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Sorptive number prediction of highly calcareous soils at different applied tensions using regression models

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Abstract

Sorptive-number (α) is of vital importance in water flow and infiltration modeling that is needed in numerous soil applications particularly in unsaturated flow conditions. Recently, alternative-indirect-approaches are used to estimate hydraulic-attributes from widely/easily available soil properties due to tedious and time consuming nature of their laboratory/field measurements. At 138 experimental locations on two calcareous soil series a set of successively applied tensions of 0.2, 0.15, 0.1, 0.06, and 0.03 m were applied for infiltration measurements using a single-disc tension infiltrometer. Sorptive number of soil was determined using the gathered infiltration data. The common physicochemical attributes were also determined at each experimental location. Regression-pedotransfer functions (PTFs) were developed to estimate the α parameters of 138 soil samples (measured at tensions of 0.03 to 0.2 m) from their corresponding physicochemical properties. The most influential investigated physical soil attributes in α predictions were sand and silt contents, bulk density (BD), initial and near-saturated water contents by volume (θ_i and θ_s, respectively) and the most influential chemical attributes were the ratio of cation-exchange-capacity to electrical-conductivity (CEC/EC_e), organic matter (OM), exchangeable-sodium-percentage (ESP), sodium-adsorption-ratio (SAR), soluble calcium (Ca_{sol}), pH, and some of their combinations. Evaluating the generated-PTFs using some statistical criteria revealed that all of PTFs-predictions were statistically acceptable; however, all of them were generally over-predicted. The most and least accurate predictions were obtained at applied tensions of 0.03 and 0.2 m, respectively. In another word, the prediction-accuracy decreased as applied tension increased. Generally, it can be concluded that PTFs predictions of α are enough accurate for the majority of applications, and consequently could rectify requirements where they are not easily-available.

Keywords: Pedotransfer functions; physico-chemeical properties; sorptive number.
Abbreviations: BD- bulk density; CCE- calcium carbonate equilibrium; CEC- cation exchange capacity; ECe- electrical conductivity of saturated paste; EKP- exchangeable potassium percentage; ESP- exchangeable sodium percentage; OM- organic matter; PTFs- Pedotransfer functions; SAR- sodium adsorption ratio; θ_i- initial water content; θ_s- saturated water content.

Introduction

Modeling infiltration and flow rate in the soil is important in numerous applications of soil science including contaminant fate and transport in the vadoze zone, irrigation management, and rainfall-runoff prediction (Nachabe, 1996). Successful applications of these models can be achieved only if reliable estimates for analytical expressions of hydraulic attributes e.g., sorptive number (α) is available. The importance of α is well documented in the literature on soil physics. Sorptive number is equal to inverse of macroscopic capillary length which is equivalent to the wetting front suction or the effective capillary drive in the Green and Ampt model of infiltration (Nachabe 1996). This hydraulic attribute also is the single parameter in the exponential (or the quasi-linear) hydraulic conductivity function, which is used to linearize and solve the multidimensional, transient Richards' equation (Wooding 1968; Philip 1985). This hydraulic parameter emerges directly from the tedious, costly, time-consuming, and labor intensive field or laboratory measurements and these measurement techniques give only local scale results (Mermoud and Xu 2006; Moosavi and Sepaskhah 2012a). Point measurement of soil hydraulic attributes may produce inaccurate results due to highly spatio-temporal variability. Therefore, large numbers of soil samples have to be collected. Furthermore, published information on soils around the world may have data on soil particle size distribution, organic matter content and bulk density, but the data on soil hydraulic properties may be incomplete or missing. Due to these reasons, recently a great deal of research has been devoted to develop alternative indirect approaches to estimate soil hydraulic attributes (Timlin et al. 2004) e.g., α or the other soil characteristics like soil erodibility (Neyshabouri et al. 2011) and cation exchange capacity (Kianpoor Kalkhajeh et al. 2012) from widely available or more easily measured basic soil properties, and/or limited data. Efforts have been made to relate these hydraulic properties to more easily measurable and more readily available soil properties such as particle-size distribution (sand, silt and clay content), organic matter or organic C content, bulk density, porosity, etc. Such relationships are referred to pedo-transfer functions (PTFs) (Mermoud and Xu 2006). Numerous PTFs have been developed in recent decades, such as those proposed by Cosby et al. (1984), Saxton et al. (1986), Rawls and Brakensiek (1989), Vereecken et al. (1990), Wosten (1997), and Zhuang et al. (2001) among others. Baker and Ellison (2008) stated that "Pedotransfer functions, PTFs, transfer the data we have into the data we need". Conventional regression equations (Rawls et al. 2004; Wosten et al. 1995) and artificial neural networks, ANNs, (Minasny et al. 1999; Schaap et al. 1998) are two types of pedotransfer functions. Regarding the amount of accessible soil data, two types of PTFs, namely class and continuous PTFs were recognized (Wosten 1997). The class PTFs estimate certain soil attributes based on the class (textural, horizon, etc.) to which the soil samples belong. But, continuous PTFs estimate certain soil attributes as a continuous function of measured variables (one or more variables). As mentioned earlier a summary of PTFs and their status is given by Pachepsky et al. (1999) and McBratney et al. (2002). McBratney et al. (2002) proposed a more detailed classification that accounts for the crisp/fuzzy nature of the inputs and outputs. Romano (2004) stated that PTFs seem rather flexible with respect to its local calibration and this opens new opportunities in soil hydraulic characterization using indirect methods. His results reinforced the need for detailed, but limited in number, local measurements that reflect soil hydraulic behavior and would provide an information base for calibration of PTFs. Estimation of hydraulic attributes is generally limited to the soil water retention function and soil saturated hydraulic conductivity (Mermoud and Xu 2006; Rezaee et al. 2011). There is a small number of PTFs available for estimation of unsaturated hydraulic characteristics especially at different soil water tensions. Therefore, the objective of this study was to relate the sorptive number (α) of soils at different applied tensions to the easily measurable physico-chemical properties of soils by development of PTFs.

