSD. Hwang and Powers [30] used Arya and Paris [4] model and nonlinear models of PSD to estimate the SWRC and concluded that the linear relationship between the PSD and the void size distribution (VSD) would not be appropriate for the multi-component particle systems such as soils. Their results suggested that the nonlinear relationship between the PSD and the VSD would be more appropriate and made better estimates of hydraulic properties. As a result, quantifying PSD by a fractal model and using its parameters to predict the Dexter model by regression method can be a successful method to improve the performances of the PTFs in smectitic soils. In the ANN method, fractal parameters of the PSD had no significant effect on the estimation of the Dexter model.

Using α_a, D_a and L_a along with the SCBD as estimators in PTF3 the accuracy and reliability of the Dexter model estimate significantly improved and the AIC and IRMSE decreased by using the regression method. However, the relative improvement was less than its value for PTF2. A good reason for using fractal models to investigate soil structure is to gain information on aggregation processes. We must recall that many physical properties of systems (e.g. soils) formed by aggregation depend on the scaling properties of the generated structures [38]. Fractal parameters of the ASD had no significant effect on the estimation of the Dexter model by the ANN method.

When the parameters of Fredlund *et al.* [21] PSD model were used in PTF4 as inputs in addition to the SCBD to estimate the Dexter model, substantial improvement occurred (Table 3). The AIC and IRMSE decreased significantly for both the testing and training stages. The relative improvement of the training and testing errors were 53.4 and 67%, respectively, this show substantial improvement. Comparing the PTFs shows that the parameters of Fredlund *et al.* [21] PSD model that was used in PTF4 which had the better result in comparison with PTFs in which fractal parameters of PSD were used (Table 3). The comparisons of measured and predicted values of the SWRC by the Dexter model for the two soils that were shown in Fig. 3 confirm the superiority of Fredlund *et al.* [21] PSD model parameters in the estimation of the SWRC by the regression method (Fig. 3; a and b). Fredlund *et al.* [21] PSD model is a four-parameter model, which has one parameter more than the fractal parameters of the PSD model. Perhaps that is why, Fredlund *et al.* [21] PSD model is more accurate and reliable than fractal PSD model. It seems that the influences of soil texture [15] is more than that of soil structure [20] on the estimation of the Dexter model in smectitic soils. The Dexter model is based on pore space, and on the assumption of water retention within pores by capillary action [14]. Perhaps the superiority of PTFs in which PSD parameters were used in comparison with PTFs in which ASD parameters were used is because of the high clay content that increases total porosity in smectitic soils.

The IME represents the positive and negative differences. Therefore, the IME can only be used to indicate over prediction (IME > 0) or under prediction (IME < 0) [56]. The IME values showed under prediction for most of the VG model estimates while, the over prediction was found for most of the Dexter model estimates (Table 3 and Fig. 2 and 3).

In one by one estimation of the parameters of the Dexter model, using fractal parameters as additional inputs resulted in the most accurate PTFs (data was not shown). However, when we use these parameters to simulate the Dexter model and the estimated curves were compared with measured curves, it was observed that these PTFs had low accuracy in comparison with PTFs that used Fredlund *et al*. [21] PSD parameters (Table 3 and Fig. 3 a, b, c and d). These results showed that, it was better to use an objective function that minimizes the difference between measured and estimated water contents, not the difference between measured and estimated parameters [39].

Comparing Predictability of Dexter and VG Models

Finally the comparison between the Dexter and the VG models was done based on the IRMSE and AIC in the training and testing stages. In each stage 8 PTFs were developed, 4 PTFs by ANNs and 4 PTFs by regression. The VG model PTFs had better results in the training stage but, in the testing stage the Dexter model was the superior model and 7 PTFs had better performance with the Dexter model. The superiority of the VG model in the training stage was in the ANN method. Multiple linear regression cannot be used to predict van Genuchten parameters. Scheinost *et al.* [52] found it difficult to estimate the scaling parameters of α and n of the VG equation by using the regression method. *T-test* results showed significant difference between the two models in both the testing and training stages (data was not shown).

