Upscaling soil saturated hydraulic conductivity from pore throat characteristics

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Abstract

Upscaling and/or estimating saturated hydraulic conductivity K_{sat} at the core scale from microscopic/macrosopic soil characteristics has been actively under investigation in the hydrology and soil physics communities for several decades. Numerous models have been developed based on different approaches, such as the bundle of capillary tubes model, pedotransfer functions, etc. In this study, we apply concepts from critical path analysis, an upscaling technique first developed in the physics literature, to estimate saturated hydraulic

conductivity at the core scale from microscopic pore throat characteristics reflected in capillary pressure data. With this new model, we find K_{sat} estimations to be within a factor of 3 of the average measured saturated hydraulic conductivities reported by Rawls et al. (1982) for the eleven USDA soil texture classes.

Keywords: Capillary pressure curve, Critical path analysis, Electrical conductivity, Katz and Thompson model, Saturated hydraulic conductivity

1. Introduction

Estimating saturated hydraulic conductivity K_{sat} from microscopic and macroscopic soil properties has been an intensive research area since the 1940s. Early pioneering models were developed based on the bundle of capillary tubes approach, idealizing a porous medium by replacing actual interconnected flow paths with straight cylindrical pore tubes of equal length (e.g., Purcell, 1949; Child and Collis-George, 1950). The Purcell (1949) model also included an empirical parameter called the lithological factor that accounted for tortuosity, with values ranging from 0.085 to 0.363 with an average of 0.216.

Marshall (1957; 1958) later proposed a model similar to Purcell (1949) and Childs and Collis-George (1950) that estimated (single-phase) permeability k from a measured capillary pressure curve. In the Marshall (1958) model, the capillary pressure curve is classified into n sections, each of which is assumed to correspond to a fraction $1/n$ of the total pore cross-sectional area characterized by a mean pore radius. The average cross-sectional area of the pore space is then calculated and related to permeability k .

Brutsaert (1967) derived a saturated hydraulic conductivity model by combining the Brooks and Corey capillary pressure and Childs and Collis-George (1950) permeability equations. The Brutsaert (1967) model is

$$K_{sat} = C_B \frac{(\phi - \theta_r)^2}{P_a^2} \frac{\lambda^2}{(\lambda + 1)(\lambda + 2)} \quad (1)$$

where K_{sat} is the saturated hydraulic conductivity (cm/s), $C_B = 270$ is a constant representing the effects of fluid properties and gravity, ϕ is the porosity, λ is the pore throat-size distribution index, θ_r is the residual water content, and P_a is the air entry pressure (cm H₂O) in the Brooks and Corey (1964) model. Rawls et al. (1982) evaluated Eq. (1) using average values of ϕ , λ , θ_r , and P_a determined for the eleven USDA soil texture classes and found the estimated K_{sat} values to be about one order of magnitude larger than the measured ones.

Mishra and Parker (1990) presented the following closed-form expression using the Mualem (1976) conductivity model in conjunction with the capillary pressure model of van Genuchten (1980)

$$K_{sat} = C_{MP} (\phi - \theta_r)^{5/2} \alpha^2 \quad (2)$$

where K_{sat} has units of cm/s. Mishra and Parker (1990) set $C_{MP} = 108 \text{ cm}^3/\text{s}$ by assuming a geometrical factor of 8 for cylindrical pores, a tortuosity factor of 2.5, and values for water density, viscosity, and surface tension at 20° C. They found a reasonable agreement between measured K_{sat} and values estimated with Eq. 2 (within ± 2 standard deviation error intervals) for 48 soils in Virginia, U.S., with K_{sat} values varying over three orders of magnitude. In contrast, Hoffmann-Riem et al. (1999) showed that the same approach overestimated K_{sat} for ca. 90% of 56 data entries in the UNSODA database and by more than one order of magnitude in ca. 15-20% of these cases. Nasta et al. (2013) later assumed

$\theta_r = 0$ in Eq. 2 and based on a comparison with experimental data from the GRIZZLY database found that a significantly larger tortuosity factor $((L_a/L_s)^2 = 39.1$ in which L_s is the sample length and L_a is the average tortuous flow path) than is physically realistic was needed to match the measurements. With a more realistic tortuosity factor, Eq. 2 would have systematically overestimated K_{sat} .

By means of tortuous parallel tubes, Xu and Yu (2008) developed a model similar to the Kozeny-Carman equation. In their model K_{sat} is a function of tortuosity fractal dimension D_T , maximum pore throat radius in the medium r_{max} , and porosity. Following Yu and Cheng (2002), Xu and Yu (2008) approximately set $D_T = 1.1$ and compared the Xu and Yu (2008) model to one porous sample composed of mono-sized grains (with $\phi = 0.49$) and three experiments constructed of grains of two different sizes (with $\phi = 0.52, 0.54$ and 0.56). Although Xu and Yu (2008) found K_{sat} estimated by their approach in reasonable agreement with experiments, its application in soils remains an open question, since the pore space architecture is typically much more complicated and grain-size distributions are broader.

Based on a simple capillary bundle model and the Brooks-Corey water retention equation, Laliberte et al (1968) and, more recently, Nasta et al. (2013) proposed

$$K_{sat} = 9.579 \times 10^5 \tau_N \frac{\lambda}{\lambda+2} \frac{\phi}{P_a^2} \quad (3)$$

where K_{sat} has units of cm/h and $\tau_N = (L_s/L_a)^2$ is an empirical parameter representing the effect of tortuosity and connectivity ($0 < \tau_N < 1$). Using 62 soil samples from the GRIZZLY database, Nasta et al. (2013) found $\tau_N = 0.0138$ (i.e., $(1/8.5)^2$). This means that, on average, the tortuous flow paths were nearly 8.5 times longer than straight cylindrical pore tubes (or the sample length), which seems physically unreasonable in saturated porous

media with intermediate and high porosities as well as finite size (Ghanbarian et al., 2013b). This demonstrates the importance of connectivity, which is only treated empirically in this model. If a physically reasonable value of tortuosity was selected, Eq. 3 would systematically overestimate K_{sat} . Using 197 soil samples from the HYPRES database, Nasta et al. (2013) demonstrated that Eq. (3) with τ_N fixed at 0.0138 estimated K_{sat} more accurately than the Mishra and Parker (1990) model, Eq. 2.

