

Physico-empirical methods for estimating soil water characteristic curve under different particle size

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Abstract. Soil water characteristic curve (SWCC) is an important property of soil, but directly measuring methods are costly and time-consuming. Many attempts have been made to predict the water characteristic curve indirectly from soil particle size distribution (PSD) and basic physical properties. In this study, the Arya-Paris (A-P) model and Non-similar media concept (NSMC) model were applied to predict the SWCC indirectly with six soil samples in arid regions. The objective of this study was to compare the two physico-empirical methods and assess the applicability of them under different particle size of soil. The results showed that the A-P model was superior to NSMC model on prediction precision, and more suited to predict silty sand and silt, those soils with medium texture. While using Arya-Paris method, the scaling parameter, α (parameter used to scale pore lengths based on spherical particles to natural soil pore lengths), was estimated by non-linear fitting, linear fitting and as a constant. It was found that the A-P model with non-linear α that used improved logistic growth equation was the best method to estimate SWCC, which had a maximum coefficient of determination (R^2) and minimum root mean square error (RMSE).

1. Introduction

Soil water characteristic curve (SWCC) is an important hydraulic property that can reflect the relationship between soil water quantity and energy, which plays a significant role in researching water flow and solute transport in the unsaturated zone. However, the high variability and complexity of soil make direct determination of the SWCC costly and time-consuming. Nearly 20 years of research showed that there were different degrees of correlations between the SWCC and the basic physical properties of soil. Therefore, many scholars attempted to estimate this property indirectly using the soil's basic physical properties, such as particle-size distribution (PSD), pore structure and bulk density, which was more easily available [1-4].

The indirect method can be roughly divided into two types according to its theoretical basis, namely empirical method, such as Pedo-transfer functions (PTF) [2], and physico-empirical method, such as Arya-Paris model [5]. Empirical methods were based on statistical techniques, which only analysed some relevant relations between the input and output variables instead of causal relationship, and had a poor generality, its practicality was mostly affected by the sample database. While the physico-empirical method both had a physical basis and some empirical assumptions, which had more theoretical advantages than the PTF [6]. Arya and Paris [5] first presented a physico-empirical method



to predict soil water characteristic curves using particle-size distribution data (PSD). The approach was based mainly on the similarity between the shapes of PSD curve and SWCC. In this model, Arya and Paris regarded that the water flowed along the bundle of capillary tubes in their path and assumed that the size of the soil particles and capillary pore diameter were related. The capillary volume was treated to be a function which contained particle size, the mass fraction, also, a scaling parameter, α , which used to measure the ratio of the porosity of the spherical particle length and the natural soil pore lengths. In the earlier model, Arya and Paris [5] assumed that the scaling parameter α was a constant with a value of 1.38 for different soil textures. Later investigations showed that the α varied under different textural classes, for fine textures, the value was 1.1, and 2.5 for coarse textures [7-9]. Arya *et al* [10] proposed alternative formulations with three methods to calculate the scaling parameter, α , a logistic growth equation, a linear fit equation, and a constant α , and verified these methods by experimental water characteristic curve data for five representative soil textures with three to six soil samples (sand, sandy loam, loam, clay, and silt loam). Their research greatly improved the prediction precision compared with the original method with constant α . Tyler and Wheatcraft [8] confirmed that the parameter α was analogous to the fractal dimension of a zigzag fractal, and presented a fractal model to estimate SWCC using physico-empirical method. Zhuang *et al* [1] presented a simple analytical model based on a non-similar media concept (NSMC) to estimate SWCC.

These methods were all based on the shape similarity between the PSD curve and SWCC, so for different particle size, different textures of the soil, the applicable scope of the indirect methods are also different. In order to explore the applicability and diversity of the Arya-Paris model and Non-similar media concept model, and improve the scaling parameter α with a simple logistic growth curve, this study had chosen six different textures of the soil samples, and comprehensively assessed these two methods, providing data support for accurately predict the soil water characteristic curve.

2. Theory

2.1. The Arya-paris model

Arya-paris model [5] assumed that the soil was composed of spherical particles and cylindrical capillary bundle of porous media. The PSD curve was divided into n fractions with boundaries at particle diameters of 1~2000 μm according to the Arya-Paris method, and each fraction of the solid mass was assembled to form a hypothetical, densely cube structure composed of uniform-sized spherical particles. In each assemblage, the pore volume was a function of equivalent diameter, percentage of particle mass and a scaling parameter which computed from the particle density and bulk density that obtained from the nature of the soil structure. The water content was measured on the water-filled pore volumes which continuous accumulated, and the pore radius can be converted into equivalent pressure head according to Young - Laplace equation. The pore volume, V_{vi} ($\text{cm}^3 \text{ g}^{-1}$) is described as:

$$V_{vi} = \pi r_i^2 l_i = (w_i / \rho_p) e \quad (1)$$

$$e = (\rho_p - \rho_b) / \rho_b \quad (2)$$

Where, w_i is the solid mass of the i th fraction (g g^{-1}); ρ_p is the particle density (g cm^{-3}); r_i is the pore radius (cm); e is the void ratio; l_i is the length of the pore (cm g^{-1}) and ρ_b is the bulk density (g cm^{-3}) (Arya and Paris 1981).

