Approaches for estimating unsaturated soil hydraulic conductivities at various bulk densities with the extended Mualem-van Genuchten model

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Abstract
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Keywords
soil hydraulic conductivity, water retention curve, Mualem-van Genuchten model, bulk density

Disciplines
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Approaches for estimating unsaturated soil hydraulic conductivities at various bulk densities with the extended Mualem-van Genuchten model

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Highlights:

- Soil bulk density variations significantly affect hydraulic conductivity ($K_u$).
- Parameters in the Mualem-van Genuchten soil $K_u$ model are related to bulk density.
- Four approaches are developed to estimate $K_u$ of soils over a range of bulk densities.
Approaches for estimating unsaturated soil hydraulic conductivities at various bulk densities with the extended Mualem-van Genuchten model

Abstract

The Mualem-van Genuchten model has been widely used for estimating unsaturated soil hydraulic conductivity ($K_u$) from measured saturated hydraulic conductivity ($K_s$) and fitted water retention curve (WRC) parameters. Soil bulk density ($\rho_b$) variations affect the accuracy of $K_u$ estimates. In this study, we extend the Mualem-van Genuchten model to account for the $\rho_b$ effect with $\rho_b$-related WRC and $K_s$ models. We apply two functions (A and B) that relate the van Genuchten WRC model to $\rho_b$ and two models (1 and 2) that estimate $K_s$ with various $\rho_b$. By combining the $\rho_b$-related WRC functions and $K_s$ models, we develop four integrated approaches (i.e., A1, A2, B1, and B2) for estimating $K_u$ at various $\rho_b$. $K_u$ measurements made on five soils with various textures and $\rho_b$ are used to evaluate the accuracy of the four approaches. The results show that all approaches produce reasonable $K_u$ estimates, with average root mean square errors (RMSEs) less than 0.35 (expressed in dimensionless unit because logarithmic $K_u$ values are used). Approach A2, with an average RMSE of 0.25, agrees better with $K_u$ measurements than does Approach A1 that has an average RMSE of 0.28. This is because Model 2 accounts for the WRC shape effect near saturation. Approaches A1 and A2 give more accurate $K_u$ estimates than do Approaches B1 and B2 which both have average RMSEs of 0.35, because Function A performs better in estimating WRCs than does Function B. The proposed approaches could be incorporated into simulation models for improved prediction of water, solute, and gas transport in soils.

Keywords: soil hydraulic conductivity, water retention curve, Mualem-van Genuchten model, bulk density.
1. Introduction

Variable soil bulk density ($\rho_b$, Mg m$^{-3}$) due to human disturbances and environmental effects is an important factor causing temporal and spatial variations in soil hydraulic properties (Sillon et al., 2003; Osunbitan et al., 2005; Zhang et al., 2017; Tian et al., 2018a). A decrease in $\rho_b$ caused by tillage can enhance soil infiltration capacity (Kribaa et al., 2001). After tillage, $\rho_b$ tends to increase with time under the influences of gravity, rainfall and water flow into the soil (Tian et al., 2018b), which results in a substantial decrease in the saturated soil hydraulic conductivity, $K_s$ (Osunbitan et al., 2005). The unsaturated soil hydraulic conductivity ($K_u$) response to $\rho_b$ variation induced by traffic compaction or tillage was shown to exhibit complex behaviors in space and time (Strudley et al., 2008; Alletto and Coquet, 2009). Swelling and shrinkage of clay minerals alter $\rho_b$ along with the pore system; this has been shown to have significant effects on soil water retention characteristics (Gregory et al., 2010; Salager et al., 2010). Irrigation, root growth, drying and wetting cycles, and freezing and thawing processes were also observed to alter $\rho_b$ and soil hydraulic properties (Benson and Othman, 1993; Kodešová et al., 2006; Strudley et al., 2008; Bodner et al., 2013; Zhang et al., 2017).

Obtaining accurate measurements of soil hydraulic properties, especially $K_u$, is generally difficult, costly, and time-consuming. Wind (1966) introduced an approach for measuring $K_u$ by using evaporation experiments in the laboratory. Schindler (1980) developed a simplified evaporation method for determining $K_u$. In the field, Ankeny et al. (1990) introduced a simple method to determine $K_u$ through infiltration experiments. In addition, in-situ $K_u$ dynamics can be estimated by combined use of heat pulse and water potential sensors (Tian et al., 2018a). More commonly, $K_u$ is estimated using soil water retention parameters and $K_s$ measurement, based on relative hydraulic conductivity models (Burdine, 1953; Mualem, 1976; van Genuchten, 1980;
Taking into account the effects of $\rho_b$ in the $K_u$ estimation models is increasingly important for improved simulation of water, solute, and gas transport in soils (Vereecken et al., 2016).