The parallel tube models presented in the literature (e.g., Purcell, 1949; Nasta et al., 2013) contain an empirical tortuosity-connectivity factor that must be estimated by fitting the model to experimental observations. The *tortuous* parallel tube models (e.g., Xu and Yu, 2008) also contain a parameter that must be either measured or estimated, the tortuosity fractal dimension D_T . In the literature, D_T was determined based on the box counting method and two-dimensional images (e.g., Yu and Cheng, 2002) or approximated from pore space fractal dimension, minimum and maximum pore radii, porosity and average tortuosity. The latter was commonly approximated (e.g., Feng and Yu, 2007; Li et al. 2015) based on the simplified two-dimensional model of Yu and Li (2004) that allows flow only between square solid particles in an equilateral-triangle arrangement with either the flow path changing with a specific angle that depends on the particle size and pore space, or the streamline direction changes are limited to multiples of 90° (Ghanbarian et al., 2013a). Therefore, a precise and rigorous method for D_T estimation is not yet clear and, consequently, the practical application of those models to estimate K_{sat} is questionable. In addition, parallel and tortuous parallel models are distorted idealizations of soils (Fatt, 1956; Sahimi, 2011; Hunt et al., 2013). Pore throats in real soils exist neither in series nor in parallel, but are distributed throughout an interconnected and complex multi-scale

network. A failure to properly account for the significant effects of pore connectivity is one important reason why capillary bundle models might overestimate K_{sat} in soils, if the physical basis of their parameters is respected. However, when K_{sat} scales with r_{max} ($\propto 1/P_a$) with an exponent much greater than the theoretical value of 2 (see Eqs. 1 and 3), one may expect models based upon bundle of capillary tubes underestimate K_{sat} , as we show in this study. Critical path analysis is a powerful analytical approach based on percolation theory (Sahimi, 1994; Sahimi, 2011; Hunt et al., 2014) that can account for both tortuosity and *connectivity*, thus overcoming a significant limitation of the parallel and tortuous parallel models. Although critical path analysis has been successfully tested on *rocks* (e.g., Kats and Thompson, 1986, 1987; Arns et al., 2005; Ghanbarian et al., 2016) and some characteristics of such a solution have been enumerated in soils (e.g., Hunt, 2001; Hunt and Gee, 2002a) and non-Newtonian fluid flow (Sahimi, 1993), to the best of the authors' knowledge it has never been evaluated previously in the estimation of *saturated hydraulic conductivity of soils*. The main objective of this study is, therefore, to develop a theoretical model via critical path analysis to estimate saturated hydraulic conductivity K_{sat} in soil.

2. Theory

2.1. Pore throat-size distribution and capillary pressure curve

Here, we consider a power-law distribution of pore sizes. It has been argued in the literature (e.g., Pachepsky et al., 2000) that pores in soils possess a hierarchical structure that can be represented as a fractal object. Filgueira et al. (1999), Bird et al. (2000), Hunt and Gee (2002b), and Ghanbarian-Alavijeh and Hunt (2012b) have shown that the power-

137 law pore-size distributions predicted in fractal models can be used to estimate capillary
138 pressure curves.

139 Assuming soils are fractal, the probability density function of the pore throat sizes,
140 $f(r)$, follows a power law, and is given by

$$141 \quad f(r) = \frac{D}{r_{min}^{-D} - r_{max}^{-D}} r^{-1-D} = C_p r^{-1-D}, \quad r_{min} \leq r \leq r_{max} \quad (4)$$

142 where r is the pore throat radius, r_{min} and r_{max} are the smallest and largest *accessible* pore
143 throat radii representing the lower and upper bounds of the fractal scaling, respectively, and
144 D is the fractal dimension of the pore space whose value in three dimensions is typically
145 between 0 and 3. The larger the fractal dimension D , the broader is the pore throat-size
146 distribution.

147 The volume fraction of all the pores between the lower and upper cutoffs of the
148 fractal scaling (the porosity ϕ of the porous medium) is determined by integrating $f(r)$:

$$149 \quad \phi = \int_{r_{min}}^{r_{max}} s r^3 f(r) dr = \frac{s C_p}{3-D} (r_{max}^{3-D} - r_{min}^{3-D}) \quad (5)$$

150 in which the shape factor s is assumed to be constant across all pore throat sizes.

151 The volume fraction of the pores filled by water (θ) is a function of some upper
152 limit $r \leq r_{max}$

$$153 \quad \theta = \int_{r_{min}}^r s r^3 f(r) dr = \frac{s C_p}{3-D} (r^{3-D} - r_{min}^{3-D}) \quad (6)$$

154 Note that for the sake of simplicity, we assumed that each pore throat of the porous
155 medium is occupied by only water or air. Equation (6) integrates over pore throat sizes
156 between r_{min} and r . This necessarily means that all pores with throat size r and greater are
157 collectively drained, and any entrapment of water in those pore throats during drainage is
158 ignored. Such simplicity in the pore occupancy is, however, only an approximation.