The water content ($\text{cm}^3 \text{ cm}^{-3}$) of the i th fraction, is calculated from water-filled pore volumes which continuous accumulated as:

$$\theta_{vi} = \sum_{j=1}^{j=i} V_{vj} / V_b ; i = 1, 2, \dots, n \quad (3)$$

Where V_b is the volume of the soil sample.

n_i (g^{-1}), which is the number of spherical particles for fraction of each particle size, is calculated as:

$$n_i = 3w_i / (4\pi\rho_p R_i^3) \quad (4)$$

Where R_i is the average of particle radius (cm) for the i th fraction. In an hypothetical cubic close-packed system consisting of uniform spherical particles, the pore length l_i is calculated as $l_i = 2n_i R_i$, considering the distribution of the particle shape irregularity in the natural soil, add a scaling parameter α , $l_i = 2n_i^\alpha R_i$, and the pore radius can be expressed by:

$$r_i = R_i [4en_i^{(1-\alpha)} / 6]^{1/2} \quad (5)$$

According to the principle of capillary, the pore radii, r_i , and the equivalent pressure heads, $|h_i|$ (cm H_2O) can be used to transformed by the capillary equation.

$$h_i = \frac{2\gamma \cos \phi}{\rho_w g r_i} \quad (6)$$

Where h_i is the pressure head (cm H_2O), γ is the surface tension (g s^{-2}), ρ_w is the density of water (g cm^{-3}), and ϕ is the contact angle.

2.2. Estimating scaling parameter

The relationship between the number of spherical particles, N_i (g^{-1}), and the number of spherical particles in the ideal soil, n_i (g^{-1}), which required to trace the pore length in the relevant natural soil's structure, is given by:

$$n_i^\alpha = N_i \quad \text{or} \quad \alpha_i = \log N_i / \log n_i \quad (7)$$

Equation (4) was used to calculate the values of n_i from the PSD data. N_i was calculated as:

$$N_i = 7.371 w_i e^{h_{mi}^2} / \rho_p R_i \quad (8)$$

Where h_{mi} is the measured pressure head (cm H_2O).

Arya *et al* [10] evaluated scaling parameter α with logistic growth method and similarity method. This study used three formulation methods based on Arya *et al* to calculate the α : nonlinear fitting α , linear fitting α , and constant α .

2.2.1. Nonlinear fitting. Through the observation of the data between $\log N_i$ and $\log n_i$, it was found that the relationship was in an s-shaped curve, so we can choose logistic growth equation to fit $\log N_i$ and $\log n_i$:

$$Y = a + b \exp\{-\exp[-c(X - d)]\} \quad (9)$$

In which Y represents $\log N_i$, and X is $\log n_i$, a , b , c , d respectively represent the shape parameter.

2.2.2. Linear fitting. Arya *et al* [10] found there is a linear relation between $\log N_i$ and $\log \frac{w_i}{R_i^3}$:

$$\log N_i = a + b \log \frac{w_i}{R_i^3} \quad (10)$$

Substituting $\log N_i$ for equation (10) into equation (7), we can obtain an explicit formulation about α as follow:

$$\alpha = \frac{a + b \log(\frac{w_i}{R_i^3})}{\log n_i} \quad (11)$$

2.2.3. *Constant α .* In this method, we assumed that the scaling parameter α was a constant which can be calculated by fitting the value of $\log N_i$ and $\log N_i$ with linear regression, and setting the intercept value to 0. The slope of the resulting regression line represented the value of α .

2.3. Non-similar media concept model (NSMC)

Zhuang *et al* [1] used a non-similar media concept which was proposed by Miyazaki [11] to estimate saturated hydraulic conductivity for the first time. This concept is defined as:

$$V_{v,i} = \left(\frac{w_i}{\rho_p} \right) e = N_i \left[(\bar{D}_{g,i} + \bar{D}_i)^3 - \tau_i \bar{D}_{g,i}^3 \right] \quad (12)$$

Where $\bar{D}_{g,i}$ is the average particle diameter (cm) for the i th fraction, $\bar{D}_i$ is the average pore diameter (cm) generated by these i th fraction particles, τ is calculated by the ratio of the solid phase volume and the total soil volume, which be called a shape factor of the solid phase. For a cube, the value of τ is 1.0, and $\pi/6$ for a sphere, the meaning of the w_i , ρ_p , e is the same as the equation (1).

The relationship between the average pore diameter, $\bar{D}_i$, and the average particle diameter, $\bar{D}_{g,i}$, is described as:

$$\bar{D}_i = \bar{D}_{g,i} [(\tau_i e + \tau_i)^{1/3} - 1] \quad (13)$$

Assuming that the shape factor τ_i can be calculated by a logistic function of the average particle diameter $\bar{D}_{g,i}$ as follows:

$$\tau_i = [1 + e \exp(\delta \bullet \bar{D}_{g,i})]^{-1} \quad (14)$$

The parameter δ is obtained by:

$$\delta = \begin{cases} n\alpha & \text{for sand} \\ \alpha & \text{for loam and clay} \end{cases} \quad (15)$$

Where n and α are obtained from fitting the PSD curve using the van-Genuchten model [12,13].

The equivalent capillary pressure head, h_i (cm H₂O), which with respect to the i th fraction, can be described as:

$$\psi_i = \frac{4\gamma \cos \phi}{\rho_w g D_{g,i} [(\tau_i e + \tau_i)^{1/3} - 1]} \quad (16)$$

The meaning of the parameters is the same as the equation (6).

The water content of the i th particle size fraction is calculated from water-filled pore volumes which continuous accumulated as equation (3).

