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原著

토양수분특성 추정을 위한 입자크기분포 모형들의 비교

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Comparison of Particle-Size Distribution Models for Estimating Water Retention Characteristic

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요 약 문

불포화토양내 물의 흐름과 유기오염물질의 이동현상을 예측하기 위해서는 불포화토양의 토양수분곡선을 구하는 것이 필수적이다. 입자크기분포로부터 토양수분곡선을 직접 구하는 물리경험적 방법이 많은 연구자들에 의해 제안되고 적용되어왔다. 이 방법은 공극크기분포가 직접적으로 입자크기분포와 상호연관되어있다는 개념을 이용한 것으로, 입자크기분포곡선을 산정하는 방법이 토양수분곡선추정에 영향을 미칠 수 있다는 것을 의미한다. 본 연구에서는 Arya-Paris 모형을 이용한 토양수분곡선 추정이 어떠한 입자크기분포모형을 선택하는가에 따라 영향을 받는지를 알아보고자 하였다. 1~4의 추정변수를 갖는 4개의 입자분포곡선 모형을 사용한 결과, 단지 1개의 추정변수를 갖는 Jaky모형이 더 많은 추정변수를 가진 모형보다 토양수분곡선을 잘 예측하였다. Jaky모형의 우월한 예측력은 아마도 현장토양이 가지는 구조적 특성때문인 것으로 사료된다.

주제어 : 입자크기분포, 토양수분곡선, Arya-Paris 모형, Jaky모형

ABSTRACT

Knowledge of soil water retention characteristic is essential for many problems involving water

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flow and organic solute transport in unsaturated soils. A physico-empirical approach based on the translation of the particle-size distribution (PSD) into a corresponding water retention curve has been accomplished by others using the concept that the pore-size distribution is directly related to PSD. This approach implies that details of a PSD curve may affect the estimation of water retention characteristic (WRC). To determine whether the WRC estimation using the Arya-Paris model could be affected by the selection of a PSD model, four PSD models with one to four fitting parameters were used. The Jaky model with only one fitting parameter had greater WRC estimation ability than other models with greater number of fitting parameters. The better performance of the Jaky model may be explained by the effect of soil structure in field soils.

Key Words : Particle-size distribution, water retention characteristic, Arya-Paris model, Jaky model.

1. INTRODUCTION

Soil water retention characteristic is one of fundamental hydraulic properties necessary to understand water flow and mass transport phenomena in unsaturated soils. Soil water retention measurements are relatively time-consuming in laboratory and field conditions. Hence, statistical techniques have been used to estimate this property indirectly using particle-size distribution (PSD) and other soil properties. However, these techniques have limited applicability and accuracy for various reasons[1), 2), 3), 4)].

A physico-empirical approach, which is based on the translation of the PSD into a corresponding water retention curve, has been accomplished using the concept that the pore-size distribution is directly related to PSD[5), 6), 7), 8)]. This approach implies that details of a PSD curve may affect the estimation of water retention characteristic (WRC). Arya et al.[7)] suggested that PSDs comprised of at least twenty fractions were a reasonable number of fractions for the calculation of the WRC with their own model. However, experimental PSD data usually has a limited number of data points. For example, the Korean soil database containing 1,387 soils had seven PSD data points for each soil[9)]. Soils in the UNSODA database used by Arya et al.[7)] usually had from four to eleven PSD data points. This indicates that a procedure is needed to generate detailed PSD from limited number of experimental PSD data points to provide adequate prediction of the WRC through application of the physico-empirical approach.

Arya and Paris[5)] and Arya et al.[7)] did not describe explicitly how detailed PSD data were generated from experimental PSD data points. On the other hand, Haverkamp and Parlange[6)] adopted a functional relationship of the van Genuchten[10)] type to fit the experimental PSD data. Zhuang et al.[8)] adopted two functional relationships, i.e. the van Genuchten[10)] type for sand and loamy sand soils and a logarithm function for the other textural soils, to generate detailed PSD.