Combining Eqs. (5) and (6) with the Young-Laplace equation ($P_c = A/r$, where P_c is the capillary pressure and A is $2\gamma\cos(\omega)$ in which γ is the air-water surface tension and ω is the air-water contact angle), results in the fractal capillary pressure model given by

$$\theta = \phi - \beta \left[1 - \left(\frac{P_c}{P_a} \right)^{D-3} \right], \quad |P_a| \leq |P_c| \leq |P_{max}| \quad (7)$$

where P_a is the air entry pressure ($=A/r_{max}$), P_{max} is the maximum capillary pressure ($=A/r_{min}$), and β is $\phi r_{max}^{3-D} / (r_{max}^{3-D} - r_{min}^{3-D})$. Note that Eq. (7) is similar to the Perrier et al. (1996) and Bird et al. (2000) models, albeit with different terminology.

2.2. Critical path analysis

Critical path analysis (CPA), introduced by Ambegaokar et al. (1971) and Pollak (1972), is a powerful approach for understanding transport in random (uncorrelated) systems. According to CPA, transport in a randomly disordered system is controlled by conductances with magnitudes slightly less than the threshold conductance, where the threshold conductance is the smallest possible value of the conductance for which the set of all larger conductances still forms an infinite connected cluster.

Katz and Thompson (1986, 1987) were first to apply critical path analysis to link permeability, k , to electrical conductivity and critical pore radius. They expressed permeability k as

$$k = \frac{1}{C_{KT}} \frac{\sigma_b}{\sigma_w} r_c^2 = \frac{1}{C_{KT}} \frac{1}{F} r_c^2 \quad (8)$$

where σ_b is bulk electrical conductivity, σ_w is saturating fluid electrical conductivity, F is the formation factor, r_c is the critical pore diameter, and C_{KT} is a constant equal to 56.5.

In what follows, we show how parameters r_c , σ_b/σ_w , and ultimately K_{sat} ($=f_f k = \rho g_A k / \mu$ in which f_f is fluidity factor, ρ is fluid density, g_A is gravitational acceleration, μ is dynamic

fluid viscosity and k is given by Eq. (8)) may be estimated from pore throat characteristics and capillary pressure measurements.

- Critical pore radius r_c

Using concepts from critical path analysis, one may define the critical volume content of percolation, θ_t , under fully saturated conditions as follows (Ghanbarian-Alavijeh and Hunt, 2012a):

$$\theta_t = \int_{r_c}^{r_{max}} sr^3 f(r) dr = \frac{SC_p}{3-D} (r_{max}^{3-D} - r_c^{3-D}) \quad (9)$$

where r_c is the critical pore radius below which pores do not substantially contribute to fluid flow and permeability.

Given that $\beta = \phi r_{max}^{3-D} / (r_{max}^{3-D} - r_{min}^{3-D})$, rewriting Eq. (9) yields,

$$r_c = r_{max} \left[1 - \frac{\theta_t}{\beta} \right]^{\frac{1}{3-D}} \quad (10)$$

where r_{max} can be estimated from the air entry pressure ($P_a = A / r_{max}$). Therefore, if r_{max} , θ_t , β , and D are known, one may calculate the critical pore radius r_c via Eq. (10). In Eq. (10), the greater the critical water content θ_t , the smaller is the critical pore radius r_c . We should also point out that when $\theta_t = 0$, the critical pore radius would be equal to the maximum accessible pore radius ($r_c = r_{max}$).

- Electrical conductivity σ_b / σ_w

The ratio of the electrical conductivity of water to the electrical conductivity of bulk, known as formation factor ($F = \sigma_w / \sigma_b$), is typically measured in rocks to estimate

permeability. However, if not measured, the electrical conductivity σ_b/σ_w can be approximated from the capillary pressure curve. Katz and Thompson (1987) proposed

$$\frac{\sigma_b}{\sigma_w} = \frac{r_{max}^e}{r_c} \phi S(r_{max}^e) \quad (11)$$

where r_{max}^e is the pore throat radius corresponding to optimum path for electrical conductivity, $S(r_{max}^e)$ is the fractional volume of connected pore space involving pore throats of size r_{max}^e and greater. Katz and Thompson (1987) argued that when the pore throat-size distribution is broad, r_{max}^e can be estimated from $[1 - t/(1 + t)]r_c$ in which t is a critical exponent from percolation theory and equal to 2 in three dimensions (Stauffer and Aharony, 1994). Accordingly, r_{max}^e would be *roughly* $r_c/3$.

Analogously to how we derived Eq. (13), one may define $S(r_{max}^e)$ as follows:

$$S(r_{max}^e) = \frac{1}{\phi} \int_{r_{max}^e}^{r_{max}} sr^3 f(r) dr = 1 - \left(\frac{r_{max}^e}{r_{max}} \right)^{3-D} \quad (12)$$

Approximating r_{max}^e by $r_c/3$ and combining Eqs. (11) and (12) gives

$$\frac{\sigma_b}{\sigma_w} = \frac{\phi}{3} \left[1 - \left(\frac{r_c}{3r_{max}} \right)^{3-D} \right] \quad (13)$$

Equation (13), developed using concepts from critical path analysis, is a new electrical conductivity model estimating σ_b/σ_w from pore throat characteristics r_{max} , r_c , and D , as well as porosity ϕ .

- Saturated hydraulic conductivity K_{sat}

Substituting the critical pore radius r_c and electrical conductivity σ_b/σ_w from Eqs. (10) and (13) into Eq. (8) yields the saturated hydraulic conductivity based on critical path analysis as follows

$$K_{sat} = f_f \frac{A^2 P_a^{-2} \phi}{C_{KT}} \frac{1}{3} \left[1 - \left(\frac{1}{3} \right)^{3-D} \left(1 - \frac{\theta_t}{\beta} \right) \right] \left(1 - \frac{\theta_t}{\beta} \right)^{\frac{2}{3-D}} \quad (14)$$

Recall that C_{KT} is a constant coefficient equal to 56.5 (Katz and Thompson, 1986; 1987), A is the constant coefficient in the Young-Laplace equation ($=2\gamma\cos(\omega)$), P_a is the air entry pressure, f_f is the fluidity factor ($=\rho g_A/\mu$), θ_t is the critical water content for percolation, and ϕ is the porosity.