To account for the effect of $\rho_b$ in hydraulic conductivity estimation models, the $K_s$ value and soil water retention parameters should be related to $\rho_b$. Several approaches have been developed to relate $K_s$ to $\rho_b$ or the total soil porosity (Mualem and Assouline, 1989; Or et al., 2000; Flint and Selker, 2003; Assouline, 2006a; Guarracino, 2007; Assouline and Or, 2008). The $K_s$ values under different $\rho_b$ conditions can be estimated with $\rho_b$-related models based on the Kozeny-Carman equation (Or et al., 2000). Mualem and Assouline (1989) estimated soil $K_s$ with various $\rho_b$ by using a water retention curve (WRC) function and a $K_s$ measurement at a reference $\rho_b$. This method performed well when combined with the Brooks and Corey (1964) and Assouline et al. (1998) WRC models (Assouline, 2006a). Methods for modeling the relationship between $\rho_b$ and soil water retention parameters have also been reported (Ahuja et al., 1998; Assouline, 2006b). Assouline (2006b) introduced approaches that correlate the Brooks and Corey (1964) and Assouline et al. (1998) model parameters to $\rho_b$. The studies of Assouline (2006a, 2006b) have made it possible to estimate $K_u$ for soils at different $\rho_b$ values through a joint use of the $\rho_b$-related $K_s$ estimates and water retention parameters.

In terms of soil water flow simulation, the Mualem-van Genuchten (1980) hydraulic conductivity estimation model has been widely used (Jansson, 1998; Šimůnek et al., 2005). There is a need to relate the Mualem-van Genuchten (1980) model parameters to $\rho_b$ for an improved understanding of water transport in dynamic soil systems. Tian et al. (2018c) related the parameters used in the van Genuchten (1980) WRC model to $\rho_b$ using a series of $\rho_b$-related empirical functions. Two approaches for estimating WRCs of soils at various $\rho_b$ values were
developed by Tian et al. (2018c). The Mualem and Assouline (1989) method has the potential to be combined with the van Genuchten (1980) WRC function for estimating $K_s$ of soils at various $\rho_b$, but it has not been evaluated with measured $K_s$ values. The Tian et al. (2018c) approaches and the Mualem and Assouline (1989) method are promising for application to the Mualem-van Genuchten (1980) hydraulic conductivity estimation model for taking into account the effect of $\rho_b$.

The objectives of this study are to: (1) relate the Mualem-van Genuchten (1980) soil hydraulic conductivity estimation model parameters to $\rho_b$; (2) introduce four approaches to estimate $K_u$ for soil over a range of $\rho_b$ values; and (3) evaluate and compare the performance of the four approaches for estimating $K_u$ using measured values.

2. Materials and Methods

2.1 Model development

The Mualem-van Genuchten model has been widely used for describing soil hydraulic properties (van Genuchten, 1980). In this model, the soil WRC is expressed by

\[
S = \begin{cases} 
\frac{\theta - \theta_r}{\theta_s - \theta_r} \left[ \frac{1}{1 + (\alpha |\psi|)^n} \right]^m, & \psi \leq 0 \\
1, & \psi > 0
\end{cases}
\]  

(1)

where $S$ is the effective degree of saturation, $\theta$ is the volumetric soil water content (m$^3$ m$^{-3}$) at soil water matric potential $\psi$ (kPa), $\theta_r$ and $\theta_s$ are the residual and saturated water contents (m$^3$ m$^{-3}$), respectively, and $\alpha$ (kPa$^{-1}$), $n$, and $m$ are empirical shape parameters, in which $m$ is commonly expressed as $m = 1 - 1/n$ to derive a closed-form solution for the Mualem (1976) relative hydraulic conductivity model.

The Mualem-van Genuchten (1980) hydraulic conductivity function is given as follows,
\[ K(S) = \begin{cases} K'S^L \left[ 1 - (1 - S^{n/(n-1)})^{1-1/n} \right]^2 & \psi \leq 0 \\ K' & \psi > 0 \end{cases} \] (2)

where \( K \) is the hydraulic conductivity (mm h\(^{-1}\)), \( K' \) is a matching point at saturation (mm h\(^{-1}\)), and \( L \) is an empirical pore-connectivity parameter. A measured \( K_s \) is commonly used for \( K' \), while \( L \) is fixed at 0.5 (Mualem, 1976). The \( K_u-\theta \) or \( K_u-\psi \) relationship is obtained by combining Eqs. (1) and (2).

Variation in \( \rho_b \) can have a significant effect on the estimation of \( K_u \) (Assouline, 2006a). Thus, it is necessary to relate the Mualem-van Genuchten (1980) model to \( \rho_b \) for improved prediction of water movement in soil systems with spatially- and/or temporally-variable \( \rho_b \). Tian et al. (2018c) extended the four parameters in Eq. (1) to account for the \( \rho_b \) dependence with the following equations,

\[ \theta_s = \left( \frac{\rho_s - \rho_b}{\rho_s - \rho_{bo}} \right) \theta_{s0} \] (3)

\[ \theta_r = \frac{\rho_b}{\rho_{bo}} \theta_{r0} \] (4)

\[ \alpha = \alpha_0 \left( \frac{\rho_b}{\rho_{bo}} \right)^{-3.97} \] (5)

