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RE-EVALUATION OF HYDRAULIC CONDUCTIVITY ESTIMATION OF UNSATURATED SOILS WITH PARTICLE-SIZE DISTRIBUTION MODELS

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Abstract : Knowledge on the unsaturated hydraulic conductivity function of soils is essential for many problems including water flow and solute transport in unsaturated soils. Recently, Arya et al. [12] developed a model to compute unsaturated hydraulic conductivity directly from particle-size distribution (PSD) of a soil. This model implies that details of a PSD curve may affect the estimation of unsaturated hydraulic conductivity. To determine whether the unsaturated hydraulic conductivity estimation using the Arya et al. 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 showed better performance for estimating the unsaturated hydraulic conductivity than other models with more fitting parameters. It indicates that both inherent measurement errors in the soil database used in this study and difference between gross textural characteristics and hydrophysical behavior of individual soils could eliminate the effect of more detailed and accurate PSD representation obtained with models with more fitting parameters.

Key Words : Arya et al. model, Jaky model, particle-size distribution, unsaturated hydraulic conductivity, unsaturated soil

INTRODUCTION

Knowledge on the unsaturated hydraulic conductivity function as a function of water content, *K*(θ), or pressure head, *K*(*h*) is essential for many problems including water flow and solute transport in unsaturated soils. Direct measurements of the unsaturated hydraulic conductivity are relatively time-consuming in both laboratory and field conditions. Hence, considerable efforts have been devoted to the indirect estimation of the unsaturated hydraulic conductivity.$^{1,2)}$

Estimation of the unsaturated hydraulic conductivity function is typically based on the models that take into account the pore-size distribution of a soil.$^{3\sim6)}$ Input data for these types of models generally include a measured or estimated soil water retention function, $h(\theta)$ and the saturated hydraulic conductivity, K_s. The utility of pore-size distribution models to predict $K(\theta)$ from $h(\theta)$ and K_s implies that $K(\theta)$ can be related to the same basic soil properties that are commonly used to characterize $h(\theta)$ and K_s. Hence, much effort has been focused on relating parameters of mathematical functions to the basic soil properties.$^{7\sim11)}$

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Recently, Arya et al.[12)] developed a model to compute $K(\theta)$ directly from the particle-size distribution (PSD). The model is based on the assumption that soil pores can be represented by equivalent capillary tubes and that the water flow rate is a function of pore size. Unlike other models, the measurements for the $h(\theta)$ and K_s are not necessary. They found that the shapes of the predicted $K(\theta)$ functions were similar to those of the measured data and the average of root mean square errors (RMSEs) for all textures was similar to that which have been observed with other hydraulic conductivity prediction models.[13)]

Since this model computes $K(\theta)$ directly from the PSD of a soil, details of a PSD curve may affect the ultimate $K(\theta)$ estimation. Arya et al. suggested that PSDs comprised of at least twenty fractions are necessary to reasonably calculate the $K(\theta)$ function. However, Arya et al. did not describe explicitly how detailed PSD data were generated from experimental PSD data points. 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.[14)] Soils in the UNSODA database used by Arya et al. 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 $K(\theta)$ through application of this model.

Many PSD models have been proposed to generate detailed PSD from experimental PSD data points.[15~19)] Hwang et al.[14)] compared the capability of seven PSD models with different underlying assumptions to be fitted on experimental PSD data of 1,387 different soils in the Korean soil database. They found that the four-parameter Fredlund et al. model[16)] performed best for the PSD prediction. Nemes et al.[17)] 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.

The objectives of this study were (1) to determine whether the $K(\theta)$ estimation using the Arya et al. model could be affected by the selection of a PSD model, and (2) to determine if the use of a PSD model with better goodness-of-fit represents better experimental $K(\theta)$ data. To achieve these objectives, four models were used to generate detailed PSD curves from experimental PSD data in the UNSODA database. The $K(\theta)$ predicted with these detailed PSD curves and the Arya et al. model was then compared with experimental $K(\theta)$ data.

BACKGROUND

The Arya et al. Model

The model is based on the premise that flow in soil pores is a function of the pore radius which is determined by the PSD. Additionally, it is assumed that the hydraulic conductivity of a soil, at a given saturation, is made up of contributions from flow in pores that remain completely filled with water at that saturation; that is, the contribution of partially drained pores to overall flow is insignificant.