Results and discussion

Descriptive statistics

The main descriptive statistics of measured physicochemical and hydraulic soil attributes of entire dataset along with the datasets were used for generating and testing the PTFs were presented in Table 2. The GMD and $\alpha_{0.2}$ showed the highest variability (CV) among the physical and hydraulic soil attributes of all datasets, respectively. The highest variability of $\alpha_{0.2}$ may be due to high variability of pores taking apart in water movement process. Soluble Mg showed the highest variability among the chemical attributes of entire and PTFs-generating datasets and Na_{sol} was the most variant chemical attribute in PTFs-testing dataset. The high variability of soluble Mg may correspond to highly variable nature properties of soils in the studies area. Whereas, θ_s, pH, and $\alpha_{0.0.3}$ showed the lowest variability (CV) among physical, chemical, and hydraulic soil attributes, respectively. Since studied locations belong to the neighbor soil series with the same parent materials, pH of soil samples showed the lowest variation among all of chemical attributes. The lowest variability of θ_s and $\alpha_{0.0.3}$ may correspond to the lowest variability of soil porosity in the studied areas that plays key rule in the mentioned soil parameters. The results of the present study were the same as those found by Moosavi and Sepaskhah (2012a, 2012b). The W statistic of Shapiro and Wilk (1965) test that compares the distribution of a set of measured data against the normal distribution was determined for each soil attributes at the probability level of 0.9. The W statistics of greater than or close to 0.9 mean that the data are normally distributed. In another word the closer W value is to 1.0 indicating the higher probability for normal distribution of the data. Results showed that the W statistics for almost all of soil attributes were close to 0.9 indicating that the normal distribution can be considered, so there was no need to data transformation in statistical analysis for PTFs generation. The soil parameters of high W statistics (e.g., clay content and BD) and the ones of low W statistics (e.g., $\alpha_{0.2,}$ $\alpha_{0.15,}$ GMD or pH) have the minimum and the maximum deviation from normal distribution, respectively (Table 1). The results were in agreement with the findings of Moosavi and Sepaskhah (2012a, 2012b) for all of the mentioned soil attributes and with the results of Shouse et al. (1995) for BD and clay content.

Results showed that the mean values of α increased as applied tension decreased. The SD of α parameters increased as moving from severe unsaturated water entry condition (i.e., ψ of 0.2 m) toward the near saturated conditions (i.e., ψ of 0.03 m) excepting for $\alpha_{0.1}$. Since the CV of α at each applied tension is calculated by dividing the SD of α to its corresponding average value and the average values of α increased as applied tension decreased, therefore, the CV of α parameters followed the contrary pattern of variation with change in applied tensions in comparison to SD. Moosavi and Sepaskhah (2012a) concluded that the higher variability of the measured α at lower applied tensions in comparison to the higher ones may be related to the higher amounts of soil macro pores taking apart in water flow process during lower applied tensions.