2.4. Particle-size distribution curve (PSD)

The key to estimating soil water characteristic curve used physico-empirical methods is to obtain the whole PSD curve. However, the result of conventional soil particle analysis is only a few data points, which greatly limits the prediction accuracy and practicability of the indirect method. This study used MLog model [13] to fit the whole PSD curve, which has the form:

$$m = \frac{1}{1 + a \exp(-bD^c)} \quad (17)$$

Where D is the particle diameter (cm), m is cumulative mass fractions of the particles with the diameter smaller than D , a , b , c is the shape parameter of the curve.

3. Materials and methods

3.1. Research materials

Six soil samples with four typical textures in arid and semi-arid regions were selected as the experimental samples, which were medium sand, silty sand, silt, and silty clay. These soils are taken from the Key Laboratory of Subsurface Hydrology and Ecological Effect in Arid Region from Chang'an University, Xi'an, China. The basic physical properties of the soil sample included the bulk density, and grain size composition were obtained according to the geotechnical test procedures. Which were shown in table 1, and figures 1(a)-1(d) shown the real photos of the six samples of soils.

Table 1. Some basic properties of the soil samples.

Soil Texture	particle-size distribution (mm.%)							Mean particle size D50	Dry density g·cm ⁻³
	>0.5	0.5 ~ 0.25	0.25 ~ 0.075	0.075 ~ 0.05	0.05 ~ 0.01	0.01 ~ 0.005	<0.005		
Medium sand	27.9	45.7	23.9	2.5	0	0	0	0.4	1.57
Silty sand	0	0	52.8	14.3	28.9	2.1	1.9	0.08	1.47
Silt-1	0	0	40.5	21.7	33.7	2.1	2	0.063	1.43
Silt-2	0	0	1.8	14.4	73.3	5.5	5	0.03	1.32
Silty clay-1	0	0	9.2	7.3	75.6	4.1	3.8	0.02	1.37
Silty clay-2	0	0	0	4.3	66.3	12.5	16.9	0.02	1.57

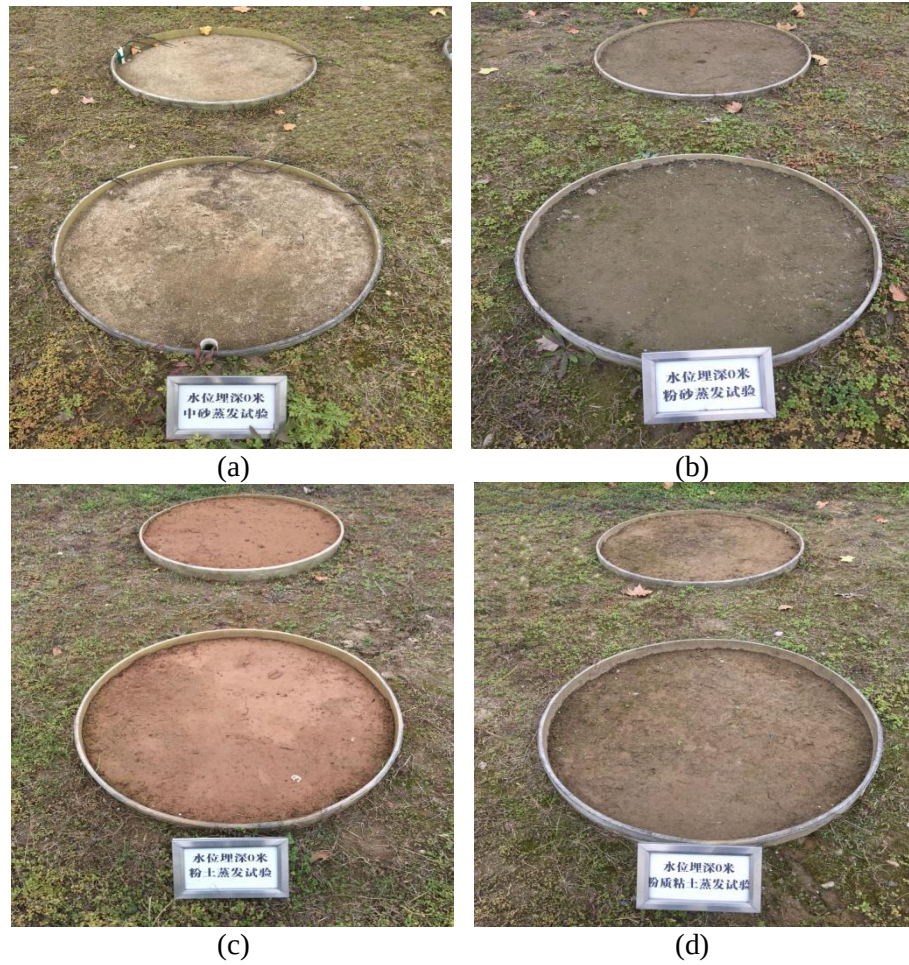


Figure 1. Photos of the soil samples. (a) medium sand, (b) silty sand, (c) silt and (d) silty clay.