The volumetric water content, θ_i (cm^3 cm^{-3}), can be calculated from PSD, porosity, and maximum measured water content information, according to

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

where ϕ is the total porosity (cm^3 cm^{-3}), S_w is the ratio of measured saturated water content to the total porosity, and w_j is the mass fraction (g g^{-1}) in the jth particle-size fraction. To compute w_j, the PSD is divided into n fractions, and the difference in cumulative mass corresponding with successive particle sizes is used to compute w_j. Further information on scaling water content from the PSD can be found in Arya and Paris[20)] and Arya et al.[21)]

The hydraulic conductivity of the sample, K

(θ_i) (cm s^{-1}), corresponding with water content θ_i (cm^3 cm^{-3}), is given explicitly in terms of parameters of the PSD and packing characteristics of the sample

$$K(\theta_i) = \frac{c\psi_e}{\pi} \sum_{j=1}^{j=i} R_j^{(x-2)} w_j \, [0.667 e n_j^{(1-\alpha j)}]^{(x-2)/2} \; ; \quad i = 1, 2, \ldots, n \qquad (2)$$

where c and x are parameters which can be evaluated empirically using experimental $K(\theta_i)$ data, φ_e is the effective porosity given by $\varphi_e = S_w[1-(\rho_b/\rho_s)]$ where ρ_s is the particle density (g cm^{-3}) and ρ_b is the bulk density (g cm^{-3}), R_j is the mean particle radius (cm) for the jth particle-size fraction, e is the void ratio of the natural-structured soil sample equal to $(\rho_s-\rho_b)/\rho_b$, n_j is the number of equivalent spherical particles in the jth particle-size fraction (g^{-1}) which is given by,

$$n_j = 3w_j/(4\rho_s R_j^3) \qquad (3)$$

and α_j is the scaling parameter defined by Arya et al.[21] as

$$\alpha_j = \log N_j / \log n_j \qquad (4)$$

where N_j (g^{-1}) represents the scaled number of hypothetical spherical particles of radius R_j required to trace the tortuous pore length contributed by n_j natural particles in the actual sample. The N_j can be obtained from the PSD using the empirical relationship[21]:

$$\log N_j = a + b\log(w_j/R_j^3) \qquad (5)$$

Table 1 summarizes parameters a, b, c, and x required in equations (2) and (5), and the goodness of fit, r^2, for four soil textures included in the study of Arya et al..[12,21] Arya et al. provides detailed of their own model.

Particle-Size Distribution Models

To estimate $K(\theta)$ from a PSD using the Arya et al. model, first of all, it is needed 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 take an approach for representing the PSD. For this approach, 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, then providing different predicted $K(\theta_i)$ pairs (e.g., see equations (1) and (2)). Three lognormal models were chosen from PSD models previously studied by Buchan et al.[15] and Hwang et al.[14]: the Jaky model with one parameter[22]; a simple lognormal model with two parameters (SL)[23]; and one modified lognormal model with three parameters, i.e. an offset-nonrenormalized lognormal model (ONL).[15] Buchan et al.[15] provides details of the three lognormal models. The Fredrund et al.[16] model was tested as four-parameter model. The four models considered in this study are listed in Table 2.

Table 1. Parameters of equations (2) and (5) and the goodness of fit, r^2, for four soil textural classes*

Textural class	Arya et al.[21]				Arya et al.[12]			
	Soils	a	b	r^2	Soils	log c	x	r^2
Sand	6	-2.478	1.490	0.882	5	1.849	3.999	0.913
Sandy loam	6	-3.398	1.773	0.952	4	-0.871	3.063	0.964
Loam	4	-1.681	1.395	0.936	4	2.647	4.258	0.972
Clay	5	-2.600	1.305	0.954	3	-0.488	3.506	0.976

* cf. Arya et al.[12,21]

Table 2. Particle-size distribution models tested for texture data of 12 soils

Name	Model*	Parameters
Jaky,[22]	$F(d) = \exp\left\{-\frac{1}{p^2}\left[\ln\left(\frac{d}{d_o}\right)\right]^2\right\}$	p (d_o=2 mm)
Simple Lognormal (SL),[23]	$G(\ln d) = F_n\left(\frac{\ln d - \mu}{\sigma}\right)$ where $F_n(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} \exp(-\frac{x^2}{2})dx$ **	μ, σ
Offset-Nonrenormalized Lognormal (ONL),[15]	$H(\ln d) = G(\ln d) + c$ ($G(\ln d)$ defined by the SL model)	μ, σ, c
Fredlund,[16]	$J(d) = \frac{1}{\left\{\ln\left[\exp(1) + \left(\frac{\alpha}{d}\right)^n\right]\right\}^m} \left\{1 - \left[\frac{\ln\left(1+\frac{d_f}{d}\right)}{\ln\left(1+\frac{d_f}{d_m}\right)}\right]^7\right\}$	α, n, m, d_f (d_m=0.0001 mm)