where the subscript 0 refers to parameters under a reference \( \rho_b \) condition, and \( \rho_s \) is the soil particle density (Mg m\(^{-3}\)). A linear relationship between parameter \( n \) and \( \rho_b \) has been reported by several studies (Assouline et al., 1997; Fu & Shao, 2007; Jiang et al., 2017),

\[ n = a \rho_b + b \] (6A)

where \( a \) and \( b \) are empirical parameters that vary with soil type. To obtain \( a \) and \( b \), at least two \( n \) values at two reference bulk densities are needed. Tian et al. (2018c) observed a relatively moderate relationship (compared to the linear relationship) between \( n \) and \( \rho_b \) as follows,
\[ n = 1 + (n_0 - 1) \left( \frac{\rho_b}{\rho_{b0}} \right)^{-0.97+1.28f_{\text{silt}}/f_{\text{clay}}} \]

(6B)

where \( f_{\text{silt}}/f_{\text{clay}} \) is the ratio between the soil silt content and clay content that are determined according to the USDA soil textural classification, and \( n_0 \) is the fitted \( n \) value at the reference \( \rho_{b0} \) condition. Unlike Eq. (6A), Eq. (6B) estimates \( n \) values at various \( \rho_b \) using only one reference \( n_0 \) value, and thus it has the advantage of simplicity.

By substituting Eqs. (3) - (6) into Eq. (1), the van Genuchten (1980) WRC model is extended to take into account the effects of \( \rho_b \). To simplify the expression of the model function, we set the value of \( \rho_{b0} \) to be 1.0 Mg m\(^{-3}\), then the \( \rho_b \)-related Eq. (1) is normalized as follows,

\[
S = \begin{cases} 
\frac{\theta - \rho_b \theta_{r0}}{(\rho_s - \rho_b \theta_{r0})} & \text{if } \Psi < 0 \\
\frac{1}{1 + (\rho_b^{-3.97} a_0 |\Psi|)^n} & \text{if } \Psi > 0 
\end{cases} 
\]

(7)

where \( n \) is expressed as Eq. (6A) or Eq. (6B) with \( \rho_{b0} = 1.0 \text{ Mg m}^{-3} \). Note, \( \rho_b \), \( \rho_{b0} \), and \( \rho_s \) in Eq. (7) are assumed to be unitless parameters to make units match.

The \( K_s \) also varies with \( \rho_b \) (Jabro, 1992). After comparing eight different models that related \( K_s \) to \( \rho_b \), Assouline (2006b) concluded that the following Kozeny–Carman equation-based model had the best agreement with \( K_s \) measurements.

\[
K_s = K_{s0} \left( \frac{\eta}{\eta_0} \right)^{3} \left( \frac{\rho_b}{\rho_{b0}} \right)^{\delta-7}
\]

(8)

where \( \eta = 1 - \rho_b/\rho_s \) is the soil total porosity, and \( \delta \) is an empirical parameter. Assouline (2006b) observed that \( \delta = 4 \) gave the best overall agreement with the \( K_s \) measurements for soils used in his study. \( K_{s0} \) and \( \eta_0 \) are parameters under the reference \( \rho_{b0} \) condition. By setting \( \rho_{b0} \) to 1.0 Mg m\(^{-3}\), Eq. (8) is normalized as
\[ K_s = K_{s0} \left( \frac{\rho_s - \rho_b}{\rho_s - 1} \right)^3 \rho_b^{-3} \]  

(9)

In addition, Mualem and Assouline (1989) developed a semi-theoretical model to estimate \( K_s \) under various \( \rho_b \) conditions using soil WRC model functions,

\[ K_s = K_{s0} \left( \frac{\theta_s - \theta_r}{\theta_s - \theta_{r0}} \right)^{L+2} \left( \int_0^1 \frac{1}{|\psi|^{-1} dS(\psi)} \right)^2 \]  

(10)

where \( S(\psi) \) represents a WRC model function (e.g., the Brooks and Corey (1964) model) and \( S_0 \) is the effective degree of saturation at the reference \( \rho_{b0} \). The empirical pore-connectivity parameter \( L = 0.5 \), also used in Eq. (2), is adopted in Eq. (10). Assouline (2006a) combined Eq. (10) with the Brooks and Corey (1964) and the Assouline et al. (1998) WRC functions for estimating soil \( K_s \) of at various \( \rho_b \) values. In the present study, the van Genuchten (1980) WRC function is applied to this model. By substituting Eqs. (1), (3), and (4) into Eq. (10), performing integration (details about the integral calculation are shown in the Appendix), and setting \( \rho_{b0} \) to 1.0 Mg m\(^{-3}\), we derive a new \( K_s \) model as follows,

\[ K_s = K_{s0} \left( \frac{\rho_s - \rho_b}{\rho_s - \rho_{b0}} \theta_{s0} - \theta_{r0} \theta_{r0} \right)^{2.5} \rho_b^{-3.97+2} \]  

(11)