3.2. Research methods

The estimated soil water characteristic curve was calculated as shown in figure 2 (A-P model for example):

3.3. Reliability of results

To rigorously determine the precision to the Arya-Paris model and the Non-similar Media Concept Model (NSMC), we use the root mean square error (RMSE) and coefficient of determination (R^2) to compare the statistical results. The RMSE and R^2 values are calculated by experimental pressure head (h_{exp}) and the estimated pressure head (h_{est}) under the same water content value. The formulae are:

$$RMSE = \left[\frac{1}{N} \sum_N (Y_i - Y_p)^2 \right]^{1/2} \quad (18)$$

$$R^2 = \left[\frac{\sum (Y_i - \bar{Y}_i)(Y_p - \bar{Y}_p)}{\sqrt{\sum (Y_i - \bar{Y}_i)^2 \sum (Y_p - \bar{Y}_p)^2}} \right]^2 \quad (19)$$

Where Y_i is the experimental pressure head (h_{exp}), Y_p is the estimated pressure head (h_{est}) by different methods, $\bar{Y}_i$ is the mean experimental pressure head, $\bar{Y}_p$ is the mean estimated pressure head, and N is the number of experimental groups of the pressure head.

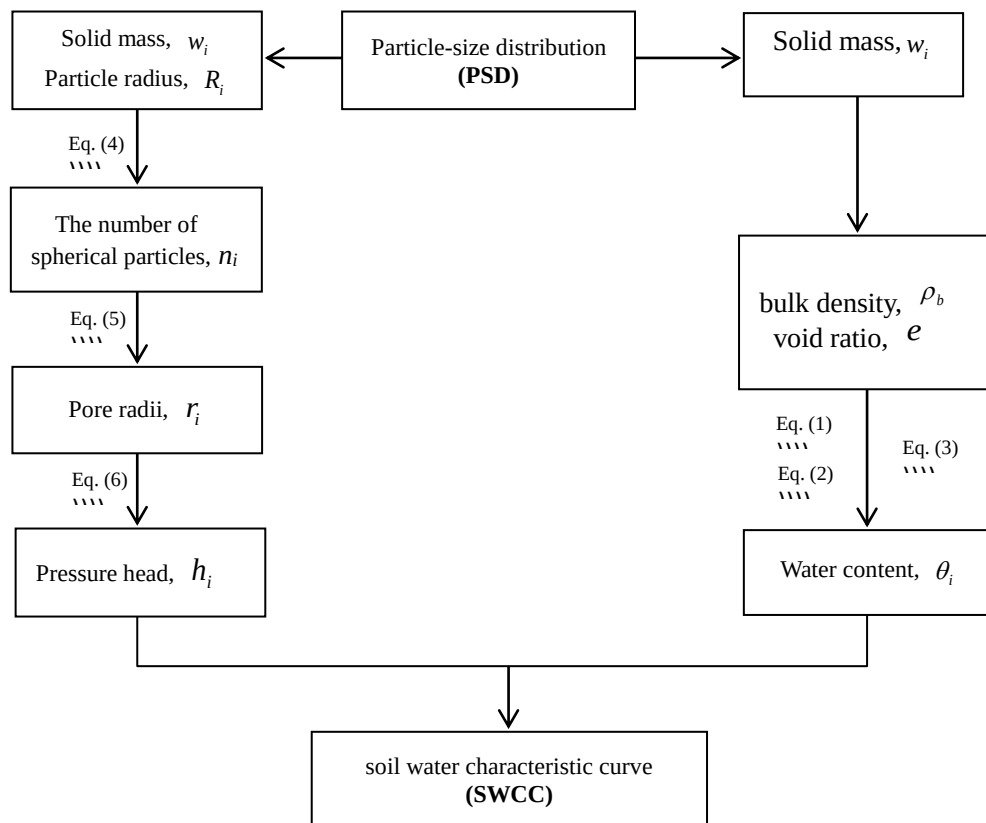
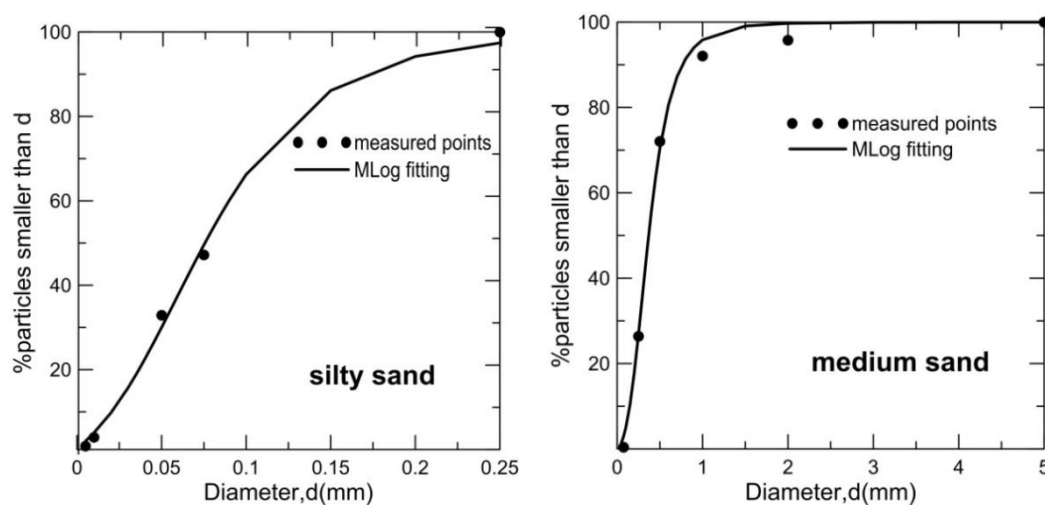


Figure 2. Calculation flow chart (Arya-Paris model e.g.).