*d: particle diameter in mm, **$F_n(x)$ = cumulative normal distribution function

RESEARCH METHODS

The UNSODA Hydraulic Property Database

Experimental $K(\theta)$, PSD, bulk density, and particle density data were obtained from the UNSODA hydraulic property database.[24] For this study, twelve data sets, representing a range of textures that include sand, sandy loam, loam, and clay, were selected from the UNSODA hydraulic property database (Table 3). These data sets were taken from those that Arya et al. used to calibrate and test their model. Soils used in this study had the experimental PSD data points ranging from four to eleven and experimental $K(\theta)$ data points ranging from five to forty-four in each soil.

Calculation of Hydraulic Conductivity Function, $K(\theta_i)$

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 non-linear regression procedure was used to find the values of the fitting parameters that give the 'best fit' between the PSD model and the experimental PSD data. This procedure was done using the SOLVER routine of Microsoft Excel software.[14]

Table 3. Textural classes and UNSODA codes for soils used for testing unsaturated hydraulic conductivity function based on different PSD models*

Textural classes	UNSODA codes
Sand	1050, 1460, 4650
Sandy loam	1130, 1381, 4160
Loam	1370, 2531, 4610
Clay	1400, 4121, 4681

*cf. Arya et al.[12]

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, 600, 800, 1,000, 1,500, and 2,000 μm.[12,21] 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 w_i was converted to an equivalent number of spherical particles, n_i, using equation (3). The scaled number of spherical particles, N_i, was calculated for each w_i using equation

(5) and Table 1. Particle numbers obtained from equations (3) and (5) were used in equation (4) to calculate the scaling parameter, α_i for each w_i. Mean R_i, n_i, and α_i for each w_i, e, φ_e, and c and x taken from Table 1 were used to compute $K(\theta_i)$ using equation (2). The corresponding water content, θ_i, was obtained by using equation (1).

Selection of the Best PSD Model for *K(θ)* Estimation

It is necessary to determine if the $K(\theta)$ estimation using the Arya et al. model could be affected by the selection of a PSD model. Three PSD models (Jaky, SL, ONL) used in this study have the same underlying assumption that the PSD in soil is lognormal, implying the possibility of identical performance among these models in the $K(\theta)$ estimation. Therefore, to determine if statistically identical estimations resulted in between the PSD model pairs, including the Fredlund model, paired *t*-tests were conducted on each log-transformed predicted $K(\theta_i)$ values at the same θ_i.

To determine whether a PSD model with better fitting ability represents better experimental the hydraulic conductivity data, r^2 and RMSEs were used as statistical comparison of the results. The r^2 and RMSEs were computed using log-transformed experimental and predicted $K(\theta_i)$ at the same experimental θ_i. Van Genuchten[6] function was employed to calculate predicted $K(\theta_i)$ at the same experimental θ_i from twenty $K(\theta_i)$ data points calculated from the Arya et al. model. The SOLVER routine of Microsoft Excel software was used again for this nonlinear regression.

RESULTS AND DISCUSSION

Goodness-of-fit of Particle-Size Distribution Models

In all of the soils and all of the models, values of r^2 for the PSD models fit to experimental PSD data ranged from 0.932 to 1.000 (Figure 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. This result consists with that of Hwang et al..[14]

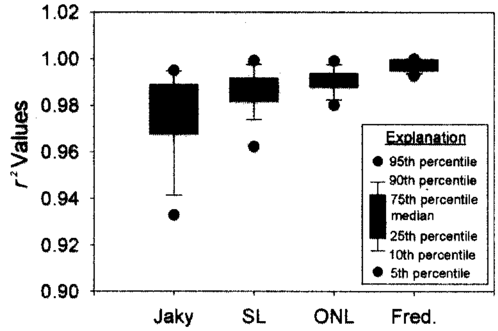

Figure 1. Box plot for r^2 percentiles as the goodness-of-fit of four PSD models for all soils.

Effect of PSD Models on *K(θ)* Estimation

Typical examples of predicted and experimental $K(\theta)$ curves for sand, sandy loam, loam, and clay soils as affected by the PSD models are presented in Figure 2, showing that all four PSD models adequately predict shape of the experimental $K(\theta)$ data. The estimation of the $K(\theta)$ curve seemed to be a little different when different PSD models were used (Figure 2); the accuracy of $K(\theta)$ estimation may be affected by the selection of a PSD model.