2.2 Approaches for estimating \( K_u \) for soils at various \( \rho_b \) values

So far, we have introduced two van Genuchten WRC functions (i.e., Eqs. (7) + (6A) and Eqs. (7) + (6B), designated as Function A and Function B, respectively) that relate model parameters to \( \rho_b \) and two \( K_s \) models (i.e., Eqs. (9) and (11), designated as Model 1 and Model 2, respectively) that include \( \rho_b \) as a variable. Tian et al. (2018c) indicated that Function A gave more accurate WRC estimates than did Function B, while Function B had the advantage of simplicity over Function A. Model 1 was developed based on the Kozeny–Carman equation, while Model 2
included WRC model functions as variables. By combining these WRC functions and $K_s$ models with Eq. (2), we obtained the following four approaches that can be used to estimate $K_u$ for soils at various $\rho_b$ values: Approaches A1 (Eq. 2+Function A and Model 1), A2 (Eq. 2+Function A and Model 2), B1 (Eq. 2+Function B and Model 1), and B2 (Eq. 2+Function B and Model 2).

Water retention curve parameters and $K_{s0}$ value at the reference $\rho_{b0}$ of 1.0 Mg m$^{-3}$ are required for the proposed approaches, but they can be obtained using measurements made on samples with any known $\rho_b$. For example, parameters $\theta_{s0}$ and $\theta_{r0}$ at $\rho_{b0}$ of 1.0 Mg m$^{-3}$ can be calculated from $\theta_s$ and $\theta_r$ measurements on soil samples with a known $\rho_b$ by solving Eqs. (3) and (4). Note, considering that $\theta_r$ is the water content at which soil $K_u$ approaches zero, we set $\theta_r$ as the $\theta$ determined at -1500 kPa following Tian et al. (2018c). When $\theta$ measurements at -1500 kPa are not available, the best-fit values are used.

For Function A, three unknown parameters $\alpha_0$, $a$ and $b$ are obtained by fitting Eqs. (6A) + (7) to WRC measurements simultaneously with the least-squares method. For a specific soil, both $a$ and $b$ rely on $\rho_b$, thus at least two WRC curves at two markedly different $\rho_b$ values are required to derive the best-fit $a$ and $b$ values (Tian et al., 2018c). For Function B, $n$ depends on $\rho_b$ and soil texture ($f_{silt}/f_{clay}$). Thus, unknown parameters $\alpha_0$ and $n_0$ can be obtained by fitting Eqs. (6B) + (7) to one WRC measurement at a known $\rho_b$ value (Tian et al., 2018c). In this case, $\rho_b$ can be any specific value.

The $K_s$ at the required $\rho_b$ condition can be directly calculated with Eq. (8) or Eq. (10) from a $K_s$ measurement with a known $\rho_b$ or it can be obtained by using the normalized $K_s$ model (Eq. 9 or 11). The $K_{s0}$ in Eq. (9) is estimated from the $K_s$ measurement at a known $\rho_b$ by solving Eq. (9). Likewise, the $K_{s0}$ in Eq. (11) can be estimated from $\theta_{s0}$ and $\theta_{r0}$ estimates and a $K_s$ measurement made on soil with a known $\rho_b$ by solving the equation.
2.3 Experimental validation

To evaluate the performance of the four approaches for estimating soil $K_u$ with variable $\rho_b$, the measurements of $K_s$, $K_u$, and WRC made on five soils with different textures and $\rho_b$ values were used as validation datasets. Table 1 presents the basic physical properties of the soils. The datasets of soils 1-3 were from Laliberte et al. (1966) who measured the main drying WRCs of the soils at three or four $\rho_b$ values, and the $K_s$ and $K_u(\psi)$ values were determined at another five $\rho_b$ conditions (Table 1). The different $\rho_b$ conditions were achieved by packing soil columns with a vibrating device.

For soils 4 and 5, we measured the WRC, $K_s$ and $K_u(\psi)$ values at various $\rho_b$ values (Table 1). The soil samples were air-dried, passed through a 2-mm screen, mixed with predetermined amounts of water, and then packed uniformly into stainless-steel containers at different $\rho_b$ values. The WRCs of soils 4 and 5 were determined at a range of $\psi$ values (-0.5, -1, -2, -4, -6, -8, and -10 kPa) with a tension table (Eijkelkamp, Giesbeek, the Netherlands), and at -30, -50, -100, -500, and -1500 kPa with a pressure plate apparatus (Soilmoisture Equipment Corp., Santa Barbara, CA). These WRCs have been reported in Tian et al. (2018c). The $K_s$ of soil samples at different $\rho_b$ were determined by using the constant head method (Klute and Dirksen, 1986). Three replicated WRC and $K_s$ measurements were made for each soil and each $\rho_b$. The $K_u(\psi)$ curves of soils 4 and 5 were determined with a HYPROP device (UMS GmbH, Munich, Germany) following the simplified evaporation method (Schindler, 1980; Peters et al., 2005).