4. Results and discussions

4.1. Particle-size distribution curve (PSD)

The PSD curves of the experimental soil samples used by Mlog model are shown in figure 3.



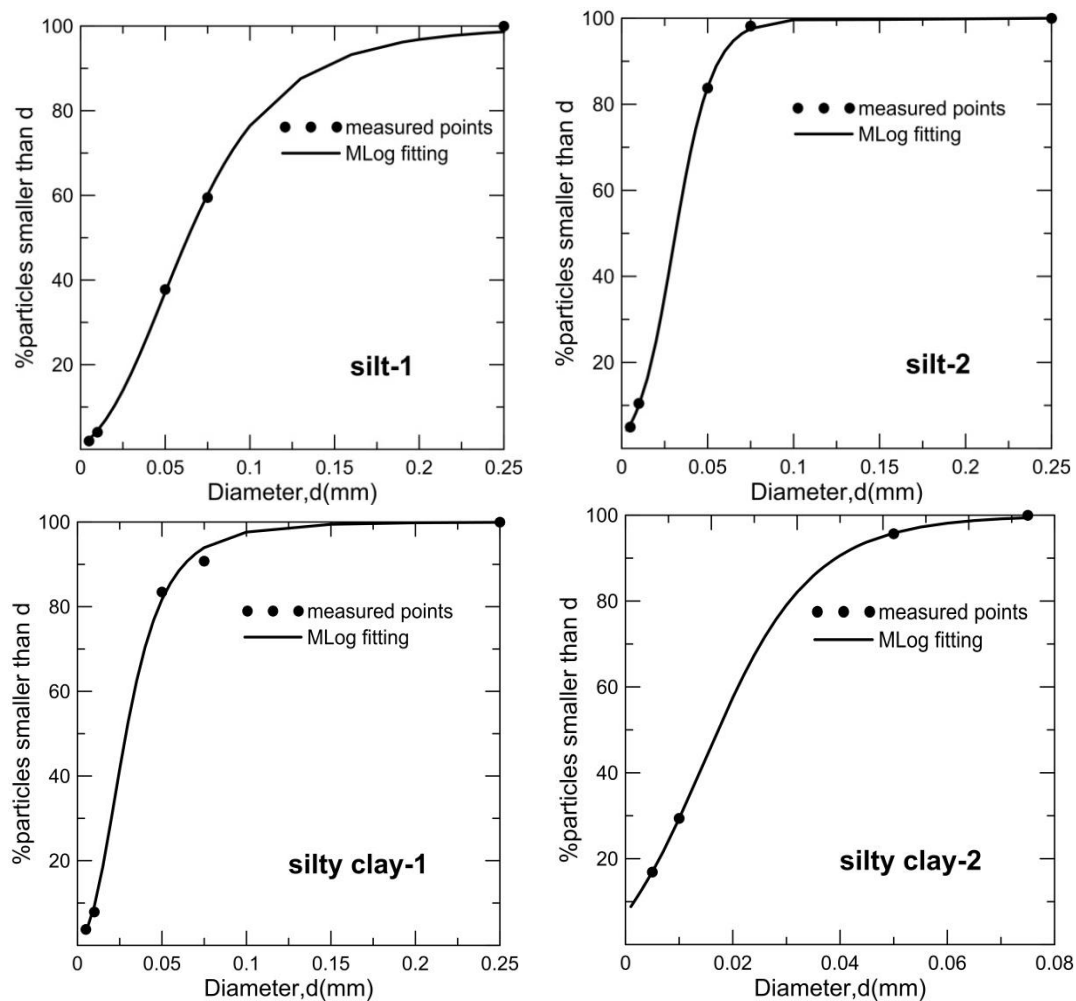


Figure 3. Particle-size distribution curve of Mlog model.

4.2. Estimated soil water characteristic curve (SWCC)

4.2.1. Estimated SWCC by Arya-paris model. The estimated SWCC by Arya-paris model with three different approaches of scaling parameter were shown in figure 4. As was shown in figure 4, the three fitting methods can well estimate the SWCC. The best way to fit the measured and estimated SWCC was the nonlinear α method, the linear method take second place, and constant α was the worst choice. The nonlinear method had minimum error between the predicted values and measured values, and can better predict the volume water content and pressure head at inflection point, so it can estimate the trend of the whole curve. Using linear α and constant α usually resulted in underestimate the water content in the dry range (high tension region) and overestimate it in the wet range (low tension region), which had a relatively larger error near the point that the curve had a sharp change. This may be due to the limitations of soil structure and the capillary theory. Near saturated region, moisture in the soil mainly depends on the water stored in the large pore, and the porosity of the large particle size level in the PSD plays a decisive role in the prediction results. While near the dry region, the soil moisture content is close to the residual water content, and water mainly remain in the small pores, where the porosity of the small particle size level plays a controlling role in the prediction results. Therefore, when dividing the particle size fraction in the process of predicting SWCC, the extreme particle size has a great influence on prediction results. It is recommended to divide the particle size fraction reasonably when using the Arya-Paris model.