As shown in Figure 2, the SL and ONL models showed nearly identical performance for the $K(\theta)$ estimation. Therefore, it is necessary to determine if any PSD model pair has statistically identical performance in the $K(\theta)$ estimation. To do this, paired *t*-tests were conducted on log-transformed $K(\theta)$ predictions with all possible six PSD model pairs. It was found that only SL-ONL pair had statistically identical performance for the $K(\theta)$ estimation at 95% significance level. Other PSD models did not result in statistically identical $K(\theta)$ estimation.

The differences between predicted and

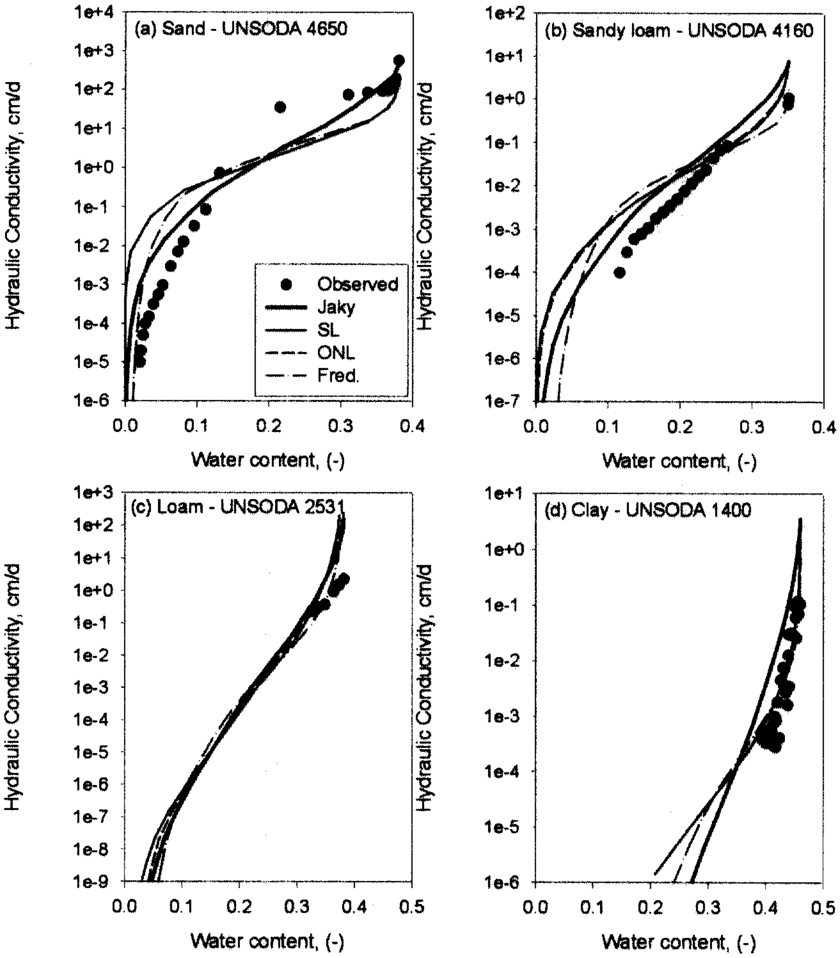

Figure 2. An illustration of experimental and predicted unsaturated hydraulic conductivity curves using four PSD models for each textural class (sand, sandy loam, loam, and clay soils).

experimental *K(θ)* varied in magnitude from a textural class to other textural classes. Especially, the Jaky model showed the best performance in sand whereas it showed a little worse performance in a clay soil (Figure 2(a), (d)). The Fredlund model, which showed the best PSD prediction among the models, did not show the best performance for estimating *K(θ)* (e.g., Figure 2(a), (b)). This trend was confirmed by the r^2 and RMSE analyses on the predicted and experimental *K(θ)* data for each PSD model (Figure 3).

Figure 3 shows a comparison of the logarithms of experimental vs. predicted *K(θ)* values for all soils on a 1:1 scale. The r^2 values were 0.765 for the Jaky model, 0.613 for the SL model, 0.638 for the ONL model, and 0.688 for the Fredlund model. And the RMSE values were 1.066 for the Jaky model, 1.332 for the SL model, 1.284 for the ONL model, and 1.099 for the Fredlund model. The one-parameter Jaky model performed better than other models with more fitting parameters. This result indicates that the PSD model showing better PSD fitness could not guarantee better *K(θ)* prediction.