The WRCs at the lowest and highest $\rho_b$ values (Table 1) were applied to calculate the $\theta_{s0}$ and $\theta_{r0}$, and to obtain the best-fit $a_0$, $a$, and $b$ values in Approaches A1 and A2. The $a_0$ and $n_0$ values in Approaches B1 and B2 were obtained by fitting Eqs. (6b) + (7) to the WRC measurements at the lowest $\rho_b$. Then, WRC parameters at the $\rho_b$ for determining $K_u$ were estimated using the
proposed functions. The $K_{s0}$ values in Eqs. (9) and (11) were determined by using a $K_s$ measurement at a known $\rho_b$. Substantial variation usually occurred in $K_s$ measurements on the same soil (van Genuchten et al., 1991). In consideration of this variability, all $K_s$ measurements at different $\rho_b$ were applied for the calculation of $K_{s0}$, and the average values were used to estimate $K_u$. The $K_u(\psi)$ values for each soil at different $\rho_b$ were then estimated accordingly and compared with the measured data. The root mean square error (RMSE) and bias between the estimated and measured $K_u$ values were used to evaluate the performance of the approaches.

$$\text{RMSE} = \sqrt{\frac{\sum (\log_{10} K_u(\text{estimated}) - \log_{10} K_u(\text{measured}))^2}{N}}$$ (12)

$$\text{Bias} = \frac{\sum (\log_{10} K_u(\text{estimated}) - \log_{10} K_u(\text{measured}))}{N}$$ (13)

where $N$ is the number of data points. Logarithmic values of $K_u$ were used in Eqs. (12) and (13) to avoid deviations toward high conductivities in the wet range. The RMSE and bias are presented as dimensionless numbers because logarithmic conductivity values were used.

We also calculated the best-fit $K_s$ values to evaluate the performance of Models 1 and 2 for estimating $K_s$. The best-fit $K_s$ was obtained by fitting Eq. (2), in which the parameters $S$ and $n$ were estimated using Function A, to measured $K_u(\psi)$ values using the least squares method. The goodness of fit was quantified with the RMSE between estimated and measured $K_u$ values. The best-fit $K_s$ represents the most suitable value for the matching point at saturation, i.e. $K'$ in Eq. (2).

3. Results and Discussion

3.1 Soil WRC estimates at various $\rho_b$ values
Fig. 1 presents the WRC estimates of the five soils using Function A and Function B. Instead of the conventional θ-ψ relationship, the WRCs presented here show ψ as a function of S because the $K_s(\psi)$ estimations are needed in this study, and thus only the $S(\psi)$ term in Eq. (7) is necessary. The $\rho_b$ variation had a significant effect on the shape of the WRC estimates. In general $S$ of soils at relatively low $\rho_b$ values changed over $\psi$ more considerably, compared to those of soils at relatively high $\rho_b$ values, in the near-saturation $\psi$ range. However, the changes of the $S(\psi)$ curve shape showed opposite trends in mid-range $\psi$ (Fig. 1). In terms of WRCs from different estimation functions, Function B gave slightly higher $S$ than did Function A in the wetter range of the WRCs, but the opposite trend was observed in the drier range of the WRCs. For soils 1-3, most of the water was drained at relatively large $\psi (> -30 \text{ kPa})$, and the two functions produced quite similar WRCs except on samples with the lowest $\rho_b$ values. For soils 4 and 5, the full-range (0 to -1500 kPa) WRCs were measured, the WRCs estimated with Function A differed considerably from that of Function B when $S$ decreased rapidly with the reduction of $\psi$. Tian et al. (2018c) showed that Function A produced more accurate WRC estimates than did Function B in most cases, which was caused by the fact that Function A used reference measurements on samples at two different $\rho_b$ values, whereas Function B used only one WRC measurement. Conversely, Function B has the advantage of being less time consuming for data collection as compared to Function A, and it is preferred when limited WRC measurements are available.

3.2 Soil $K_s$ estimates at various $\rho_b$ values

Fig. 2 shows the measured, best-fit, and estimated (using Models 1 and 2) $K_s$ values as a function of $\rho_b$ for the five soils. The $\rho_b$ variation had a significant effect on $K_s$ measurements. Generally, $K_s$ decreased with increasing $\rho_b$, and $K_s$ of soils at the highest and lowest $\rho_b$ values differed by up to one order of magnitude (Fig. 2). The $\rho_b$ also affected the accuracy of the best-fit
$K_s$ values. For samples with relatively high $\rho_b$, the best-fit $K_s$ values were close to measured $K_s$; for samples with relatively low $\rho_b$, however, the best-fit $K_s$ values were greater than measured ones (Fig. 2). Some studies reported that the measured $K_s$ might not be the optimal $K'$ for estimating $K_u$ with the original Mualem-van Genuchten model (Schaap et al., 2001; Schaap and van Genuchten, 2006). Other studies pointed out that the measured $K_s$ should be fixed at a small negative value of the pressure head because Eq. (2) failed to capture the macro-pore flow (Luckner et al., 1989; Vogel and Cislerova, 1988), and the $K_u(\psi)$ curve estimated with the original Mualem-van Genuchten model could exhibit an abrupt drop at water contents just below saturation when the change of the WRC shape near saturation was significant (Vogel et al., 2000). In other words, the best-fit $K_s$ at saturation could be substantially greater than the measured $K_s$ when the shape of the WRC changed considerably at matric potentials near saturation. This was evident in Fig. 1: in the near saturation range of the WRCs, the degree of saturation $S$ declined quickly with $\psi$ for soil samples with relatively low $\rho_b$, while the $S$ changes were relatively small for soil samples with relatively high $\rho_b$. Consequently, the curve fitting procedure overestimated $K_s$ at low $\rho_b$ values due to significant changes in the WRC shape near saturation.