In what follows, we evaluate our proposed saturated hydraulic conductivity model, Eq. (14), in the estimation of K_{sat} from soil pore space properties and fluid characteristics.

3. Materials and Methods

To evaluate the proposed model Eq. (14) – estimating the saturated hydraulic conductivity from capillary pressure data – we use the Rawls et al. (1982) database, including undisturbed cores for 1323 non-structured soils with 5371 horizons from 32 US states. Rawls et al. (1982) reported the average value of the Brooks and Corey (1964) capillary pressure curve model parameters, total porosity, and saturated hydraulic conductivity for eleven USDA soil texture classes. More specifically, the number of samples and the arithmetic average value of ϕ , θ_r , λ , P_a and K_{sat} for the Rawls et al. (1982) database are presented in Table 1. We should point out that both geometric and arithmetic mean values for air entry pressure P_a and pore throat-size distribution index λ were reported by Rawls et al. (1982). However, to be consistent with the arithmetic average ϕ , θ_r , and K_{sat} values (W.J. Rawls 2016, personal communication), we use the arithmetic mean of P_a and λ .

In Table 1 we also present the calculated largest accessible pore throat radius r_{max} , critical pore radius r_c and electrical conductivity σ_b/σ_w ($=1/F$). r_{max} was determined from the value of P_a (given in Table 1) and the Young-Laplace equation. For the sake of simplicity,

we assume that surface tension $\gamma = 0.0728$ (N/m), air-water contact angle $\omega = 0$ and pores are cylindrical. That results into the approximation $r_{\max} \approx 0.149/P_a$, in which P_a is in cm H₂O. However, presuming cylindrical pores and $\omega = 0$ in the complex pore space geometry of natural soils may yield uncertainties in the K_{sat} estimations. We discuss in further details the effect of contact angle in the Discussion section. r_c was calculated from Eq. (10) and assuming that $\beta = \phi$, $\theta_t = \theta_r$ and $3 - D = \lambda$. σ_b/σ_w was estimated via Eq. (13) given that $3 - D = \lambda$.

Rawls et al. (1982) used the Brooks and Corey (1964) model to describe the capillary pressure curve, while the model we developed in section 2.1 is a fractal-based model with power-law pore-size distribution. Equation (7), however, would be *approximately* equivalent to the empirical Brooks and Corey (1964) model, if $\beta = \phi$ and $\lambda = 3 - D$ (Perrier et al., 1996), i.e.,

$$\frac{\theta - \theta_r}{\phi - \theta_r} = \left(\frac{P_c}{P_a} \right)^{-\lambda}, \quad |P_a| \leq |P_c| \leq |P_{\max}| \quad (15)$$

Recall that λ is the pore throat-size distribution index, P_a is the air entry pressure, and θ_r is the residual water content (Brooks and Corey, 1964). We should emphasize that the proposed fractal capillary pressure curve model, Eq. (7), would be fully consistent with the Brooks and Corey (1964) model only if the residual water content is zero in Eq. (15), which is unlikely in fine-textured soils typically showing a non-zero residual water content (see Table 1). However, inaccurate characterization of the capillary pressure curve at low water contents by *approximately* equating Eq. (7) to Eq. (15) should not greatly affect K_{sat} estimates in our calculations because K_{sat} is mainly controlled by soil structural pores (macropores) rather than soil textural pores (micropores) in the undisturbed samples collected by Rawls et al. (1982).

Therefore, one may estimate K_{sat} from the Brooks-Corey model parameters by replacing $3 - D$ and β with respectively λ and ϕ in Eq. (14) to have

$$K_{sat} = f_f \frac{A^2 P_a^{-2}}{C_{KT}} \frac{\phi}{3} \left[1 - \left(\frac{1}{3} \right)^\lambda \left(1 - \frac{\theta_t}{\phi} \right) \right] \left(1 - \frac{\theta_t}{\phi} \right)^{\frac{2}{\lambda}} \quad (16)$$

Note that replacing β with ϕ necessarily means that $r_{min} \rightarrow 0$. The critical volume fraction for percolation (θ_t) is not a priori known in soils, but can be roughly *approximated* by the residual water content θ_r , the maximum amount of water in a soil that will not contribute to liquid flow because of blockage from the flow paths or strong adsorption onto the solid phase (Luckner et al., 1989; van Genuchten et al., 1991).

To assess the accuracy of Eq. (16) in the estimation of K_{sat} statistically, the root mean square log-transformed error (RMSLE) parameter is calculated as follows

$$RMSLE = \sqrt{\frac{1}{N} \sum_{i=1}^N [\log(K_{sat})_{cal} - \log(K_{sat})_{meas}]^2} \quad (17)$$

where $N = 11$ is the number of values, and $(K_{sat})_{cal}$ and $(K_{sat})_{meas}$ are the calculated (estimated) and measured saturated hydraulic conductivities, respectively.