Predictor soil attributes

Table 2 shows the derived PTFs for prediction of α. The most influential investigated physical soil attributes in prediction of α were sand and silt contents, BD, θ_i, and θ_s, and the most influential investigated chemical attributes were CEC/EC_e, OM, ESP, SAR, Ca_{sol}, pH, and some of their combinations. Results indicated that the soil texture components and the soil attributes affecting soil structure, dispersion and flocculation play significant rules in water movement process and consequently in α prediction. Wagner et al. (2001) also reported that the bulk density and organic matter content were influential inputs in prediction of soil hydraulic parameters using eight well known equations. Saxton and Rawls (2006) reported that soil texture has dominant effect on soil water retention characteristics. However, they included four additional inputs (OM, bulk density, gravel, salinity) that can have significant effects in the complete prediction method. They reported that OM was included in the regression equations, thus its effect was directly represented by the regression equations. They stated that soil structure and distribution of large pores strongly influenced by soil density, and consequently has a significant effect on hydraulic conductivity. The inverse relation between α and OM at applied tension of 0.1 to 0.2 m reveal that the increase in OM result in a decrease in α parameter and consequently, an increase in unsaturated soil hydraulic conductivity. This is probably due to the fact that the soil OM positively affects the water holding capacity of soil and soil hydraulic conductivity. The results were in agreement with the findings

Table 1. Statistics for the entire data set along with the data set used for generating and testing of pedotransfer functions (PTFs).

	Entire dataset						PTFs-generating dataset					PTFs- testing dataset				
Soil attribute**	Min.*	Max.	Avr.	SD	CV	W	Min.	Max.	Avr.	SD	CV	Min.	Max.	Avr.	SD	CV
Sand (g kg^{-1})	74.00	449	217	74	34.16	0.95	74.00	411	219	73.81	33.65	94.00	449	213	75.67	35.51
Silt (g kg^{-1})	84.32	660	358	224	62.67	0.94	84.32	660	356	229	64.21	91.72	630	361	218	60.23
Clay (g kg^{-1})	93.15	316	215	54	25.32	0.98	109	316	214	52.59	24.57	93.15	316	216	58.32	27.00
Gravel (g kg^{-1})	0.01	629	210	224	107	0.93	0.01	629	211	224	106	0.01	629	210	228	109
MWD ($\times10^{-3}$, m)	0.09	3.29	1.24	1.12	90.37	0.94	0.09	3.29	1.24	1.12	90.11	0.11	3.29	1.23	1.13	91.90
GMD	-1.97	1.65	0.08	0.48	569	0.76	-1.54	1.62	0.09	0.47	523	-1.97	1.65	0.07	0.51	686
BD (Mg m^{-3})	0.98	1.80	1.36	0.20	14.37	0.98	0.98	1.73	1.35	0.20	14.51	0.98	1.80	1.37	0.19	14.21
θ_i (m^3 m^{-3})	0.01	0.10	0.03	0.01	43.32	0.85	0.01	0.10	0.03	0.01	48.98	0.01	0.04	0.03	0.01	26.28
θ_s (m^3 m^{-3})	0.24	0.44	0.34	0.05	13.58	0.93	0.24	0.44	0.34	0.05	13.99	0.24	0.41	0.34	0.04	12.86
OM (g kg^{-1})	10.21	42.19	23.19	5.17	22.30	0.86	10.21	42.19	22.76	4.88	21.43	14.29	40.83	24.06	5.67	23.58
pH	7.06	8.23	7.84	0.15	1.91	0.84	7.06	8.23	7.85	0.15	1.93	7.06	8.03	7.84	0.15	1.88
EC_e (dS m^{-1})	0.46	0.91	0.67	0.08	11.45	0.88	0.47	0.91	0.67	0.07	10.99	0.46	0.91	0.68	0.08	12.41
CEC ($cmol_+$ kg^{-1})	36.17	51.78	46.46	3.59	7.73	0.94	36.17	51.78	46.38	3.62	7.80	37.23	50.72	46.62	3.58	7.68
CCE (g kg^{-1})	313	490	408	23.33	5.71	0.97	338	490	412	22.46	5.45	313	439	402	23.88	5.94
Na_{sol} (mmol L^{-1})	0.09	3.42	0.64	0.38	60.29	0.95	0.09	1.75	0.61	0.30	49.72	0.29	3.42	0.70	0.51	72.70
K_{sol} (mmol L^{-1})	0.03	0.12	0.06	0.02	32.57	0.95	0.03	0.12	0.06	0.02	33.69	0.03	0.12	0.06	0.02	30.61
Ca_{sol} (mmol L^{-1})	6.40	24.00	11.50	3.43	29.79	0.94	6.40	24.00	11.50	3.63	31.55	7.20	19.20	11.50	3.02	26.23
Mg_{sol} (mmol L^{-1})	0.40	36.40	8.07	5.17	64.09	0.96	0.80	36.40	8.24	5.57	67.60	0.40	26.40	7.72	4.29	55.61
Na_{exch} ($cmol_+$ kg^{-1})	0.17	2.69	1.49	0.43	28.93	0.90	0.17	2.69	1.50	0.45	29.75	0.21	2.23	1.47	0.40	27.43
K_{exch} ($cmol_+$ kg^{-1})	0.13	0.23	0.16	0.02	9.57	0.89	0.13	0.23	0.16	0.02	10.41	0.13	0.19	0.16	0.01	7.59
ESP	0.39	5.40	3.20	0.89	27.79	0.92	0.39	5.40	3.22	0.92	28.44	0.44	4.44	3.16	0.84	26.64
EKP	0.28	0.52	0.35	0.04	12.40	0.87	0.30	0.52	0.36	0.05	12.94	0.28	0.45	0.35	0.04	11.23
SAR ($mol^{0.5}$ $L^{-0.5}$)	0.04	1.50	0.29	0.16	54.29	0.95	0.04	0.71	0.27	0.12	42.13	0.14	1.50	0.32	0.22	67.70
$\alpha_{0.2}$ ($\times10^{-2}$, m^{-1})	0.27	15.73	2.07	2.67	128	0.82	0.27	15.73	2.14	2.84	133	0.27	9.29	1.95	2.31	118
$\alpha_{0.15}$ ($\times10^{-2}$, m^{-1})	0.38	12.12	2.57	2.69	105	0.82	0.38	12.12	2.66	2.96	112	0.62	8.11	2.39	2.03	85.16
$\alpha_{0.1}$ ($\times10^{-2}$, m^{-1})	0.74	12.77	3.19	2.68	84.10	0.87	0.83	12.77	3.26	2.76	84.67	0.74	10.14	3.06	2.55	83.45
$\alpha_{0.06}$ ($\times10^{-2}$, m^{-1})	1.06	23.10	5.00	4.22	84.53	0.86	1.06	23.10	5.09	4.46	87.62	1.17	15.67	4.82	3.75	77.92
$\alpha_{0.03}$ ($\times10^{-2}$, m^{-1})	4.77	44.06	13.91	6.47	46.48	0.91	4.77	32.05	13.67	6.12	44.75	4.77	44.06	14.40	7.16	49.73