Fig. 2 also shows that Models 1 and 2 give quite different $K_s$ estimates, especially in the small $\rho_b$ value range. The Model 1-estimated $K_s$ curves (black solid lines) were in good agreement with $K_s$ measurements for the five soils (on average, RMSE = 0.08). This was also confirmed by Assouline (2006a) in which Model 1 gave the most accurate $K_s$ estimates compared to measured $K_s$ values among eight different models. The Model 2-estimated $K_s$ curves (red solid lines) were close to measured $K_s$ at large $\rho_b$ values, but they deviated from measurements at small $\rho_b$ values.
(RMSE = 0.20). Thus, Model 1 estimated $K_s$ values were closer to $K_s$ measurements than were Model 2 estimates.

When comparing with best-fit $K_s$ values, alternately, Model 2 produced more accurate estimates (RMSE = 0.29) than did Model 1 (RMSE = 0.37). Model 2 better accounted for the shape effect of WRCs near saturation at low $\rho_b$ values than did Model 1. This is reasonable because Model 2 is developed based on the WRC model function (see Eq. 10), and the shape effect is included by substitution of Eq. (1) into Eq. (10).

It should be noted that the reference $K_{s0}$ is a key factor in determining $K_s$ as a function of $\rho_b$ using Model 2. The dashed lines in Fig. 2 are the estimated $K_s$ curves using $K_{s0}$ derived from each single $K_s$ measurement at different $\rho_b$ values. When a $K_s$ measurement was close to the best-fit $K_s$ at the same or similar $\rho_b$, the $K_s$ curves based on this $K_s$ measurement approached the other best-fit $K_s$ values at different $\rho_b$ values. The optimal $K_s$ measurements for calculating $K_{s0}$ using Model 2 were those made on samples with relatively high $\rho_b$ values. The $\rho_b$ value should be greater than 1.5 Mg m$^{-3}$ for coarse-texture soils (e.g., soils 1 and 4), and greater than 1.3 Mg m$^{-3}$ for fine-texture soils (e.g., soils 2, 3, and 5). In consideration of the large variability of $K_s$ measurements, multiple measurements over a wide range of $\rho_b$ are preferred for calculating $K_{s0}$ in Model 2. In our study, the $K_s$ curves derived from the average $K_{s0}$ values (the solid red lines in Fig. 2) were used in the estimation of $K_u$, although they might not be the optimal values for all soils. This was similar to the approach of Model 1, where average $K_{s0}$ values were used.

3.3 Soil $K_u$ estimates at various $\rho_b$ values

Four approaches, which combine two WRC functions and two $K_s$ models, were used to estimate $K_u$ of the five soils at various $\rho_b$ values. Fig. 3 compares the estimated $K_u$ versus measured $K_u$ values using Approach A1. The RMSE and bias values between estimated and
measured $K_u$ values at a specific $\rho_b$ are listed in Table 2. On the whole, Approach A1 gave accurate $K_u$ estimation for soils 1-4, with average RMSE ranged from 0.17 to 0.34, and average bias ranged from -0.23 to 0.09. On soil 5, however, Approach A1 generally underestimated $K_u$ under all three $\rho_b$ conditions, with an average RMSE of 0.89 and an average bias of -0.71. The underestimation was especially clear in the low $K_u$ range. The results in Fig. 3 and Table 2 also indicate that compared to measurements, Approach A1 tends to give lower $K_u$ values under the relatively low $\rho_b$ range, but no consistent trends are observed in the relatively high $\rho_b$ range. This happened because Approach A1 used Model 1 for estimating $K_s$, and the estimations were generally lower than the best-fit $K_s$ values under relatively low $\rho_b$ conditions (Fig. 2).