4. Results

The saturated hydraulic conductivity K_{sat} and the estimated electrical conductivity σ_b/σ_w (or $1/F$) as a function of the calculated critical pore radius r_c are shown in Figure 1 for the eleven USDA soil texture classes from Rawls et al. (1982). As can be observed, although K_{sat} is highly correlated to r_c with $R^2 = 0.94$, σ_b/σ_w does not show a strong dependency on r_c ($R^2 = 0.26$). Fitting a power law to the $K_{sat}-r_c$ and σ_b/σ_w-r_c data yielded exponents slightly less than 2 (i.e., 1.9) and slightly greater than zero (i.e., 0.128), respectively. The obtained results are consistent with the fact that water flow is strongly controlled by both

geometrical (e.g., pore-size distribution, pore shape, surface area) and topological (e.g., connectivity) characteristics of the porous medium, while the flow of electricity is more dominated by topology. Comparison of hydraulic conductance $g_h \propto r^4$ with electrical conductance $g_e \propto r^2$ in a perfectly cylindrical tube also confirms that saturated hydraulic conductivity is more dominated by pore space properties than is the case for electrical conductivity.

Note that such a weak dependency of σ_w/σ_b on r_c (exponent 0.128 and $R^2 = 0.26$) does not mean that one can estimate σ_w/σ_b from Archie's law, i.e. $\sigma_w/\sigma_b = \phi^2$, in which σ_w/σ_b is only a function of porosity and *independent* of r_c ; see e.g., Eq. 1 in Kamath (1992) or Eq. 1 in Nelson (2009). In the Results section, we discuss how estimation of σ_w/σ_b by Archie's law in the CPA model of Katz and Thompson (1986; 1987) would yield inaccurate estimates of K_{sat} .

The product of K_{sat} and the formation factor $F (= \sigma_w/\sigma_b)$ versus r_c is presented in Figure 2. The best-fit power law to the data has an exponent of 1.774 with $R^2 = 0.97$, which is not in perfect agreement with the theoretical results from critical path analysis (Eq. 8). We should, therefore, expect such a discrepancy between the theoretical and experimental exponents (2 vs. 1.774) to result in an overestimation of K_{sat} when the Katz and Thompson model Eq. (8) is used, if Eq. (13) estimates σ_b/σ_w reasonably accurately. This is demonstrated in the following.

We also show K_{sat} as a function of the maximum accessible pore radius r_{max} in Figure 3. As can be seen, K_{sat} is highly correlated to r_{max} with $R^2 = 0.97$. The exponent 3.28 of the power law fit to the experimental data is very different (by a factor of 1.64) from the value that would be expected theoretically, $K_{sat} \propto r_{max}^2 \propto P_a^{-2}$ (see e.g., Eqs. 1, 3 and 14).

315 However, K_{sat} estimation is affected by several factors: tortuosity-connectivity and the
 316 exponent scaling K_{sat} with r_{max} in the bundle of capillary tubes model and constant C_{KT} ,
 317 formation factor F and the exponent scaling K_{sat} with r_c in CPA. Plotting K_{sat} estimated by
 318 the bundle of capillary tubes (Eq. 3) and critical path analysis (Eq. 16) models versus
 319 maximum accessible pore radius r_{max} and fitting a power law to the data gave exponents of
 320 2.66 ($R^2 = 0.99$) and 3.55 ($R^2 = 0.96$), respectively (results not shown). The exponent for
 321 the capillary bundle model is larger than the theoretical value of 2 (see Eq. 3) because λ is
 322 significantly correlated to r_{max} (i.e., $\lambda \propto r_{\text{max}}^{0.81}$ with $R^2 = 0.88$) in the Rawls et al. (1982)
 323 database. However, it is still much smaller than the value of 3.28 derived from the data
 324 (Fig. 3). In contrast, the value obtained from the CPA analysis (i.e. 3.55) is much closer to
 325 the experimental value, which indicates that CPA scales K_{sat} with microscopic soil
 326 characteristics e.g., r_{max} in a physically more appropriate way than the bundle of capillary
 327 tubes model. Figure 4 compares the saturated hydraulic conductivity estimated using CPA
 328 (Eq. 16) and the bundle of capillary tubes (Eq. 3) model with the experimental data from
 329 Rawls et al. (1982). Both critical path analysis and the Nasta et al. (2013) model with $\tau_N =$
 330 0.0138 estimated K_{sat} within a factor of three of the measured conductivity. However, Eq.
 331 (16) with $\text{RMSLE} = 0.315$ provided slightly better estimations than Eq. (3) with $\text{RMSLE} =$
 332 0.320. We should point out that Eq. (3) was previously calibrated using data from the
 333 GRIZZLY database and the parameter τ_N was optimized by Nasta et al. (2013), while Eq.
 334 (16) is not calibrated and has no optimized parameter. Note also that using the same
 335 database, Rawls et al. (1982) found that the Brutsaert (1967) model (Eq. 1) estimated K_{sat}
 336 much less accurately: estimated values were one order of magnitude larger than measured
 337 values. Mishra and Parker (1990) also found errors in the K_{sat} estimates within a factor of

near 15 (see their Fig. 1). Nasta et al. (2013) evaluated the Mishra and Parker (1990) and Guarracino (2007) models using 197 soil samples from the HYPRES databases. They found K_{sat} estimations mainly within a factor of a hundred of measurements (see their Fig. 3).

Fig. 4 shows that critical path analysis overestimated K_{sat} , while the bundle of capillary tubes model of Nasta et al. (2013) mainly underestimated. Interestingly, critical path analysis estimated K_{sat} of fine-textured soils more accurately than that of coarse-textured ones (see Fig. 4). This is in agreement with concepts from critical path analysis, which is an appropriate upscaling method for porous media with broad pore throat-size distributions and negligible surface conduction. However, the term “broad” has not been satisfactorily defined in the literature. Regarding the validity of the critical path analysis approach, Shah and Yortsos (1996) stated that, “The basic argument underlying this theory [critical path analysis] is that because of the large exponent in the pore conductance-pore [throat] radius relationship, $g \sim r^4$, natural porous media, even though moderately disordered in pore [throat] size, possess a wide conductance distribution.” Therefore, even for sandy soils whose pore sizes only span one or two orders of magnitude, one may expect critical path analysis to be reasonably accurate. This, however, needs to be investigated through further experiments.