The superiority of the Jaky model for predicting *K(θ)* may be explained by (1) inherent errors of *K(θ)* measurements in the UNSODA database used in this study and (2)

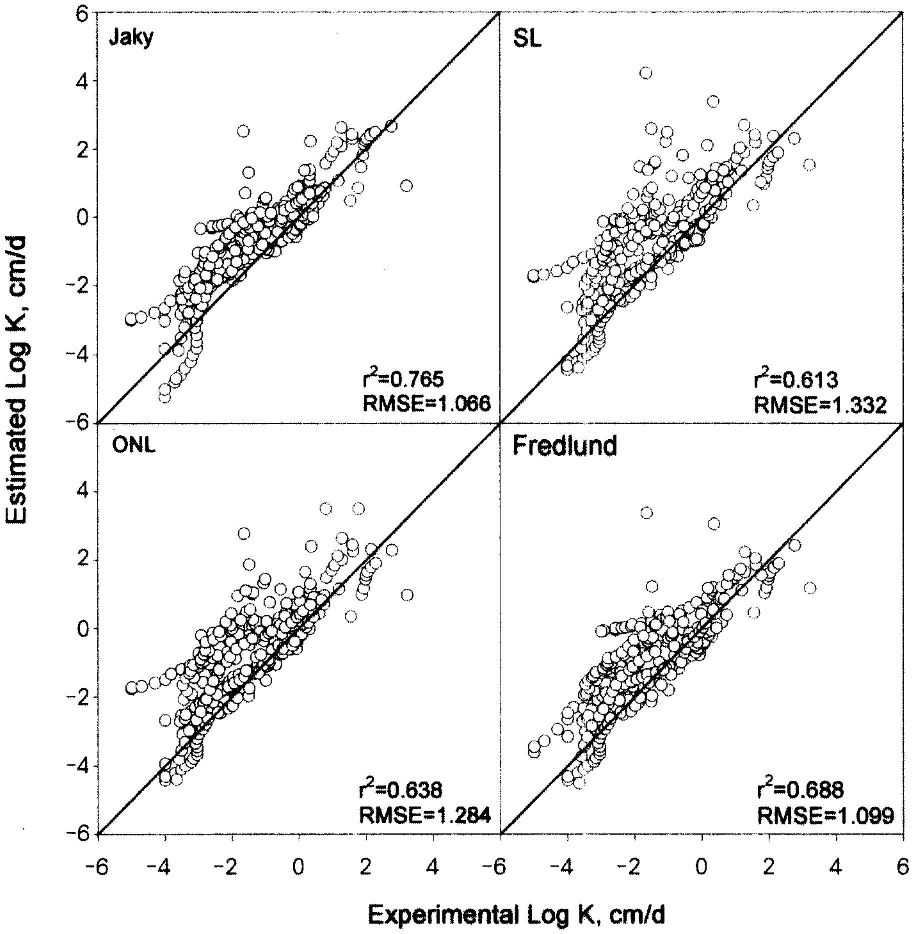

Figure 3. Comparison of experimental and predicted hydraulic conductivity for four PSD models. Test results for 12 soils are pooled.

possible difference between gross textural characteristics (e.g., PSD and bulk density) and hydrophysical behavior of individual soils.

The *K(θ)* measurement is typically difficult, and large differences in experimentally measured *K(θ)* data between replicated samples of the same soil are common.[25] Also, the UNSODA data used in this study were very heterogeneous because they were collected from regions with various geological origins around the world and different experimental procedures were used for each data set.[24] Variable experimental procedures may introduce additional noise in the *K(θ)* data.

The Arya et al. model is based on the assumption that the water flow rate is a function of pore size which is determined primarily by size of the particles and the bulk density. Therefore, the only input data required were a PSD and bulk density. However, real 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 the PSD and bulk density data. Therefore, both inherent measurement errors in the UNSODA database and difference between gross textural characteristics and hydrophysical behavior of individual soils could eliminate the effect of more detailed and accurate PSD representation on the *K(θ)* prediction.

CONCLUSIONS

To determine whether estimates of the *K(θ)* using the Arya et al. model could be affected by the selection of a PSD model, four PSD models were used to generate detailed PSD. These detailed PSDs were then used as input to predict the *K(θ)*. The use of input data from the Jaky model, with only one fitting parameter, resulted in better predictions for *K(θ)* than other PSD models with greater numbers of fitting parameters. The quality of predictions based on the Jaky model indicates that both inherent measurement errors in the UNSODA database and difference between gross textural characteristics and hydrophysical behavior of individual soils could eliminate the effect of more detailed and accurate PSD representation obtained with models with more fitting parameters.

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