Although the Mualem-van Genuchten (1980) hydraulic conductivity model has been used extensively, it has several limitations when the default $K'$ and $L = 0.5$ are used in Eq. (2). In the present study, $L$ was taken as 0.5, an optimal value obtained from a data set of 45 disturbed and undisturbed samples (Mualem, 1976). Several studies have indicated that $L$ varied over a wide range, and it could be negative (Yates et al., 1992; Schuh and Cline, 1990; Leij et al., 1997; Schaap and Leij, 2000). Schaap and Leij (2000) showed that using $L = -1$ produced more accurate $K_u$ estimates for a data set of 235 soil samples than did $L = 0.5$. Fig. 4 evaluates the effects of parameter $L$ on the original Mualem-van Genuchten (1980) model, in which measured $K_s$ at $\rho_b$ of 1.09 Mg m$^{-3}$ and WRC parameters at $\rho_b$ of 1.10 Mg m$^{-3}$ (Table 1) were used to estimate $K_u$ of soil 5 at $\rho_b$ of 1.13 Mg m$^{-3}$. For the original Mualem-van Genuchten (1980) model, it was observed that $L = -1$ is a more suitable model parameter than $L = 0.5$ for soil 5 (Fig. 4). Similarly, setting $L = -1$ (instead of $L = 0.5$) in the $\rho_b$-related model (Approach A1) improved the accuracy of estimates for soil 5 (Fig. 3). The average RMSE was decreased from 0.89 to 0.35 and the average bias changed from -0.71 to -0.02 (Table 2). Thus, for soil 5, using an $L$ value of -
Approach A1 produced more accurate $K_u$ estimates than did using $L = 0.5$. It is difficult to determine which $L$ is optimal for a specific soil because $L$ is affected by soil texture and several other physical properties (Schaap and Leij, 2000). Despite this, our results showed that using the same $L$ in the $\rho_b$-related model produced accurate $K_u$ estimates when the $L$ value was suitable for the original Mualem-van Genuchten (1980) model (i.e., the model not accounting for $\rho_b$ effects).

A comparison between measured and estimated $K_u$ values using Approach A2 for the five soils is presented in Fig. 5. Except for soil 5, the estimated $K_u$ values agreed well with the $K_u$ measurements. Similar to that of Approach A1, taking $L = -1$ (instead of the default $L = 0.5$) improved the accuracy of Approach A2 significantly on soil 5: the average RMSE decreased from 0.78 to 0.25, and the average bias changed from -0.65 to -0.01. Further analysis showed that Approach A2 produced better $K_u$ estimates as indicated by the lower (on soils 1, 2, 4, and 5) or the same (on soil 3) average RMSEs compared to those of Approach A1 (Table 2). This is because Approach A2 accounted for the shape effect of WRCs near saturation under relatively low $\rho_b$ conditions for most soils. Across the five soils, Approach A2 gave $K_u$ estimates with an average RMSE and an average bias of 0.25 and -0.03, respectively.

The measured $K_u$ data versus estimated $K_u$ values using Approaches B1 and B2 are presented in Figs. 6 and 7, respectively. In both cases, the WRC parameters were obtained by using Function B in which soil texture data and one WRC measurement were used. Tian et al. (2018c) indicated that Function B gave less accurate WRC estimates than did Function A. Consequently, the $K_u$ values from Approaches B1 and B2 had larger average RMSE values (0.35 for both approaches) on all five soils than did those from Approaches A1 and A2 (average RMSE values of 0.28 and 0.25, respectively; Table 2). No consistent difference was observed between Approaches B1 and B2. On soils 1, 2, and 5, approach B2 gave more accurate $K_u$ estimates than
did Approach B1, especially under relatively low $\rho_b$ conditions. On soils 3 and 4, however, Approach B1 produced $K_u$ data with lower average RMSE than did those from Approach B2.

In summary, among the four approaches, Approach A2 performed the best, followed by Approach A1, and both gave more accurate results than did Approaches B1 and B2. On the other hand, Approaches B1 and B2 required fewer WRC measurements for estimation of model parameters, which might be an advantage in some situations where the cost or availability of data collection is an important issue. For all four approaches, the accuracy of WRC estimates was a key factor that determined the accuracy of $K_u$ estimates, especially in the lower $K_u$ range. Besides, we observed that parameter $L$ played a critical role in estimating $K_u$ with the Mualem-van Genuchten model. The default $L$ of 0.5 was reasonable for soils 1-4, while an $L$ of -1 was better for soil 5. Thus, future studies are required to further improve the model accuracy by introducing soil-specific $L$ values or texture-dependent $L$ models.

4. Conclusion

Changes in $\rho_b$ affect the accuracy of the Mualem-van Genuchten (1980) $K_u$-estimation model. In this study, we applied two functions for relating WRC parameters to $\rho_b$ and two models for correlating $K_s$ with $\rho_b$. By assembling the functions and models, four approaches were developed to estimate $K_u$ of soils at various $\rho_b$ values. Evaluation using $K_u$ measurements on five soils showed that among the four approaches, Approach A2 gave the most accurate $K_u$ estimates for all soils. Approach A1 produced less accurate $K_u$ estimates compared to Approach A2, but performed better than did Approaches B1 and B2. Approach A2 performed better than did Approach A1 because the $K_s$-estimation model used in Approach A2 accounted for the shape effect of WRC near saturation under relatively low $\rho_b$. Approaches A1 and A2 gave more accurate $K_u$ estimates than did Approaches B1 and B2 because more accurate WRC estimates
were used. On the whole, all four approaches gave reasonable $K_u$ estimates with average RMSEs lower than 0.35. Thus, the approaches developed herein have potential for improving simulation of transient and variable soil water, solute, and gas transport processes that depend on $\rho_b$. 
Acknowledgements