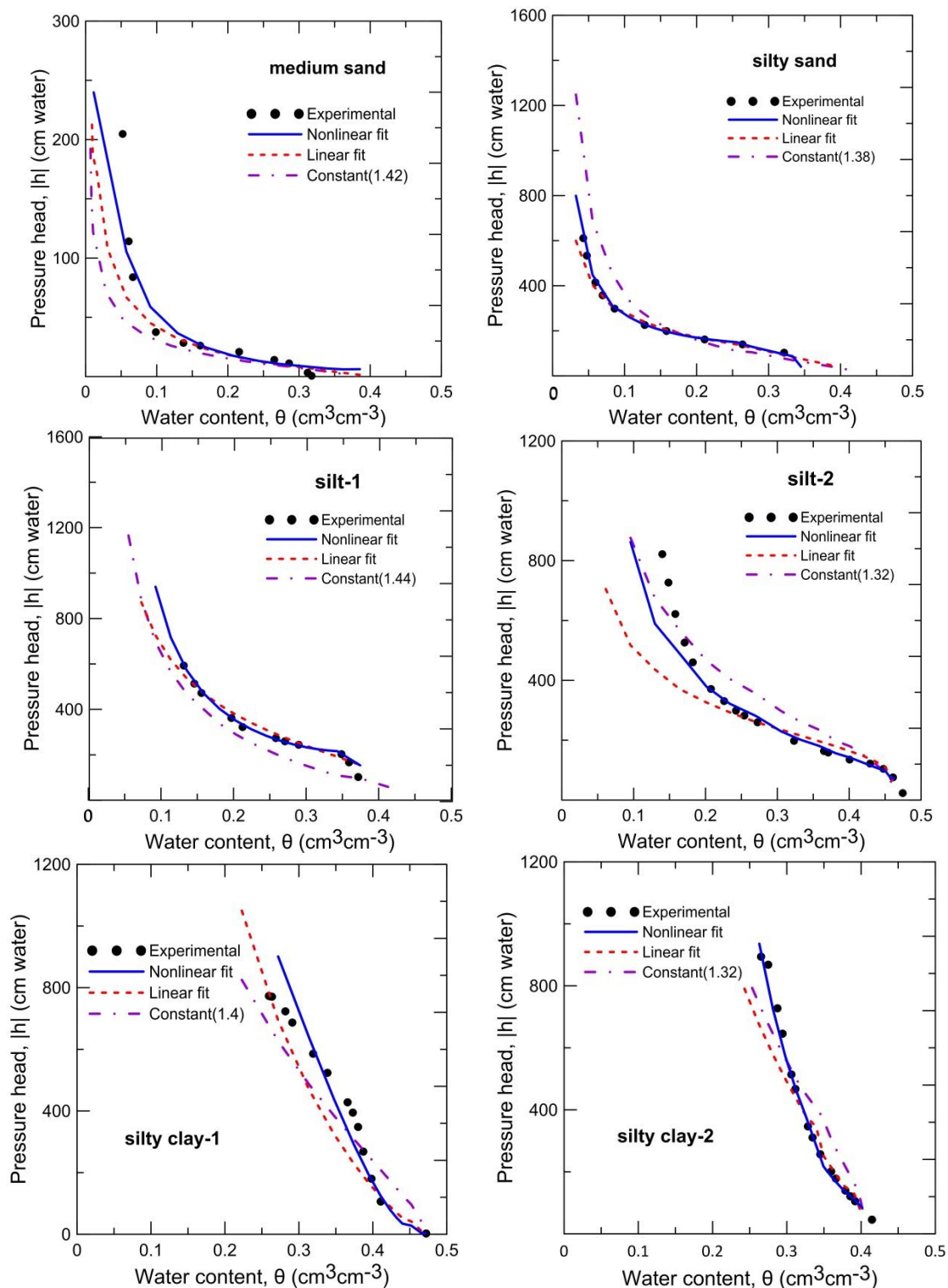
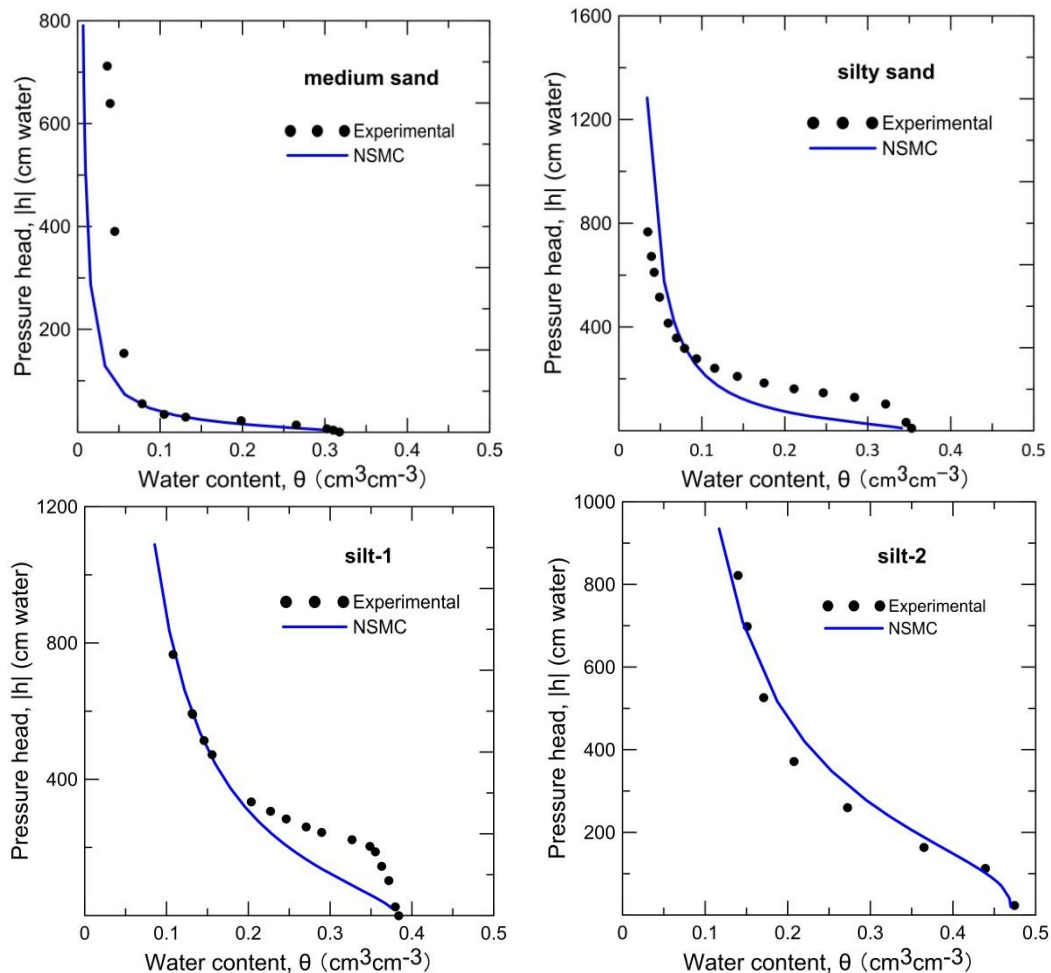