Other diverse PSD models have been proposed to generate detailed PSD from experimental PSD data points[11), 12), 13), 14), 15)]. Hwang et al.[9)] compared the capability of seven PSD models with different underlying assumptions to fit experimental PSD data of 1,387 different soils in the Korean soil database. They found that the four-parameter Fredlund et al. model[12)] performed best even when three statistical criteria that impose a penalty for additional fitting parameters were used to assess the quality of the fit. Nemes et al.[13)] evaluated four different procedures to interpolate PSDs to achieve compatibility within soil databases. A loglinear interpolation procedure was the least accurate for estimating missing particle size classes for the soil databases they studied.

Since the WRC estimation by the physico-empirical approach is based mainly on the similarity between shapes of PSD and water retention curves, the estimation of WRC may be affected by the selection of a PSD model. The objectives of this study were (1) to determine whether the estimation of the WRC using the physico-empirical approach could be affected by the selection of a PSD model, and (2) to determine if the use of a PSD model with better fitting ability represents better experimental WRC data. To achieve these objectives, four models were used to generate detailed PSD curves from experimental PSD data in the UNSODA database. The WRC predicted with these detailed PSD curves and the Arya and Paris[5)] and Arya et al.[7)] physico-empirical models were then compared with the experimental WRC data.

2. BACKGROUND

2.1 The Arya-Paris model

The model assumes that the pore-size distribution is directly related to PSD. Firstly, the PSD curve is divided into n fractions, and the difference in cumulative mass fraction corresponding with successive particle sizes is used to obtain the solid mass in each fraction. The pore volume associated with the solid mass in each fraction is calculated on the basis of the assumption that the bulk and particle densities of the bulk sample apply to each fraction. The pore volumes generated by each fraction are progressively summed and considered filled with water. The volumetric water content at the upper bounds of successive mass fractions is obtained by summations of the individual pore volumes divided by the bulk volume of the sample. An equivalent pore radius is calculated for each fraction and converted to soil water pressure head using the capillary equation. Calculated pressure heads are sequentially paired with calculated water contents to obtain a soil water characteristic curve. The basic assumptions and equations of the model are as follows.

The volumetric water content, θ_i (cm³ cm⁻³), can be calculated from PSD, porosity, and maximum measured water content information, according to

$$\theta_i = (\varphi S_w) \sum_{j=1}^{j=i} w_j ; \qquad i = 1,2,\ldots\ldots, n \qquad (1)$$

where φ is the total porosity ($\mathrm{cm^3\ cm^{-3}}$), S_w is the ratio of measured saturated water content to the total porosity, and w_i is the mass fraction ($\mathrm{g\ g^{-1}}$) in the ith particle-size fraction.

The number of spherical particles for the ith particle-size fraction (g^{-1}), n_i, is given by

$$n_i = 3w_i / (4\pi\rho_s R_i^3) \qquad (2)$$

where ρ_s is the particle density (g cm^{-3}) and R_i is the mean particle radius in the ith particle-size fraction (cm). Pore radii for a natural soil (cm), r_i, are given by

$$r_i = 0.816 R_i / \sqrt{e n_i^{(1-\alpha i)}} \qquad (3)$$

where e is the void ratio given by $(\rho_s - \rho_b)/\rho_b$, ρ_b is the bulk density of the soil (g cm^{-3}), and α_i is the scaling parameter which is to be determined empirically and equal to log N_i/log n_i where N_i is the scaled number of spherical particles in the corresponding natural structure soil (g^{-1}).

Pore radii, r_i (cm), are converted to equivalent pressure head, h_i (cm water), using the Young-Laplace equation describing capillary rise in a cylindrical pore :

$$h_i = \frac{2\gamma \cos\theta}{\rho_w g r_i} \cong \frac{A}{r_i} \qquad (4)$$

where γ is the surface tension of water, θ is the contact angle, ρ_w is the density of water, and g is the acceleration due to gravity. The value of A for air-water-soil systems is 0.149 cm^2. Details of the Arya-Paris model are provided by Arya and Paris[5] later improved by Arya et al.[7].