The Dexter model is a five-parameter model, which has one parameter more than the van Genuchten model. Maybe that is why Dexter is more accurate than the van Genuchten model in the testing stage.

The Dexter model is a bimodal model. It is probable that one of the factors behind the superiority of the predictability of this model is that the studied soils had bimodal pore size distribution. In well-aggregated natural soils the pore system is frequently partitioned into intra-aggregates or textural pores and inter-aggregates or structural pores [55]. Thus, the result of pore-size distributions is often bimodal [16]. Another factor proving the efficiency of this model is the number of the parameters of this model, as the accuracy of the experimental data of R^2 increases with the rise in the number of parameters, the simplicity of usage of the model decreases [9].

Unimodals like VG and BC are suitable for those soil types which have homogeneous pores.

CONCLUSIONS

1. This paper has displayed the development and validation of the PTFs for estimation of soil hydraulic parameters from basic soil properties, the PSD and ASD fractal parameters and Fredlund *et al*. [21] PSD model parameters using ANNs and regression methods and the comparison of the predictive capabilities of these methods using some evaluation criteria. The overall performance of ANNs has been better than that of regression. According to this study the ANNs method can be most accurate for parametric PTFs.

2. Aggregate size distribution affect many soil functions. Fractal parameters of the ASD has had a considerable impact on the estimation of the VG model. Fractal theory can be invoked to model the physics of Vertisols. This study shows that the fractal is a useful tool for the prediction of the SWRC in Vertisols.

3. Using parameters of Fredlund *et al*. [21] PSD model in the PTFs, in order to estimate the Dexter model, brings about better results in comparison with PTFs in which fractal parameters of PSD are used. PSDs are of paramount importance in understanding soil physical properties as they are used to estimate soil hydraulic properties.

4. The Dexter model is a bimodal model and the VG is a unimodal model. The result of the prediction of the Dexter model is better than those of the VG model. In well-aggregated natural soils, which often exhibit bimodal pore-size distribution, the parametric formulation of water retention proposed by the VG leads to the representation of water retention ignoring the transition between pore systems frequently indicated by the retention data.

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ZDOLNOŚĆ FUNKCJI PEDOTRANSFEROWYCH DO SYMULOWANIA ZACHOWANIA GLEB SMEKTYTOWYCH W MODELACH KRZYWEJ RETENCJI WODNEJ GLEB

W celu kształtowania przepływów w warunkach nienasyconych możliwe jest użycie właściwości hydraulicznych, których bezpośrednie uzyskanie jest kosztowne i czasochłonne z uwagi na wysoką zmienność i złożoność systemów glebowych. Funkcje pedotrasferu w glebach smektytowych nie zostały obszernie zbadane. Co więcej, użyteczność parametrów fraktalnych w przewidywaniu krzywej retencji wodnej gleb nie zostało zbadane na przedmiotowych glebach. W niniejszym badaniu ustalono funkcje pedotransferu w celu określenia parametów modelu van Genuchtena (VG) oraz modelu Dextera przy użyciu metody regresyjnej oraz metody sztucznych sieci neuronowych. 69 próbek zebranych zostało w prowincji Guilan w Iranie. Model fraktalny i niefraktalny zostały dopasowane do rozkładu wielkości cząsteczek i rozkładu agregatowego (ASD) oraz obliczono ich parametry. W celu stworzenia funkcji pedotransferu, parametry modeli PSD i ASD użyte zostały jako estymatory. Zestawienie wyników uzyskanych przy pomocy dwóch modeli Dextera oraz VG wykazało nadrzędność modelu Dextera w odniesieniu do gleb smektytowych. Wyniki pokazały odpowiednio przewagę parametrów modelu PSD Fredlund'a i współautorów oraz parametrów fraktalnych ASD w ocenie modeli krzywej retencji wodnej gleb (SWRC) Dextera i VG. Uzyskany rezultat może być związany z wyższą dokładnością modelu PSD Fredlund'a w opisie danych PSD w glebach gliniastych. Jednakże, większa liczba parametrów uzyskanych z tego modelu w porównaniu z liczbą parametrów modelu fraktalnego może stanowić kolejny powód.