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Appendix

Inverse solution of Eq. (1) gives,

$$|\psi|^{-1} = \alpha \left( S^{-1/m} - 1 \right)^{-1/n} \quad (A1)$$

Substitution of $S = x^m$ into the integrals of Eq. (10) leads to

$$\int_0^1 |\psi|^{-1} dS(\psi) = \alpha \int_0^1 mx^{m-1}(x^{-1} - 1)^{-1/n} \, dx \quad (A2)$$

Since $m = 1 - 1/n$, so,

$$\int_0^1 |\psi|^{-1} dS(\psi) = \alpha \int_0^1 m(1 - x)^{m-1} \, dx \quad (A3)$$

Substitution of $x = 1 - y$ into Eq. (A3) leads to

$$\int_0^1 |\psi|^{-1} dS(\psi) = \alpha \int_0^1 -my^{m-1} \, dy = \alpha \quad (A4)$$

Thus, the ratio of the two integrals in Eq. (10) is

$$\frac{\int_0^1 |\psi|^{-1} dS(\psi)}{\int_0^1 |\psi|^{-1} dS_0(\psi)} = \frac{\alpha}{\alpha_0} = \left( \frac{\rho_b}{\rho_{bo}} \right)^{-3.97} \quad (A5)$$
References


Table 1. Texture, particle-size distribution, particle density ($\rho_s$), bulk density ($\rho_b$), and saturated hydraulic conductivity ($K_s$) of the soils used for predicting unsaturated hydraulic conductivity ($K_u$).

<table>
<thead>
<tr>
<th>ID</th>
<th>Texture</th>
<th>Particle-size distribution</th>
<th>$\rho_s$</th>
<th>$\rho_b$ (for WRC)</th>
<th>$\rho_b$ (for $K_s$)</th>
<th>Measured $K_s$</th>
<th>$\rho_b$ (for $K_u$)</th>
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<td>Sand</td>
<td>90 6 4</td>
<td>2.71</td>
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<td>2270 2420 2210 2100</td>
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</tr>
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<td>1.18 1.26 1.37 1.41</td>
<td>48 31 16 12</td>
<td>1.18 1.26 1.37 1.41</td>
</tr>
<tr>
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<tr>
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<td>1.10 1.21 1.30 1.41</td>
<td>151 125 44 33</td>
<td>1.13 1.24 1.41 1.41</td>
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Table 2. The root mean square error (RMSE) and bias between Approaches A1, A2, B1, and B2 estimated and measured unsaturated hydraulic conductivity values of the five soils used in this study.

<table>
<thead>
<tr>
<th>ID</th>
<th>Texture</th>
<th>(\rho_b) (Mg m(^{-3}))</th>
<th>Approach A1</th>
<th>Approach A2</th>
<th>Approach B1</th>
<th>Approach B2</th>
</tr>
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<tr>
<td></td>
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<td><strong>0.33</strong></td>
<td><strong>-0.22</strong></td>
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<tr>
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<td><strong>Average</strong>*</td>
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<td><strong>-0.03</strong></td>
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</table>

* Average of all five soils (for soil 5, \(L = -1\)) as a whole.
Fig. 1. Estimated relationships between degree of saturation ($S$) and water matric potential ($\psi$) for five soils at various bulk densities (values listed in legend) based on Functions A and B.
Fig. 2. Estimated saturated hydraulic conductivity ($K_s$) for five soils as a function of soil bulk density ($\rho_b$) using Model 1 and 2 (average $K_{s0}$ values were used). Measured and best-fit $K_s$ values were also included in the figure. Dashed lines were Model 2 estimates using $K_{s0}$ from each $K_s$ measurement at various $\rho_b$ values.
Fig. 3. Approach A1 estimated unsaturated hydraulic conductivity ($K_u$) for five soils at various bulk densities (values listed in legend) compared with corresponding measured data. For soil 5, parameter $L = -1$ was also tested.
Fig. 4. Comparison of measured unsaturated hydraulic conductivity ($K_u$) of soil 5 at bulk density of 1.13 Mg m$^{-3}$ to original Mualem-van Genuchten model estimated $K_u$ with both $L = 0.5$ and -1.
Fig. 5. Approach A2 estimated unsaturated hydraulic conductivity ($K_u$) for five soils at various bulk densities (values listed in legend) compared with corresponding measured data. For soil 5, parameter $L = -1$ was also tested.
Fig. 6. Approach B1 estimated unsaturated hydraulic conductivity ($K_u$) for five soils at various bulk densities (values listed in legend) compared with corresponding measured data. For soil 5, parameter $L = -1$ was also tested.
Fig. 7. Approach B2 estimated unsaturated hydraulic conductivity ($K_u$) for five soils at various bulk densities (values listed in legend) compared with corresponding measured data. For soil 5, parameter $L = -1$ was also tested.
Highlights:

- Soil bulk density variations significantly affect hydraulic conductivity ($K_u$).
- Parameters in the Mualem-van Genuchten soil $K_u$ model are related to bulk density.
- Four approaches are developed to estimate $K_u$ of soils over a range of bulk densities.