2.2 Particle-size distribution models

To estimate WRC from a PSD using the Arya-Paris model, firstly, it is necessary that (1) the PSD curve is divided into n fractions and (2) the w_i is calculated from the difference in cumulative mass fraction corresponding with successive particle sizes. To estimate cumulative mass fraction corresponding with successive particle sizes from limited number of experimental PSD data points, it is necessary to have an approach for representing the PSD. To do this, parametric PSD models can be used because they can provide complete information on the soil PSD. Four unimodal parametric models were tested to generate w_i for each soil. Each PSD model may yield different w_i, providing different predicted $\theta(h_i)$ pairs (see equations (1) through (4)). Three lognormal models were chosen among models previously studied by Buchan et al.[11] and Hwang et al.[9]: the Jaky one-parameter model[16] with a sigmoid half of a Gaussian lognormal distribution; a simple lognormal model with two parameters (SL)[17]; and one modified lognormal model with three parameters, i.e. an offset-nonrenormalized lognormal model (ONL)[11]. Buchan et al.[11] provides details of the three lognormal models. The Fredrund et al.[12] model was tested as four-parameter model. The four models considered in this study are listed in Table 1.

Table 1. Textural Classes and UNSODA Codes for Soils Used for Testing the Estimation of Water Retention Characteristic Based on Different PSD Models

Textural classes	UNSODA codes
Sand	1050, 1460, 2100, 3132, 3340, 4650
Sandy loam	1130, 1131, 1381, 3310, 4160
Loam	1370, 2531, 4610
Silt loam	1341, 4081, 4510, 4531, 4670
Clay	1400, 2361, 3282, 4121, 4681

(From Arya et al., 1999)

3. RESEARCH METHODS

3.1 The UNSODA hydraulic property database

Experimental WRC, PSD, bulk density, and particle density data were obtained from the UNSODA hydraulic property database[18]. For this study, twenty-four data sets, representing a range of textures that include sand, sandy loam, loam, silt loam, and clay, were selected from the UNSODA hydraulic property database (Table 2). These data sets were same as those that Arya et al.[7] used to formulate three methods to estimate the scaling factor α_i of their own model. Soils used in this study had four to eleven experimental PSD data points and experimental $\theta(h_i)$ data points ranged from six to thirty in each soil.

3.2 Calculation of water retention curve, $\theta(h_i)$

The number of PSD experimental data points ranged from four to eleven in soil database. To estimate a full range of PSD from limited number of experimental PSD data points, four PSD models were fitted to the experimental PSD data points in each soil. To optimize parameters of a PSD model, an iterative nonlinear regression procedure was applied to evaluate the values of the fitting parameters that give the 'best fit' between the PSD model and the experimental PSD data (SOLVER routine of Microsoft Excel software[9]).

A PSD curve for each soil was divided into twenty size fractions (i.e. $n = 20$) with fraction boundaries at particle diameters of 1, 2, 3, 5, 10, 20, 30, 40, 50, 70, 100, 150, 200, 300, 400,

Table 2. Particle-Size Distribution Models Tested for Texture Data of 24 soils

Name	Model†	Parameters
Jaky (Jaky, 1944)	$F(d) = \exp\left\{-\frac{1}{p^2}\left[\mathrm{in}\left(\frac{d}{d_0}\right)\right]^2\right\}$	p ($d_0 = 2$ mm)
Simple Lognormal (SL) (Buchan, 1989)	$F(X) = \left(1+erf\left[\left(X-\mu\right)/\sigma\sqrt{2}\right]\right)/2\ (X \geq \mu)$ ‡ $F(X) = \left(1-erf\left[\left(X-\mu\right)/\sigma\sqrt{2}\right]\right)/2\ (X < \mu)$ $X = \mathrm{In}(d)$	μ, σ
Offset-Nonrenormalized Lognormal (ONL) (Buchan et al., 1993)	$G(X) = F(X) + c$ ($F(X)$ defined by SL model)	μ, σ, c
Fredlund (Fredlund et al., 2000)	$F(d) = \frac{1}{\left\{\ln\left[\exp(1)+\left(\frac{a}{d}\right)^n\right]\right\}^m}\left\{1-\left[\frac{\ln\left(1+\frac{d_f}{d}\right)}{\ln\left(1+\frac{d_f}{d_m}\right)}\right]^7\right\}$	α, n, m, d_f ($d_m = 0.0001$ mm)

† d: particle diameter in mm.

‡ erf [ ]=error function.