*. Min., Max., Avg., SD, CV, and W are the minimum, maximum, average, standard deviation, coefficient of variation (%), and Shapiro and Wilk's (1965) W statistic for normality test, respectively. *. Sand, silt, clay, gravel, MWD, GMD, BD, θ_i, θ_s, OM, pH, EC_e, CEC, CCE, Na_{sol}, K_{sol}, Ca_{sol}, Mg_{sol}, Na_{exch}, K_{exch}, ESP, EKP, and SAR are the sand, silt, clay, and gravel contents, mean weight diameter and geometric mean diameter of primary particles, bulk density, initial and saturated volumetric water contents, organic matter content, pH of saturated paste, electrical conductivity of saturated extract, cation exchange capacity, calcium carbonate equivalent, soluble sodium, potassium, calcium and magnesium, exchangeable Na and K, exchangeable sodium percentage, exchangeable potassium percentage, and sodium adsorption ratio in the given units, respectively.
**. $\alpha_{0.2}$, $\alpha_{0.15}$, $\alpha_{0.1}$, $\alpha_{0.06}$, and $\alpha_{0.03}$ are sorptive number of soil measured at applied tensions of 0.2, 0.15, 0.1, 0.06, and 0.03 m, respectively.

of Hudson (1994) who concluded that increase in soil OM generally produced a soil with increased water retention capability and conductivity, mainly as a result of its effect on aggregation and pore space distribution. The generated PTFs show that there are positive relations between α and sand content of soil. In the other word, the value of α is increased as soil texture is became coarser. The positive relations between α and sand is probably due to the higher saturated and lower unsaturated hydraulic conductivity of sand particles in comparison to those of clay particles. This is due to fact that the large pores which taking apart in saturated flow process is more abundant in sand particles than in clay ones. Reynolds et al. (1985) also reported the higher values of α for coarse texture soil than the finer ones. Precision evaluation of predicted α using statistical indices Table 2 also shows R^2, NRMSE, GMER, and GSDER values correspond to predictions of testing data set. Based on R^2, NRMSE, GMER, and GSDER values of predictions for testing data set (Table 2), it can be concluded that all of predictions for α were statistically acceptable, e.g., the GMER values for prediction of α at different applied tensions were somehow close to 1.0 indicating that the acceptable predictions were obtained. The GSDER value, as an indicator of data scatter, was generally lowest for the PTFs predictions of α at lower applied tensions i.e., 0.03 m, while it showed quite large values indicating a larger scatter for the PTFs predictions of α at higher applied tensions especially 0.2 m. The mentioned statistics of predictions revealed that the most and the least accurate predictions were obtained for measured α at tensions of 0.03 and 0.2 m, respectively (the accuracy of PTFs predictions decreased as applied tensions increased). The large GSDER values, indicating a larger scatter for the PTFs predictions of α at higher applied tensions especially 0.2 m than the lower applied tensions. This is may be due to the fact that in lower applied tensions almost all of soil pores participate in water flow and consequently, more soil factors can affect the soil hydraulic attributes.