Figure 4. The estimated SWCC by Arya-paris model.

In addition, the same method also has different results to predict different textures of the soil. It can be seen from figure 4 that the three methods of calculating scaling parameter α all showed good agreement on silty sands and silt, which have the medium particle size (0.05~0.25 mm), but for the relatively large particle size such as medium sand (>0.25 mm) and small particles size such as silty

clay (<0.02 mm), the prediction results were less desirable. This may be due to the relatively uniform and continuous of the pore structure for the medium texture soil, which has little particle size differences, using the theory of capillary to predict soil water characteristic curve can eliminate the extreme particle size deviation. It is concluded that the Arya-Paris model is more suited to predict the medium texture of soil, but is not suitable for predicting coarse and fine-textured soils.

4.2.2. Estimated SWCC by non-similar media concept model (NSMC). Figure 5 compared the SWCC measured by experimental values and calculated values for the NSMC model for 6 different soil samples. This figure shows that the NSMC model estimated the SWCC is reasonable, however, it cannot describe the tendency of the curve accurately at inflection point, thus cannot predict the air entry value accurately near saturation of the soils and the residual water content at the dry region. Relatively speaking, the NSMC model is more suited to be used to predict the medium sand and silty sands, but is not suitable for predicting the silt and silty clay, which can be seen in figure 5.



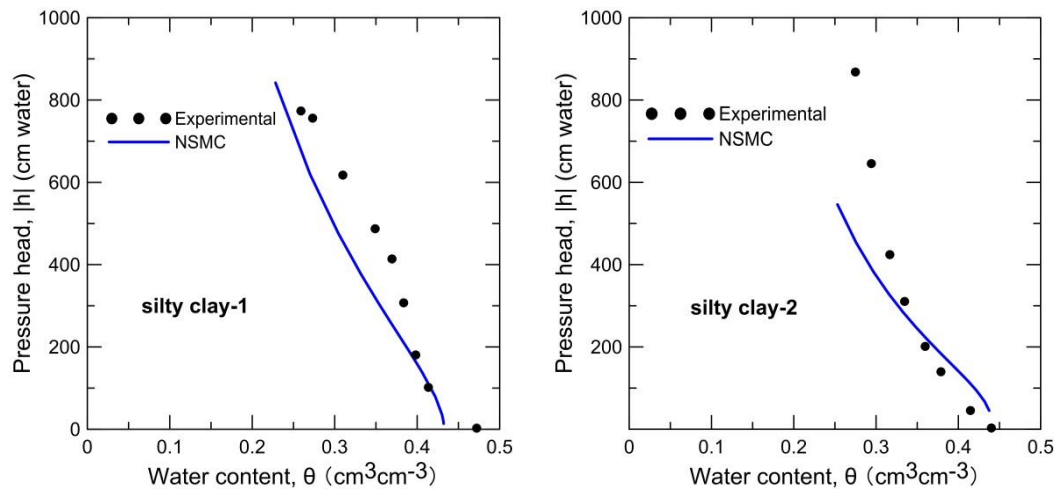
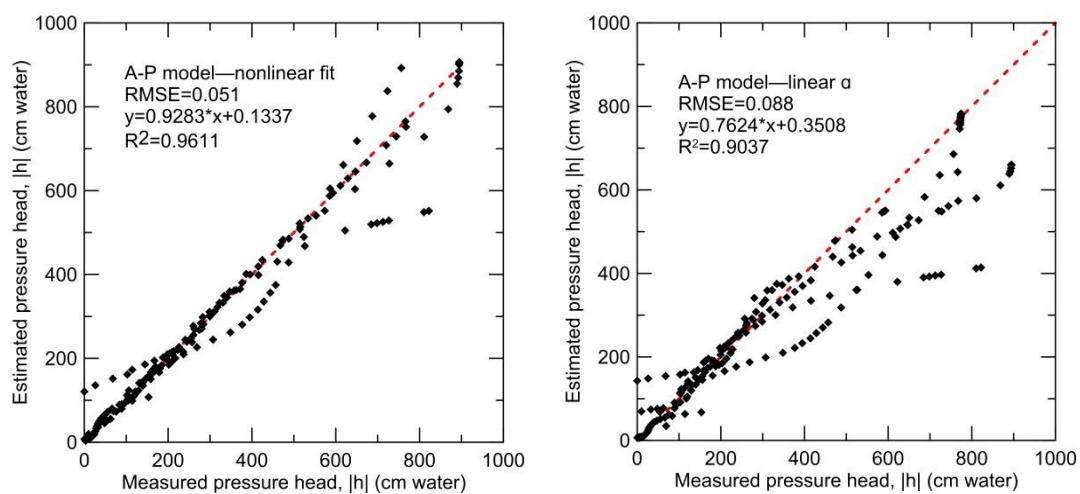


Figure 5. The estimated SWCC by NSMC model.