600, 800, 1000, 1500, and 2000 μm[7]. Cumulative mass fraction at each fraction boundary was estimated using the above fitting results for four PSD models. This yielded twenty corresponding pairs of mass fraction, w_i, and mean particle radii, R_i for each PSD model. Each PSD model may yield different w_i. Each w_i was converted to an equivalent number of spherical particles, n_i, using equation (2). To calculate mean pore radii, r_i, in equation (3), it is necessary to estimate one additional parameter, α_i.

The Arya-Paris model[5] assumed that α_i is a constant (=1.38) for all soil textural classes. Arya et al.[7] proposed three methods to estimate α_i. The first method was to relate log N_i and log n_i using a logistic growth curve. The second method was to relate log N_i and log (w_i/R_i^3) linearly. The parameters used in both methods were obtained by fitting the model to measured $\theta(h_i)$ data of twenty-four soil samples. The third method was to give α_i a single value for each representative soil texture by fitting a linear regression with zero intercept to the plot of log N_i vs. log n_i. In this study, all three methods proposed by Arya et al.[7] were tested.

The pressure head, h_i, was calculated using equation (4). And then corresponding water content, θ_i, was obtained by using equation (1).

3.3 Performance of different PSD models in WRC estimation

Three PSD models (Jaky, SL, ONL) used in this work have same underlying assumption that the PSD in soil is lognormal, implying the possibility of identical performance among these models in the estimation of WRC. Therefore, to determine whether statistically identical estimates resulted between the PSD model pairs, including the Fredlund model, paired t-tests were conducted on each log-transformed predicted h_i values at same water content.

To determine whether a PSD model with better fitting ability represents better experimental WRC, r^2 value was used as a statistical comparison of the results. The r^2 values were computed using log-transformed experimental and predicted h_i at the same experimental θ_i. Van Genuchten[10] function was chosen to calculate predicted h_i at the same experimental θ_i from twenty $\theta(h_i)$ data points calculated from the Arya-Paris model. The SOLVER routine of Microsoft Excel software was used for this nonlinear regression. The r^2 values for all PSD models and three α_i estimation methods were calculated.

4. RESULTS AND DISCUSSION

4.1 Fitting ability of particle-size distribution models

Among all of the soils and all of the models, values of r^2 for the PSD models fit to experimental PSD data ranged from 0.867 to 1.000 (Fig. 1). As expected, the model with greater number of parameters had higher r^2 values than those with smaller number of parameters. For example, the lowest r^2 values were obtained with the one-parameter Jaky model whereas the Fredlund model with four fitting parameters had the highest r^2 values. Also, the r^2 values were higher for the ONL model than for the SC model. This result

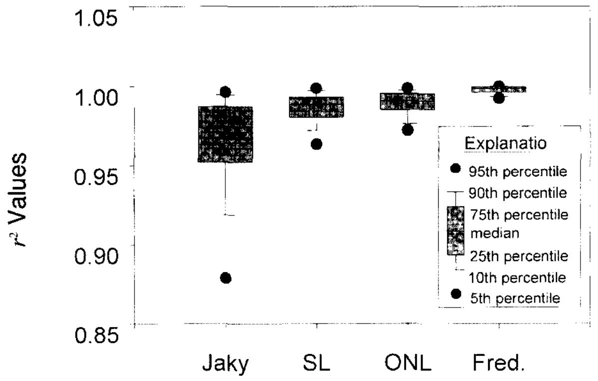

Fig. 1. Box plot for r^2 percentiles as the goodness-of-fit of four PSD models for all soils.

conforms to that of Hwang et al.[9].

4.2 Effect of PSD models on estimated soil water characteristic

Arya et al.[7] used three methods to estimate the scaling factor α_i in their model. They found that Method 1 using variable α_i was the best to estimate the WRC. However, in this work, Method 3 using constant α_i showed the best WRC estimation in all PSD models (e.g. as an example, Fig. 2 for the Jaky model). The difference between two results is considered to be due to differences in the approach used to generate the detailed PSD. Also, Zhuang et al.[8] found, using the UNSODA plus China and Japan soil data set (total 130 soil data), that Method 3 was better than the other two in the WRC estimation. Therefore, Method 3 was adopted herein as the best estimation for α_i.