Friedman and Seaton (1998) evaluated critical path analysis and more specifically the relationship between permeability and electrical conductivity in 3D pore networks of various coordination numbers and lognormal pore throat-size distribution widths. Friedman and Seaton (1998) concluded that, “Comparing the CPA prediction to the computed actual k - EC [permeability-electrical conductivity] relationship reflects a reasonable agreement for

a wide range of average coordination numbers and broadness of the pore [throat] size distribution. The agreement is excellent for low-coordination numbers, likely to be characteristics of many sedimentary rocks and soil textures. However, as the coordination number increases, the CPA estimate diverges from the actual k - EC [permeability-electrical conductivity] relationship, especially for moderate broadness of the pore [throat] size distribution. The CPA argument is expected to be applicable also to pore systems with pore shapes different than cylindrical, as the influence of the pore shape on the k - EC ratio proved to be small by comparing the permeabilities and electrical conductivities of cylindrical and slit-shaped pore networks.” However, further evaluation of critical path analysis e.g., Skaggs (2011) and Ghanbarian et al. (2016) indicated that k estimations from electrical conductivity using cylindrical pores were greater by a factor of 1.35 than those estimated using slit-shaped pores.

We should point out that critical path analysis is valid when surface conduction is negligible. This means most of the electric current flows through water in the pores. In the presence of surface conduction, the percolation threshold for electrical conductivity would be small (if not zero) because pore surfaces contribute effectively to electric current but not to water flow. Consequently, the percolation threshold for electrical flow would be less than that for water flow, in contrast to one key assumption in the Katz and Thompson (1986; 1987) model, that the percolation threshold for the two transport mechanisms is the same.

It is also worth mentioning that the coefficient $C_{KT} = 56.5$ in the Katz and Thompson (1986,1987) model Eq. (8) is only an approximate value, which should vary with different pore geometries. Subsequent analyses by Le Doussal (1989) and Skaggs

(2011) indicated that its value depends not only on pore shape (e.g., cylindrical or slit), but also is a function of the relationship between pore radius r and length l (e.g., $l \propto r$). Both Le Doussal (1989) and Skaggs (2011) suggested that C_{KT} should be ca. 3 to 4 times smaller than the value of 56.5 proposed by Katz and Thompson (1986, 1987). However, in the soils studied here, we found that $C_{KT} = 56.5$ rendered more accurate estimates of K_{sat} than those other smaller values suggested in the literature. Ghanbarian et al. (2016) recently tested the accuracy of alternative permeability models based on critical path analysis in estimating k in tight-gas sandstones and found that the Skaggs (2011) model performed the best.

We also estimated K_{sat} from Eq. (8), using r_c values reported in Table 1, and with electrical conductivity approximated by the Archie law (i.e., $\sigma_b/\sigma_b = \phi^2$). Results (not shown) indicated that Archie's law resulted in substantial overestimation of K_{sat} , with a calculated RMSLE of 0.894.

We should caution that K_{sat} overestimation with Eq. (16) (shown in Fig. 4) might be due to underestimation of the formation factor (or σ_b/σ_w overestimation) with Eq. (13) in which r_{max}^e is *roughly* approximated by $r_c/3$. In fact, further investigation is required to evaluate the validity of such an approximation and Eq. (13) in the estimation of electrical conductivity of soils.

Similar to critical path analysis, the Nasta et al. (2013) model also estimated K_{sat} in fine-textured soils better than in coarse-textured soils (see Fig. 4). However, such a result is not fully consistent with assumptions presumed in the bundle of capillary tubes approach. The pore space of soils is typically heterogeneous and complex and as we mentioned earlier pores are arranged neither in parallel nor in series. Instead, they are tortuous and interconnected, and their cross-sectional area varies (known as converging-diverging

geometry). Compared to clayey soils, sandy soils are more homogeneous, and thus the bundle of capillary tubes models should be more representative and accurate in estimating the hydraulic properties of sandy soils. This is consistent with the Kozeny-Carman equation that can be derived using concepts of a bundle of capillary tubes model (Lake, 1989) and is valid in homogeneous porous media with narrow grain-size distributions. Fatt (1956), Rao et al. (1976), Jarvis (2008) and many others discussed the various shortcomings of the bundle of capillary tubes approach. For more recent detailed discussions, see, for example, Sahimi (2011) and Hunt et al. (2014).

The unexpected better performance of the Nasta et al. (2013) model in fine-textured soils might be due to the empirical parameter τ_N representing the effect of tortuosity and connectivity. Nasta et al. (2013) optimized an average single value ($\tau_N = 0.0138$) using 62 soil samples from the GRIZZLY database, although it is well known that tortuosity and connectivity factors may vary substantially from one soil to another, depending on soil structure, pore space characteristics, dead-end pores, pore connectivity and accessibility, etc. For example, Tuli et al. (2005) assumed that tortuosity and connectivity factors might be integrated into one parameter called tortuosity-connectivity. They further assumed the tortuosity-connectivity coefficient was a function of saturation to some exponent under partially saturated conditions. For the water phase, Tuli et al. (2005) reported a wide range in the exponent values, 0.003-12.22 in undisturbed and 0.00013-0.88 in disturbed soil samples. Although one should not expect a tortuosity-connectivity coefficient under fully saturated conditions to vary over the same wide range as it does when the porous medium is partially saturated, evidence in the literature suggests that its value does nevertheless change with soil texture (sandy soil versus a clayey one).