Fig 1 shows schematic description of the measured vs. predicted values of α at different applied tensions and their comparison with 1:1 line. Fig 1 confirms our judgment about the accuracy of PTFs predictions resulted from the mentioned statistics values. Fig 1 indeed gives a comparison of measured α value vs. their corresponding predictions by the proposed regression PTFs models at different applied tensions. The slopes of the linear relationships for $\alpha_{0.2}$, $\alpha_{0.15}$, and $\alpha_{0.03}$ were closer to one than the other α values which confirms our statistically based finding about the accuracy of PTFs predictions. However, the results revealed that all of the predictions were somehow over-predicted, but generally, it can be concluded that the application of proposed PTFs for prediction of α in our study resulted in enough accurate predictions (Fig 1). Because all models are calibrated with data from one database, the predictions among models and input data levels are consistent. In addition, the uncertainty of estimations provides information about the reliability of the predictions. These characteristics can be very useful to generate uncertainty estimates of water and solute transport processes, even when limited information about the soil is available (Saxton and Rawls 2006). Although prediction errors and confidence limits were often large, estimation of soil hydraulic properties e.g., α with PTFs may be accurate enough for most applications, and hence will rectify a need where this hydraulic attribute are not readily available. The dataset used for this study was probably small and also belong to a narrow range of soil textures to conclude if the generated PTFs are of general validity. However, some PTFs may perform better in other areas, where climate and geology are more similar to the soils used for derivation of the