It is necessary to determine whether the WRC estimation using the Arya-Paris model could be affected by the selection of a PSD model. As an example, Fig. 3 shows the possibility of different water retention

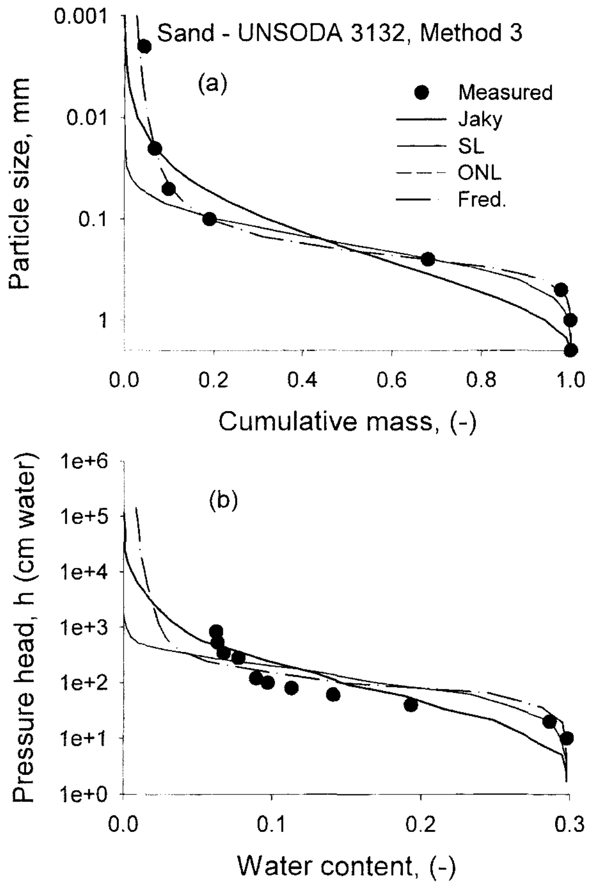

Fig. 2. Comparative fit of (a) the PSD and (b) the water retention curve using four PSD models at a sand (UNSODA No. 3132) and using Method 3 to estimate the scaling parameter α_i.

estimations according to the use of different PSD models. Note that with the Arya-Paris model, the shape of estimated water retention curve followed exactly the corresponding PSD curve (Fig. 3). This suggests that the estimation of WRC could be affected by the selection of PSD model.

As shown in Fig. 3, the SL and ONL models showed nearly identical performance in their ability to estimate both PSD and WRC. Therefore, it is necessary to determine if any

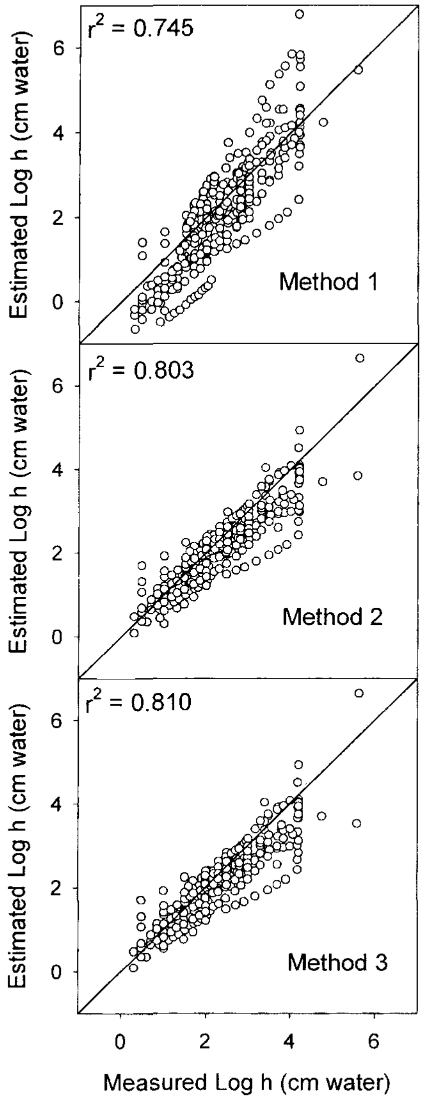

Fig. 3. **Comparison of calculated and experimental pressure heads using the Jaky model. Test results for 24 soils are pooled: (a) Method 1, (b) Method 2, and (c) Method 3.**

PSD model pair has statistically identical performance in the estimation of WRC. To do this, paired t-tests were conducted on WRC generated with all possible six PSD model pairs, using each paired log-transformed estimated h_i at the same θ_i. It was found, for all three methods to estimate α_i, that only the SL-ONL model pair showed statistically identical performance for the WRC estimation at 95% significance level.