5. Discussion

K_{sat} estimation by critical path analysis requires knowledge of the critical pore radius, electrical conductivity, pore throat-size distribution, the percolation threshold, and contact angle. In this section, we discuss plausible sources of error in K_{sat} estimation using critical path analysis and Eqs. (8), (14), or (16).

- Critical pore radius r_c

In this study, we estimated the critical pore radius r_c from Eq. (10). Figures 1 and 2 and the high correlations between K_{sat} and r_c as well as between FK_{sat} and r_c show that Eq. (10) estimated the critical pore radius reasonably well. However, rather than using Eq. (10), one may directly determine r_c from the capillary pressure curve, if measured data are available. Katz and Thompson (1986, 1987) suggested that the inflection point on the mercury intrusion capillary pressure curve corresponds to the critical pore diameter and the saturation at which a sample-spanning cluster of mercury first forms. Accurate estimation within a factor of two of measured values of permeability k in sandstones and carbonates by Katz and Thompson (1986; 1987) confirmed that the inflection point on mercury intrusion capillary pressure curves represents the critical pore radius of the porous medium. We, therefore, recommend determining r_c from mercury intrusion capillary pressure or water release characteristic curve, if measured accurately.

- Pore radius corresponding to optimum path for electrical conductivity r_{max}^e

Following Katz and Thompson (1987), we estimated $r_{max}^e = r_c/3$ assuming that the conductance distribution is sufficiently broad. Although a rough approximation, it resulted in reasonably accurate estimation of K_{sat} , as shown in Fig. 4. However, r_{max}^e may be more accurately estimated from the capillary pressure curve. Katz and Thompson (1987) proposed to multiply the volume of mercury injected into the porous medium by either r (if pore length is proportional to its radius, $l \propto r$) or r^2 (if pore length is independent of its radius). Then, the maximum of the resulting curve identifies r_{max}^e and $S(r_{max}^e)$ (see their Fig. 3 and the detailed description given in Katz and Thompson, 1987).

- Electrical conductivity σ_b/σ_w

Although electrical conductivity (or formation factor) is commonly measured on rocks in petroleum engineering, its measurement is less common in soil physics and hydrology. Therefore, we had to estimate electrical conductivity using Eq. (13) and capillary pressure data. If a detailed capillary pressure curve is available, r_c , r_{max}^e and $S(r_{max}^e)$ can be estimated more precisely, as we pointed out above. However, measuring electrical conductivity directly in soils should reduce uncertainties in K_{sat} estimation considerably. We caution that critical path analysis might not be accurate due to the significant contribution of surface conduction to electrical conductivity, especially in clay soils.

- Percolation threshold θ_t

Determination of the exact value of the percolation threshold or critical water content is extremely difficult in complicated systems such as soils. Percolation thresholds depend not only on soil structure, pore space, and pore geometry, but also on fluid characteristics and

the topology and linear size of the porous medium. In this study, we approximated θ_t by the residual water content θ_r , the stagnant amount of water that does not contribute to permeability and fluid flow, as reported in the Rawls et al. (1982) database. Again, if the pressure data were available, one could determine the critical pore radius and the critical volume fraction for percolation from the inflection point, as suggested by Katz and Thompson (1986, 1987). However, since r_c can be directly estimated from the capillary pressure, there is no need to determine θ_t . In addition to capillary pressure curve, the percolation threshold may be determined using other techniques, such as finite-size scaling analysis (see e.g., Rintoul and Torquato, 1997; Priour, 2014), Monte Carlo simulations (see e.g., Baker et al., 2002), and morphological techniques (e.g., Liu and Regenauer-Lieb, 2011).

- Contact angle ω

Estimating the critical pore throat radius r_c and consequently the saturated hydraulic conductivity K_{sat} from the capillary pressure data requires knowledge of the contact angle in the Young-Laplace equation to convert capillary pressure to pore throat radius. In this study, for the sake of simplicity we assumed $\omega = 0$ corresponding to the contact angle of pure water on smooth surfaces. However, in reality, water is typically contaminated and the soil pore-solid interface is rough, unsmooth, sub-critically water repellent and mineralogically heterogeneous. Thus, one should expect the contact angle ω to be greater than zero. Hillel (2004) stated that, “The wetting angle of pure water on clean and smooth mineral surfaces is generally zero, but where the surface is rough or coated with adsorbed

surfactants of a hydrophobic nature, the contact angle, and especially the wetting angle, can be considerably greater than zero and may even exceed 90° .”

Interestingly, if we assume $\omega = 30^\circ$ and $\gamma = 0.0728$ N/m then the constant A in the Young-Laplace equation reduces from 0.149 to 0.126. This results into smaller $r_{\max}$ and r_c values and consequently more accurate K_{sat} estimations (RMSLE = 0.202) via critical path analysis and Eq. 16 (results not shown). Therefore, for more precise estimation of K_{sat} the contact angle should be accurately characterized. Since ω may change from one soil sample to another, one should directly determine its value. For instance, Andrew et al. (2014) measured the contact angle between immiscible fluids at the pore scale through X-ray microtomography. They observed a distribution of contact angles ranging from 35 to 55° in a supercritical CO_2 -brine-carbonate system and also found the contact angle under the imbibition process greater than that under the drainage.

6. Conclusions

In this study, concepts from critical path analysis were applied to estimate the saturated hydraulic conductivity K_{sat} in soils. Theoretical models were developed to estimate the critical pore radius and the electrical conductivity from capillary pressure data. Comparisons with experimental data from the Rawls et al. (1982) database indicated that the proposed model (Eq. 16) estimated K_{sat} within a factor of three of the measured values, although it tended to overestimate. We also estimated K_{sat} using the Nasta et al. (2013) model (Eq. 3 with $\tau_N = 0.0138$) – developed based upon concepts from a bundle of capillary tubes model – which tended to underestimate. The calculated root mean log-

transformed error (RMSLE) showed that our model estimated K_{sat} slightly better than the Nasta et al. (2013) model.