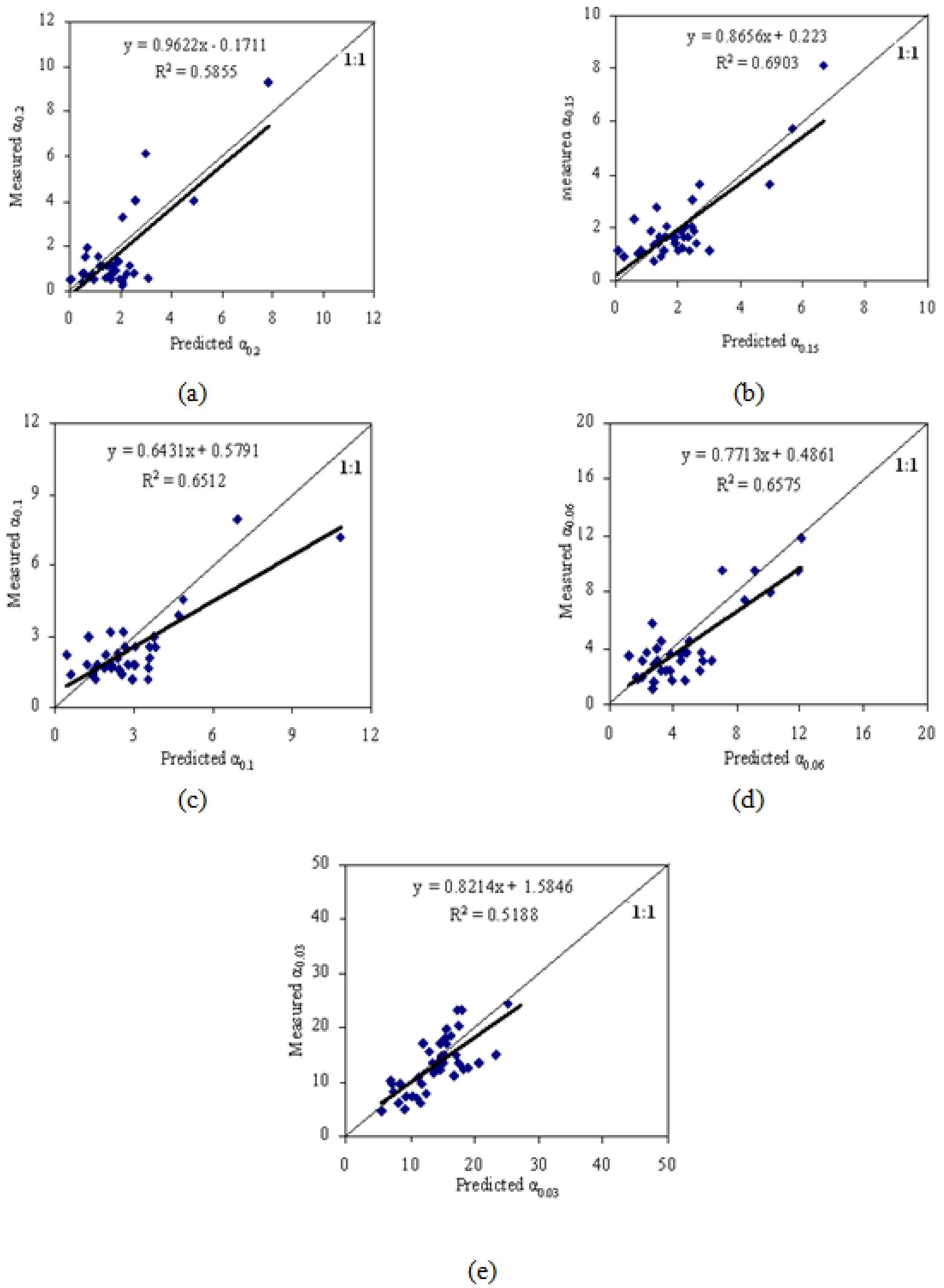

Fig 1. Measured vs. PTFs predicted values of sorptive number ($\alpha_{\psi} \times 10^{-2}$, m^{-1}) at different applied tensions (ψ, m) for testing dataset (a-e corresponds to α_{ψ} at tensions of 0.2 to 0.03 m, respectively).

respective PTFs. Saxton and Rawls (2006) stated that one of the reasons that may be responsible for the poor performance of generated PTFs in the different areas or even different runs in the same area could be the measurement technique applied in the other areas or by the other investigators.

Material and methods

Experimental location and sampling design

The study was carried out in two separate soil series [uncropped no-tilled gravelly calcareous soil of Kooye-Asatid series (loamy-skeletal, carbonatic, mesic, Fluventic Xerorthents) and uncropped non gravelly tilled calcareous soil of Daneshkadeh series (Fine, carbonatic, mesic, Typic Calcixerepts) located in Bajgah Agricultural Experimental Station, College of Agriculture, Shiraz University, I.R. of Iran (52° 32′ E, 29° 36′ N, 1810 m above the mean sea level). Measurements were conducted at 69 experimental locations on a multi-scale nested sampling design (Moosavi and Sepaskhah, 2012 a and b) in each study area. It must be noted that such a nested sampling design was used for studying the spatial variability of soil properties (Moosavi and Sepaskhah, 2012 a) and not specifically for PTFs generations. Since the more data we use the more accurate PTFs will generate, therefore, we used all of measured soil attributes together from 138 sampling locations of two studied soil series.

Determination of physico-chemical properties

In the vicinity or directly at each experimental location, selected physical and chemical attributes were measured immediately before or after the infiltration experiments. For determining the real effect of soil physical/chemical attributes on soil sorptive number, disturbed soil samples were collected in the vicinity of each experimental location immediately before the infiltration experiment and the initial volumetric water content (θ_i) was measured. Undisturbed soil samples were taken by core sampler (diameter of 0.054 m and height of 0.03 m) in order to determine the final volumetric water content, θ_s, (the water corresponded to the final supplied tension) and bulk density (BD) of soil. Collected samples remained in plastic bags before taking them to laboratory due to preventing water losses via evaporation. Gravimetric initial and final water contents of collected samples were measured using oven-drying method and multiplied to their corresponding BD to achieve θ_i and θ_s, respectively. The other soil attributes were determined in disturbed samples collected at depth of 0- 0.2 m directly underneath the disc of infiltrometer in each location quickly after infiltration experiment using the common methods as follow: soil texture components (sand, silt, and clay content) by hydrometer method, gravel content by sieving, organic matter (OM) content by wet-oxidation method, electrical conductivity of soil saturated extract (EC_e) by EC- meter, pH of soil saturated paste by glass electrode pH-meter, cation exchange capacity (CEC), exchangeable sodium (Na_{ex}) and potassium (K_{ex}) by Chapman (1986) method, soluble Na and K (Na_{sol} and K_{sol}, respectively) by ammonium acetate extraction and flame photometry, soluble calcium and magnesium (Ca_{sol} and Mg_{sol}, respectively) by titration, exchangeable sodium percentage (ESP) determined using [(Na_{ex}/CEC)×100], exchangeable potassium percentage (EKP) determined using [(K_{ex}/CEC)×100], and sodium adsorption ratio (SAR) determined using [$Na_{sol}/(Ca_{sol} + Mg_{sol})^{0.5}$], in which Na_{sol}, Ca_{sol}, and Mg_{sol} are soluble Na, Ca, and Mg (mol L^{-1}), respectively. Mean weight diameter (MWD) and geometric mean diameter (GMD) of soil primary particles were also determined (Moosavi and Sepaskhah, 2012 a)