Typical examples of predicted and experimental WRCs for sand, sandy loam, silt loam, and clay as affected by the PSD models are presented in Fig. 4. Results show that all four PSD models adequately predict shape of the experimental WRC. However, the differences between predicted and experimental h_i varied in magnitude from a textural class to other textural class. Especially, the Jaky model showed the best performance in sandy loam and silt loam soils whereas it showed a little worse performance in a clay soil (Fig. 4). Also, it was surprising to find that the Fredlund model, which had with the best fitting ability among the PSD models, did not show the best performance for estimating WRC (Fig. 4). This trend was confirmed by the r^2 analyses on the predicted and experimental h_i for each PSD model (Table 3). For all soils, the r^2 values were 0.803 for the Jaky model, 0.697 for the SL model, 0.715 for the ONL model, and 0.668 for the Fredlund model (Table 3). The one-parameter Jaky model had greater performance than other

Table 3. **r^2 values for four PSD models and each textural class**

Texture	PSD models			
	Jaky	SL	ONL	Fredlund
Sand	0.817	0.694	0.694	0.647
Sandy loam	0.831	0.771	0.754	0.696
Loam	0.944	0.973	0.973	0.954
Silty loam	0.888	0.705	0.766	0.701
Clay	0.738	0.831	0.826	0.816
Total	0.803	0.697	0.715	0.668