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677	List of symbols
678	A : Young-Laplace equation parameter ($=2\gamma\cos(\omega)$)
679	C_B : Brutsaert constant coefficient
680	C_{KT} : Katz and Thompson constant coefficient
681	C_{MP} : Mishra and Parker constant coefficient
682	C_P : power-law pore throat-size distribution coefficient
683	D : pore space fractal dimension
684	D_T : tortuosity fractal dimension
685	$f(r)$: power-law pore throat-size distribution
686	f_f : fluidity factor ($=\rho g_A/\mu$)
687	F : formation factor
688	g_A : gravitational acceleration
689	g_h : hydraulic conductance
690	g_e : electrical conductance
691	k : single-phase permeability
692	K_{sat} : saturated hydraulic conductivity
693	P_a : air entry pressure
694	P_c : capillary pressure
695	P_{max} : maximum capillary pressure
696	r : pore throat radius
697	r_c : critical pore throat radius
698	r_{min} : smallest accessible pore throat radius
699	r_{max} : largest accessible pore throat radius

700 r_{max}^e : pore throat radius corresponding to optimum path for electrical conductivity

701 s : pore shape factor

702 $S(r_{max}^e)$: fractional volume of connected pore space involving pore throats of size r_{max}^e and

703 greater

704 t : critical scaling exponent from percolation theory

705 β : fractal capillary pressure curve model parameter ($=\phi r_{max}^{3-D}/(r_{max}^{3-D} - r_{min}^{3-D})$)

706 ϕ : porosity

707 γ : surface tension

708 λ : Brooks and Corey pore throat-size distribution index

709 μ : dynamic fluid viscosity

710 ω : air-water contact angle

711 ρ : fluid density

712 σ_b : bulk electrical conductivity

713 σ_w : water electrical conductivity

714 θ : water content

715 θ_r : residual water content

716 θ_c : critical (or threshold) water content

717 τ_N : Nasta et al. tortuosity-connectivity factor

Figure captions

Figure 1. The saturated hydraulic conductivity K_{sat} and electrical conductivity σ_b/σ_w as a function of the critical pore radius r_c for 11 USDA soil texture classes in the Rawls et al. (1982) database.

Figure 2. The product of saturated hydraulic conductivity K_{sat} and electrical conductivity σ_b/σ_w as a function of the critical pore radius r_c for 11 USDA soil texture classes in the Rawls et al. (1982) database.

Figure 3. The saturated hydraulic conductivity K_{sat} as a function of the maximum accessible pore radius r_{max} determined from P_a value given in Table 1 for 11 USDA soil texture classes in the Rawls et al. (1982) database.

Figure 4. The estimated saturated hydraulic conductivity using the critical path analysis Eq. (16) with RMSLE = 0.315 and the Nasta et al. (2013) model Eq. (3) with RMSLE = 0.320 versus the measured one for the Rawls et al. (1982) database including 11 USDA soil texture classes. The red solid and dashed lines represent the 1:1 line and the factor of three boundaries, respectively.

Table 1. Brooks and Corey (1964) model parameters classified by soil texture from Rawls et al. (1982), as well as calculated maximum accessible and critical pore throat radii and electrical conductivity.

Rawls et al. (1982)							This study		
Soil texture	Samples no.	ϕ^*	θ_r	P_a (cm H ₂ O)	λ	K_{sat} (cm/h)	r_{max}^{***} (cm) $\times 10^{-3}$	r_c (cm) $\times 10^{-3}$	σ_b/σ_w (=1/F)
Sand	762	0.437	0.020	15.98	0.694	21	9.3	8.7	0.081
Loamy sand	338	0.437	0.035	20.58	0.553	6.11	7.2	6.2	0.073
Sandy loam	666	0.453	0.041	30.20	0.378	2.59	4.9	3.8	0.060
Loam	383	0.463	0.027	40.12	0.252	1.32	3.7	2.9	0.044
Silt loam	1206	0.501	0.015	50.87	0.234	0.68	2.9	2.6	0.042
Sandy clay loam	498	0.398	0.068	59.41	0.319	0.43	2.5	1.4	0.055
Clay loam	366	0.464	0.075	56.43	0.242	0.23	2.6	1.3	0.055
Silty clay loam	689	0.471	0.040	70.33	0.177	0.15	2.1	1.3	0.039
Sandy clay	45	0.43	0.109	79.48	0.223	0.12	1.9	0.51	0.060
Silty clay	127	0.479	0.056	76.54	0.15	0.09	1.9	0.85	0.040
Clay	291	0.475	0.090	85.60	0.165	0.06	1.7	0.49	0.051

* ϕ : porosity, θ_r : residual water content, P_a : air entry pressure, λ : Brooks-Corey pore throat-size distribution index, K_{sat} : saturated hydraulic conductivity, r_{max} : largest accessible pore throat radius, r_c : critical pore throat radius

** r_{max} was determined from the reported P_a value by Rawls et al. (1982) and the Young-Laplace equation assuming that surface tension $\gamma = 0.072$ (N/m), air-water contact angle $\omega = 0$ and pores are cylindrical (i.e., $r_{max} \approx 0.149/P_a$). r_c was calculated from Eq. (10) and assuming that $\beta = \phi$, $\theta_t = \theta_r$ and $3 - D = \lambda$. σ_b/σ_w was estimated via Eq. (13) given that $3 - D = \lambda$.

Fig. 1.

Fig. 2.

Fig. 3.

Fig. 4.