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Improving unsaturated hydraulic conductivity estimation in soils via percolation theory

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ABSTRACT

Accurate estimation of unsaturated hydraulic conductivity $K(S_w)$ in soils has been of great interest to soil physicists and hydrologists in the past several decades. Although various methods such as a "bundle of capillary tubes" conceptual approach were applied in the literature to theoretically model hydraulic conductivity in term of water saturation, in this study we invoke percolation theory, which quantifies the effect of the interconnectivity of pores on the macroscopic fluid flow. We incorporate the pore-solid interface roughness effect in the hydraulic conductance-pore radius (*g-r*) relationship, evaluate our $K(S_w)$ model using 104 soil samples from the UNSODA database as well as another 20 soil samples from the Rijtema database, and compare it to the Ghanbarian-Alavijeh and Hunt (2012) model. Generally speaking, we experimentally demonstrate that $K(S_w)$ estimations were improved over the entire range of water saturation when the surface roughness effect was incorporated. However, our model still underestimates the unsaturated hydraulic conductivity at low water saturations (corresponding to $K(S_w) < 10^{-4}$ cm/day). We show that after eliminating the effect of non-equilibrium conditions in the measurements $K(S_w)$ estimations were improved substantially. Other plausible sources for $K(S_w)$ underestimation are also discussed.

1. Introduction

Accurate estimate of unsaturated hydraulic conductivity $K(S_w)$ is still challenging and of great interest, particularly in two-phase flow and contaminant transport modeling in soils. Various models based on data mining techniques (e.g., Wösten and van Genuchten, 1988; Vereecken et al., 1990; Vereecken, 1995; Schaap and Leij, 1998; Weynants et al., 2009), bundle of *straight* capillary tubes (e.g., Purcell, 1949; Childs and Collis-George, 1950; Burdine, 1953; Mualem, 1976; Kosugi, 1999), bundle of *tortuous* capillary tubes (e.g., Yu et al., 2003; Liu et al., 2007; Xu et al., 2013), critical path analysis (e.g., Hunt, 2001; Hunt and Gee, 2002a,b; Hunt, 2004a; Ghanbarian-Alavijeh and Hunt, 2012; Hunt et al., 2013), effective-medium approximations (e.g., Levine and Cuthiell, 1986; Kanellopoulos and Petrou, 1988; Ghanbarian et al., 2016b), percolation theory (e.g., Larson et al., 1981; Heiba et al., 1992; Blunt et al., 1992), pore network models (e.g., Jerauld and Salter, 1990; Blunt and King, 1991; Bakke and Øren, 1997; Raoof and Hassanizadeh, 2012) and lattice-Boltzmann methods (e.g., Hazlett et al., 1998; Ramstad et al., 2010; Zhang et al., 2016) have been developed to estimate $K(S_w)$ from other porous medium characteristics, such as water retention curve (also known as capillary pressure curve), particle-size distribution, porosity, saturated hydraulic conductivity K_s, two- and three-dimensional images, etc.

The literature on unsaturated hydraulic conductivity modeling and estimation is vast and extensive. Several researchers modified the Kozeny-Carman equation to model the unsaturated hydraulic conductivity in porous media (e.g., Alpak et al., 1999; Rezanezhad et al., 2009; Khaleel, 2010). Numerous studies compared the performance of the Burdine (1953) modal with that of Mualem (1976) via experimental data (see e.g., van Genuchten and Nielsen, 1985; Alexander and Skaggs, 1986; Nimmo and Akstin, 1988; Khaleel and Saripalli, 2006; Yang and Mohanty, 2015). Even recently, Burdine (1953) and Mualem (1976) models were combined to improve unsaturated hydraulic conductivity estimation from soil water retention data (see Valiantzas, 2010). Both Burdine (1953) and Mualem (1976) models idealize a porous medium constructed of interconnected pores as a bundle of non-interconnected and straight cylindrical pore tubes. In reality pores exist neither in series nor in parallel but are typically distributed randomly throughout a complex multi-scale network.