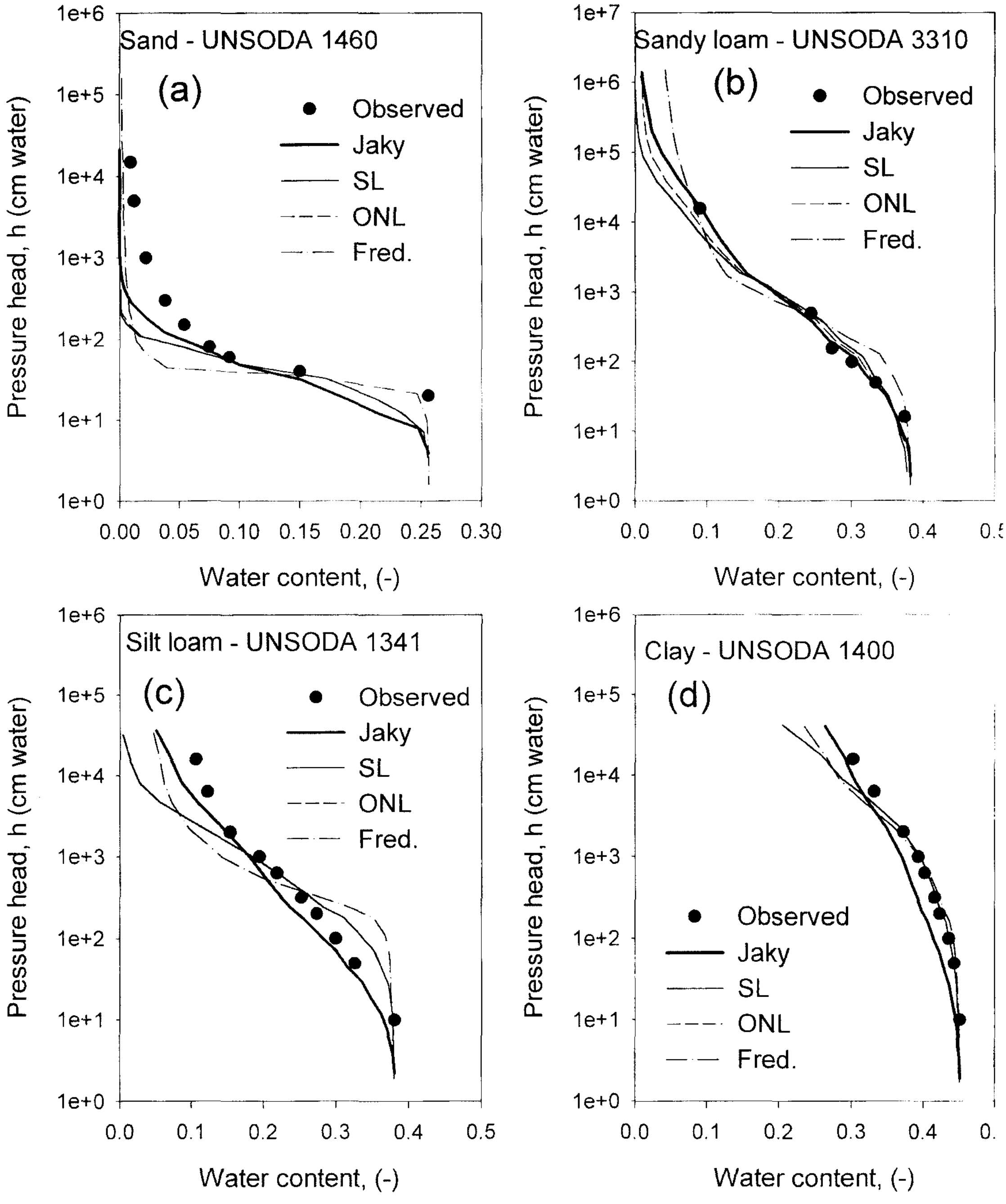

Fig. 4. Comparison of experimental and predicted water retention curves using four PSD models: (a) sand, (b) sandy loam, (c) silt loam, and (d) clay soils.

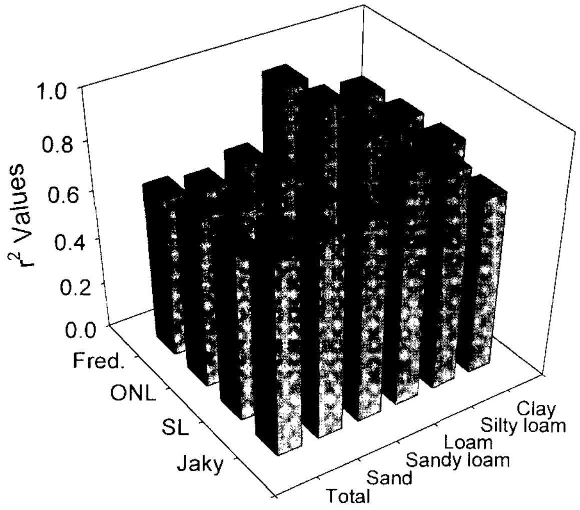

Fig.5. **r^2 plot for four PSD models and each textural class.**

models with greater number of fitting parameters. This result indicates that the PSD model with greater fitting ability could not guarantee better WRC estimation.

The superiority of the Jaky model for predicting WRC may be explained by the effect of soil structure in field soils. The Arya-Paris model was based on the assumption that the size of the particles and the bulk density are primary determinants of the pore size. Therefore, the only input data required were gross textural characteristics (e.g., PSD and bulk density). However, field soils may have aggregation of primary particles into secondary and tertiary particles, root channels, and microcracks, suggesting that these factors could not be fully represented only by gross textural characteristics. Several researchers have developed and investigated several methodologies to predict the WRC from both textural and structural information[19, 20, 21]. They found that structural features have strong effects on the WRC and that mathematical functions that consider structural information give better prediction over the texture-based model. Therefore, the existence of soil structure may cancel out the effect of more detailed and accurate PSD representation on the WRC estimation.

5. CONCLUSIONS

To determine whether estimates of the WRC using the Arya-Paris model could be affected by the selection of a PSD model, four PSD models with different number of fitting parameters were used to generate detailed PSD. It was found, using paired t-tests, that only the SL-ONL model pair showed statistically identical performance for the WRC estimation at 95% significance level. WRCs estimated with the Jaky model, which has only one fitting parameter, were better than those estimated with models that have a greater number of fitting parameters. The superiority of the Jaky model for predicting WRC may be explained by the effect of soil structure in field soils.

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