Determination of sorptive number

Infiltration experiments were carried out using a single-disc tension infiltrometer with diameter of 0.2 m (Soilmoisture Equipment Crop. P.O. Box 30025, Santa Barbara, CA 93105 U.S.A.). At each experimental location, the grasses were removed and the soil surface was leveled. Then a thin fine-sand layer (particles with diameters of 0.0001 to 0.0025 m) with thickness of approximately 0.01 m was put on the soil between the membrane of disc infiltrometer and soil surface that guarantee the good hydraulic contact. A set of successively applied tensions of 0.2, 0.15, 0.1, 0.06, and 0.03 m were used for infiltration measurements. At each applied tension, infiltration of water into the soil was recorded manually at time periods of 15 s for about first 5 min after implementation of a new tension, and later on every 1 min until achieving the steady state conditions. Soil hydraulic attributes including sorptive number were determined using the gathered infiltration data by applying the approaches proposed by Wooding (1968 after Ankeny et al. 1991).

Statistical analysis

The general moments of the empirical distribution functions (i.e. the minimum, maximum, mean, variance, coefficient of variation, skewness and kurtosis coefficients) of the measured soil attributes were determined. The normality of distribution for each studied soil attributes were checked using the Shapiro-Wilk (1965) test (after Moosavi and Sepaskhah, 2012 a and b).

Derivation of pedotransfer functions (PTFs)

Since the W statistics of Shapiro-Wilk test were close to 0.9 for almost all of the measured soil attributes; therefore, there was no need to transform the original data into normal ones. In generation of PTFs based on our measured data, we divided the entire dataset into two subsets. The first that consisted of 70 % of data (92 data) was used to generate PTFs, and the second subset that consisted of 30 % of data (46 data) was used to test the generated PTFs (validation procedure). In generation of PTFs for prediction of sorptive number (α) at each applied tension, we considered it as dependent variable and the other measured physical and chemical properties, their squares, their logarithms and some of their products as independent variables in stepwise regression modeling (using SPSS, version 16, 2007). In this study, dependent data consisted of α at tensions of 0.2, 0.15, 0.1, 0.06, and 0.03 m measured by tension disc infiltrometer. The independent data consisted of soil particle fractions (% sand, silt, clay, and gravel contents), mean weight diameter (MWD), geometric mean diameter (GMD), bulk density (BD), total soil porosity (F), initial and near saturated volumetric soil water content (θ_i and θ_s, respectively), organic matter content (OM), electrical conductivity of soil saturated extract (EC_e), pH of soil saturated paste, soluble sodium, potassium, calcium, and magnesium (Na_{sol}, K_{sol}, Ca_{sol}, and Mg_{sol}, respectively), exchangeable sodium and potassium (Na_{ex} and K_{ex}, respectively), cation exchange capacity (CEC), calcium carbonate equivalent (CCE), sodium adsorption ratio (SAR), exchangeable sodium percentage (ESP), exchangeable potassium percentage (EKP), the squared and natural logarithm value of these independent soil variables,

Table 2. Pedotransfer functions (PTFs) for prediction of sorptive number ($\alpha \times 10^{-2}$, m^{-1}) at different applied tensions along with the coefficient of determination (R^2), normalized root mean square error (NRMSE), geometric mean error ratio (GMER), and geometric standard deviation of error ratio (GSDER) of predictions for testing dataset.

Sorptive number	Predictor function*	R^2	NRMSE	GMER	GSDER
$\alpha_{0.2}$	$= 6.71 + 7.765\ (\theta_i)(\text{sand}) - 1.537\ (\text{OM}) - 1.819\ \ln(\text{ESP}) - 0.172\ (\theta_i)(\text{sand}^2) - 0.021\ (\text{silt})(\text{BD}^2)$	0.59	1.17	1.28	2.80
$\alpha_{0.15}$	$= 5.191 + 3.807\ (\theta_i)(\text{sand}) - 1.546\ (\text{OM}) - 1.247\ \ln(\text{ESP})$	0.69	0.87	1.00	2.19
$\alpha_{0.1}$	$= 3.516 + 0.105\ (\theta_i)\ (\text{sand}^2) - 0.333\ (\text{Ca}_{\text{sol.}}) - 7.314\ (\text{OM}) + 18.388\ (\theta_s^2) + 0.104\ (\text{pH}^2)(\text{OM})$	0.65	0.70	1.09	2.05
$\alpha_{0.06}$	$= 6.203 + 0.108\ (\theta_i)(\text{sand}^2) + 0.06\ (\text{CEC}/\text{EC}_e) - 1.91\ \ln(\text{ESP}) + 2.063\ \ln(\text{SAR})$	0.66	0.68	1.18	1.82
$\alpha_{0.03}$	$= -0.237 + 1.704\ (\text{OM})(\text{BD}^2) + 1.549\ (\theta_s^2)(\text{sand}) + 105.021\ (\theta_i)$	0.52	0.46	1.05	1.46
Mean		0.62	0.78	1.12	2.06