Some studies defined tortuosity-connectivity factor in the bundle of capillary tubes approach in a more rigorous way to improve $K(S_w)$ estimations (e.g., Assouline, 2001; Vervoort and Cattle, 2003; Kuang

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and Jiao, 2011). Some others considered saturated hydraulic conductivity K_s and/or tortuosity-connectivity factor as a matching point in the Mualem-van Genuchten model (e.g., Schaap and Leij, 2000; Tuli et al., 2005). Including concepts from liquid-vapor interfacial area has also improved unsaturated hydraulic conductivity in porous materials (see e.g., Or and Tuller, 1999, 2000, 2003; Tuller and Or, 2001, 2002; Zand-Parsa and Sepaskhah, 2004; Zand-Parsa, 2006).

Hunt (2001) was probably the first to apply critical path analysis (CPA), introduced by Ambegaokar et al. (1971) and Pollak (1972), to estimate the *unsaturated hydraulic conductivity of soils*, although some applications of such approach have been previously proposed to model *permeability* in disordered rocks (e.g., Katz and Thompson, 1986, 1987; David et al., 1990) and pore networks (e.g., Sahimi, 1993; Bernabé, 1995; Shah and Yortsos, 1996; Bernabé and Bruderer, 1998; Friedman and Seaton, 1998). Hunt (2001) combined the Rieu and Sposito (1991) model of pore-size distribution with CPA, estimated the unsaturated hydraulic conductivity and showed good match with experiments from the Hanford, DOE site, particularly at high water saturations. Hunt and Gee (2002a) extended the Hunt (2001) method and estimated $K(Sw)$ from particle-size distribution for Hanford data. They found good agreement with experiments over 4–6 orders of magnitude. Years later, Ghanbarian-Alavijeh and Hunt (2012) combined concepts from critical path analysis and percolation theory with the pore-solid fractal model (Perrier et al., 1999; Bird et al., 2000) and proposed a more general $K(S_w)$ model as follows

$$\frac{K(S_w)}{K_s} = \begin{cases} \left[\dfrac{\beta/\phi - 1 + S_w - S_{wc}}{\beta/\phi - S_{wc}}\right]^{\frac{\lambda}{3-D}}, & S_{wx} \le S_w \le 1 \\ \left[\dfrac{\beta/\phi - 1 + S_{wx} - S_{wc}}{\beta/\phi - S_{wc}}\right]^{\frac{\lambda}{3-D}} \left[\dfrac{S_w - S_{wc}}{S_{wx} - S_{wc}}\right]^2, & S_{wc} \le S_w \le S_{wx} \end{cases} \tag{1}$$

where $K(S_w)$ and K_s are the hydraulic conductivity under partially and fully saturated conditions, respectively, ϕ is the porosity, S_w is the water saturation, D is the pore-solid interface fractal dimension, β is the pore-solid fractal (PSF) model parameter varying between ϕ and 1, $\lambda = D$, and S_{wc} is the critical water saturation (percolation threshold for water flow). One may roughly approximate S_{wc} from water saturation at 1500 kPa tension head from the soil water retention curve (van Genuchten, 1980). Alternatively, finite-size scaling analysis (see e.g., Rintoul and Torquato, 1997; Priour, 2014), Monte Carlo simulations (see e.g., Baker et al., 2002), mercury intrusion porosimetry data (Katz and Thompson, 1986, 1987) or morphological techniques (e.g., Liu and Regenauer-Lieb, 2011) may be used to estimate the percolation threshold.

In Eq. (1) S_{wx} is the crossover point at which fractal scaling from critical path analysis switches to universal percolation scaling from percolation theory. S_{wx} can be determined by setting equal Eq. (1) top line and Eq. (1) bottom line as well as their derivatives as follows (Ghanbarian-Alavijeh and Hunt, 2012; Ghanbarian et al., 2016a):

$$S_{wx} = S_{wc} + \left[\frac{2(\beta - \phi)}{\lambda/(3 - D) - 2}\right] \tag{2}$$

The unknown parameters in Eqs. (1) and (2), such as D and β are determined by fitting the following PSF model (Bird et al., 2000) to measured soil water retention data

$$S_w = 1 - \frac{\beta}{\phi}\left[1 - \left(\frac{h}{h_{min}}\right)^{D-3}\right], \quad h_{min} \le h \le h_{max} \tag{3}$$

where h is the tension head, h_{min} is the air entry value, and h_{max} is the maximum tension head corresponding to the minimum accessible pore radius via the Young-Laplace equation. Eq. (3) – that reduces to the Tyler and Wheatcraft (1990) and Rieu and Sposito (1991) models when $\beta = \phi$ and 1, respectively – has the same form as the Perrier et al. (1996) and Ghanbarian-Alavijeh et al. (2012) models developed using different methodologies.