4.2.3. The precision of the Arya-paris model and NSMC model. In order to intuitively determine the accuracy of the method indicated, we evaluated all methods by comparing measured pressure head and estimated pressure head at the same water content on a 1:1 plot, as is shown in figure 6. The root mean square error (RMSE) and the coefficient of determination (R^2) between measured pressure head and estimated pressure head were shown in table 2. The results showed clearly that the Arya-Paris model using the nonlinear α method and linear α method to calculate the scale parameter α was more efficient and accurate than the NSMC model.

Table 2. Values of R^2 and RMSE for the methods of estimating SWCC.

	A-P model			NSMC model
	constant α	linear fit	nonlinear fit	
R^2	0.876	0.904	0.961	0.877
RMSE	0.094	0.088	0.051	0.091



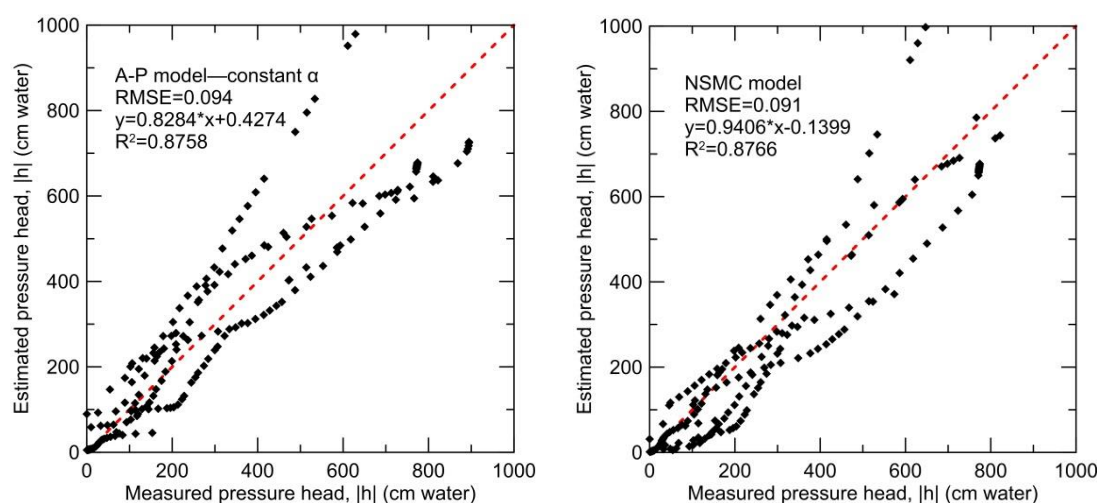


Figure 6. Comparison of measured and estimated pressure head.

When using the nonlinear α method of Arya-paris model, the measured pressure head and estimated pressure head points substantially located on 1:1 plot, and has the maximum R^2 value of 0.961 and the minimum RMSE value of 0.051, so it is the best approach to estimate the SWCC. The linear α of Arya-Paris model comes in second place, with the R^2 value of 0.904 and the RMSE value of 0.088. In contrast, the Arya-Paris model with constant α and the NSMC model are poorer, as is shown in figure 4, the measured pressure head and estimated pressure head points are relatively scattered from 1:1 plot. The values of R^2 and RMSE are 0.876 and 0.094 to Arya-Paris model with constant α , and 0.877 and 0.091 to NSMC model.

However, this research did not consider the effect of temperature upon water fate and retention behavior on the accuracy of the prediction, which should be made further research and discussion in the future.

5. Conclusions

Using the physico-empirical methods to indirectly predict soil water characteristic curve is feasible, which is much convenient and less time-consuming than directly experimental measuring method. This study recommend two physico-empirical models for estimating SWCC, that are Non-similar Media Concept Model (NSMC) and Arya-Paris (A-P) model contained three approaches for estimating the scale parameter α . These methods were verified by 6 different textures of the soil. The main conclusions obtained from this study were as follows:

Arya-Paris model with nonlinear α which used improved logistic growth equation showed good accordance between the measured and estimated SWCC, which was the best approach to estimate the SWCC. The constant α of the Arya-Paris model and the NSMC model showed poor agreement with the measured SWCC.

The same method also showed different results to predict different texture of the soil water characteristic curve. The results showed that the prediction accuracy of Arya-Paris model was superior to non-similar media approach, and more suited to predict silty sand and silt, those soils with medium particle size (0.05~0.25 mm). However, rough texture of the medium sand (>0.25 mm) and fine texture of silty clay (<0.02 mm) showed poor results. The NSMC model showed better result to predict the high sand content soil than the high silt and clay content soil.

Eventually, the results provide data support for predicting the soil water characteristic curve accurately.

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