*Sand, silt, BD, OM, θ_i, θ_s, CEC, EC_e, ESP, SAR, and $Ca_{sol.}$ are sand and silt contents (%), soil bulk density ($Mg\ m^{-3}$), organic matter content (%), initial and filed saturated volumetric water content ($m^3\ m^{-3}$), cation exchange capacity (meq $100g^{-1}$), electrical conductivity of soil saturated extract ($dS\ m^{-1}$), exchangeable sodium percentage (%), sodium absorption ratio ($mol^{0.5}\ mol^{-0.5}$), and soluble calcium content (meq l^{-1}), respectively.

and some of their product combinations. The parameters of regression models were adjusted so that the software enters each independent soil variable into regression equation automatically if its influence was statistically significant at probability level of 0.05. Consequently, α at different applied tensions were modeled as a significant function of some independent soil variables, named PTFs.

Testing the generated PTFs

Independent measured soil values of testing dataset were put into the generated PTFs to produce the PTFs predictions for α. In order to make comparisons between measured and PTFs-predicted α, the measured α of testing dataset were plotted against the PTFs predictions and their determination coefficients (R^2) were determined. The higher values of R^2 indicate the higher performance of PTFs in prediction of α and the lower ones exhibit the poor performance of PTFs. The closeness of measured-predicted pairs of data values to 1:1 line was another criterion which was used for checking the performance of generated PTFs. The more closeness of measured–predicted pairs of data to 1:1 line correspond to high performance of PTFs in prediction of α, whereas the less closeness correspond to poor performance of PTFs. Furthermore, normalized root mean squared error (NRMSE) were calculated for each PTFs-prediction of α and were considered as the other criteria in checking the performance of PTFs (Schaap and Leij 1998). The $NRMSE$ is always positive, with low and high $NRMSE$ -values representing good and poor performance of PTFs, respectively. In addition to R^2 and NRMSE, the geometric mean error ratio (GMER) and geometric standard deviation of the error ratio (GSDER) were calculated for evaluation of PTFs predictions from the error ratio, ξ, of N measured hydraulic attribute, y_m, vs. the corresponding predicted, y_p, values using the equations propoased by Tietje and Hennings 1996; and Wagner et al. 2001

The GMER yields the average factor indicating the predictions exceed or fall below the measurements. The GMER equal to 1 corresponds to an exact matching between measured and predicted values; the GMER < 1 indicates that predicted values are generally under-estimated; GMER >1 points to a general over-prediction. The GSDER yields the deviation around the mean. The GSDER equal to 1 corresponds to a perfect matching between predicted and measured values and it grows with deviation from measured data. The best model will, therefore, give a GMER close to 1 and a small GSDER (Wagner et al., 2001). In the best cases that all predicted values are the same as those of measurements the mentioned statistics yield: $R^2 = 1$, NRMSE = 0, $\xi = 1$, GMER = 1, and GSDER = 1.

Conclusion

Results indicated that the most influential physical soil attributes in prediction of α using PTFs were sand and silt contents, BD, θ_i, θ_s and the most influential investigated chemical attributes were CEC/EC, OM, pH, ESP, SAR, and Ca_{sol}. It must be noted that some combination of both physical and/or chemical soil attributes (e.g., their square or multiplication etc.) play key rule in prediction of α in addition to those attributes mentioned earlier. In the present study R^2, NRMSE, GMER, and GSDER of PTFs predictions for testing dataset varied from 0.52 to 0.69; 0.46 to 1.17; 1.0 to 1.28; and 1.46 to 2.8, respectively. Based on the results, generally it can be concluded that although prediction errors were often large, estimation of α with PTFs may be accurate enough for most applications, and hence will rectify a need where this hydraulic attribute are not readily available. Because of narrow range of soil texture for derivation of PTFs in this study it can be recommended to generate PTFs using the broader range of soils than the current study for prediction of α and validate the generated PTFs by using different independent datasets.

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