Following Hagen-Poiseuille's law, hydraulic conductance g in a perfectly cylindrical pore tube is proportional to pore radius to the fourth divided by its length (i.e., $g \propto r^4/l$). In a self-similar fractal porous medium, however, one may assume pore length proportional to its radius ($l \propto r$) and thus $g \propto r^3$ (see e.g., Katz and Thompson, 1986; Hunt, 2001). Using this methodology Hunt (2001) and Hunt and Gee (2002a) set $\lambda = 3$. To be consistent with non-universal results of Balberg (1987), Hunt (2005) later proposed $\lambda = D$, followed by Ghanbarian-Alavijeh and Hunt (2012), Hunt et al. (2014) and Ghanbarian et al. (2015).

Recently, Ghanbarian et al. (2016a) incorporated the effect of surface roughness into the hydraulic conductance in a single pore tube with unsmooth pore-solid interface, proposed $g \propto r^{2(4-D) - (3-D)/(2D-3)}$ and suggested that λ should be $2(4–D) – (3–D) / (2D–3)$ in isotropic porous media. Note that Cai et al. (2014) modified Hagen-Poiseuille's law for tortuous and irregular shaped pores but did not include the effect of surface roughness. Ghanbarian et al. (2016a) showed that $\lambda = 2(4–D) – (3–D) / (2D–3)$ resulted in more accurate $K(S_w)$ estimations than $\lambda = 3$ using 10 soil samples. Whether it can also estimate $K(S_w)$ more precisely than $\lambda = D$ is still an open question. The values of $\lambda = D$ and $2(4–D) – (3–D) / (2D–3)$ are different conceptually and affect $K(S_w)$ estimations differently since as D increases from 2 to 3, generally speaking, the value of $2(4–D) – (3–D) / (2D–3)$ decreases from approximately 3 to 2, while $\lambda = D$ increases similarly from 2 to 3. Therefore, the main objective of this study is comparing $\lambda = 2(4–D) – (3–D) / (2D–3)$ with $\lambda = D$ in the estimation of $K(S_w)$ using a large dataset i.e., 104 soil samples with various textural and structural characteristics from the UNSODA database selected by Ghanbarian-Alavijeh and Hunt (2012). In addition, we compare the performance of two λ values in the unsaturated hydraulic conductivity estimation using the Rijtema (1969) database including 20 soil samples of variety structures and textures. We also address the effects of non-equilibrium conditions, capillary number and flow rate as well as uncertainties in the determination of the pore-solid fractal model parameters β and D on $K(S_w)$ estimations from the measured drainage water retention curve.

2. Materials and methods

The Ghanbarian-Alavijeh and Hunt (2012) dataset includes 104 soil samples from the UNSODA database. The salient properties of these soils including average value of D, β, h_{min} as well as the number of samples for nine soil texture classes are given in Table 1. For soil sample distribution on the ternary diagram see Fig. 1 in Ghanbarian-Alavijeh and Hunt (2012).

The Rijtema (1969) database consists of twenty soil samples from high-permeability coarse sand to highly porous peat soil with various hydraulic characteristics. In this database, soil water content and hydraulic conductivity was measured at tensions h = 0, 2.5, 10, 31, 100, 200, 500, 2500, 16,000 and 10^6 cm H_2O. The last measured data point was, however, dropped out in this study due to possible contribution of vapor transport at such a high tension. The PSF model parameters e.g., D, β, and h_{min} were determined by directly fitting Eq. (3) to the measured soil water retention curve. Following van Genuchten (1980), we approximately set critical water saturation equivalent to saturation at 16000 cm H_2O. Table 2 presents some physical and hydraulic characteristics of each soil sample within the Rijtema (1969) database. The interested reader is referred to the original Ghanbarian-Alavijeh and Hunt (2012) and Rijtema (1969) articles for further detailed information.

In order to compare statistically the accuracy of Eq. (1) with different λ values in the estimation of $K(S_w)$, the root mean square log-transformed error (RMSLE) parameter was determined as follows