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Soil water retention curve inflection point: Insight into soil structure from percolation theory

Behzad Ghanbarian[1] | **Todd H. Skaggs**[2]

[1] Porous Media Research Lab, Dep. of Geology, Kansas State Univ., Manhattan, KS 66506, USA

[2] USDA-ARS, United States Salinity Lab., 450 W. Big Springs Rd., Riverside, CA 92507, USA

Correspondence
Behzad Ghanbarian, Porous Media Research Lab, Dep. of Geology, Kansas State Univ., Manhattan, KS 66506, USA.
Email: ghanbarian@ksu.edu

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Abstract

Quantifying soil structure has been a long-standing challenge in soil physics. Among the proposed indices and parameters, slope at the inflection point of soil water retention curve has been widely used. In this short communication, we provide theoretical insights and show that under full saturation conditions, the pore-throat radius at the inflection point (r_{inf}) is equivalent to the critical pore-throat radius within percolation theory. The inflection point, in fact, corresponds to a critical saturation (critical fraction of pore space) at which a sample-spanning cluster forms and a medium starts percolating. We discuss that r_{inf} is theoretically linked to saturated hydraulic conductivity (K_{sat}), in a power-law form within the critical path analysis framework. Using 59 soil samples from the GRIZZLY database, we show that the K_{sat} is correlated to the r_{inf}, although there exists scatter in the data. Interestingly, the experimental exponent 2.219 found from the K_{sat}–r_{inf} data is less than 5% greater than the estimated theoretical value 2.111 determined from the average fractal dimension of the measured soil water retention curves.

1 | INTRODUCTION

Soil structure is among those parameters whose quantifications have been challenging in the soil physics literature. Hillel (2003) stated that, "The arrangement or organization of the particles in the soil (i.e., the internal configuration of the soil matrix) is called *soil structure*." The structure of a soil might be characterized via different proposed parameters or indices and techniques, such as bulk density, aggregate size distribution and stability, gas adsorption, water retention curve, and imaging (Logsdon et al., 2013; Weller et al., 2021). For example, some researchers proposed the mass fractal dimension of aggregate size distribution to characterize soil structure (Chun et al., 2008; Giménez et al., 1998; Hirmas et al., 2013) and quantify its heterogeneity (Young & Crawford, 1991; Young et al., 2001). Another method proposed to evaluate soil structure and aggregate stability is high energy moisture characteristic (Childs, 1942; Levy & Mamedov, 2002). In this method, macroaggregates are either slowly or rapidly wetted under controlled rates and water retention curve is measured with 0-50-cm H_2O tension heads. A structural index is then calculated by quantifying differences between water retention curves measured under slow and fast wetting conditions. For a recent review of soil structure indicators, see Rabot et al. (2018). However, there exists no unique revealing quantity that would enable us to fully evaluate the soil structure (Armindo & Wendroth, 2016).

Saturated hydraulic conductivity (K_{sat}) is, among soil hydraulic properties, substantially affected by soil structure because highly conductive macropores can preferentially carry water (Dexter et al., 2004; Eck et al., 2016; Logsdon et al., 1990; Mossadeghi-Björklund et al., 2016). Ahuja et al. (1984) are among the first who generalized the Kozeny–Carman model by introducing the concept of an effective

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Abbreviations: CPA, critical path analysis; K_{sat}, saturated hydraulic conductivity; r_{inf}, pore-throat radius at the inflection point.

porosity as follows:

$$K_{\text{sat}} = A\phi_{\text{e}}^{\gamma} \tag{1}$$

where K_{sat} is the saturated hydraulic conductivity, A and γ are empirical parameters, and ϕ_{e} is the effective porosity. Brutsaert (1967) recommended that ϕ_{e} is approximately equal to ϕ minus the soil field capacity, commonly determined from the water content at 33 kPa suction head. In another study, Deeks et al. (2004) defined the effective porosity as the porosity of pores of size 50 μm and greater (suction head of 6 kPa and smaller). They did not find any correlation between total porosity and K_{sat} at the 95% confidence level. However, a positive relationship between effective porosity and saturated conductivity was found with $R^2 = .56$. Years later, Han et al. (2008) proposed $\phi_{\text{e}} = \phi - \theta_{\text{inf}}$ in which θ_{inf} is the water content at the inflection point of soil water retention curve.

Dexter (2004) stated that for soil drying between the saturation and the inflection point, it is mainly structural pores that are emptying. However, for soil drying below the inflection point, it is mainly textural pores that are evacuating. He proposed the slope at the inflection point, s_{inf}, as an index of soil physical quality and showed that it would be a better indicator of soil rootability than bulk density. Dexter's approach has been widely applied in the literature to quantify soil structures (Al-Kayssi, 2021; Dexter & Czyż, 2007; Farahani et al., 2019; Shekofteh & Masoudi, 2019; Silva et al., 2011).

Based on Dexter's analysis, one can determine the water saturation ($S_{\text{winf}} = \theta_{\text{inf}}/\phi$) and suction head ($h_{\text{inf}}$) and at the inflection point from the van Genuchten water retention model parameters (i.e., a, m, n, and S_{wr}) as follows:

$$S_{\text{winf}} = \left(1 - S_{\text{wr}}\right)\left[1 + \frac{1}{m}\right]^{-m} + S_{\text{wr}} \tag{2}$$

$$h_{\text{inf}} = (1/\alpha)\,(1/m)^{\frac{1}{n}} \tag{3}$$

where S_{wr} is the residual water saturation and a, m, and n are shape parameters. Dexter (2004) proposed $s_{\text{inf}} = 0.035$ as a threshold separating good structural soils ($s_{\text{inf}} > 0.035$) from poor structural soils ($s_{\text{inf}} < 0.035$).

The inflection point of the soil water retention curve and its slope have been broadly applied in the soil physics literature to evaluate the structure of soils. The effective porosity, defined as total porosity minus the water content at the inflection, has also been used to estimate the K_{sat}. The main objective of this short communication is to provide theoretical insight from percolation theory into the inflection point of the water retention curve. We demonstrate that the inflection point corresponds to the critical pore-throat radius at which a sample-spanning cluster forms and a fluid percolates. Using the critical path analysis framework and 59 soil samples from the GRIZZLY database, we experimentally show that the pore-throat radius at the inflection point (r_{inf}) is correlated to the K_{sat}.

Core Ideas

- Theory shows that the retention inflection point can be an indicator of soil structure.
- Measured K_{sat} is correlated to r_{inf}.
- Analyses of 59 soils produced an experimental scaling exponent of 2.219.
- The observed exponent 2.219 was within 5% of the estimated theoretical value 2.111.

2 | PERCOLATION THEORY

Percolation theory, introduced in its present form by Broadbent and Hammersley (1957), provides a theoretical framework from statistical physics to address the effect of interconnectivity on fluid flow in heterogeneous media such as soils and rocks. Broadbent and Hammersley (1957) studied plant disease spreading in an orchard with trees located at the intersections of a square lattice. As expected, the probability of spreading a disease decreases as the distance between aligned trees increases. Eventually the distance between trees would reach a critical value above which the disease cannot spread through the orchard (Feder, 1988).

Critical path analysis (CPA) is a promising technique from percolation theory (Ambegaokar et al., 1971; Pollak, 1972). Based on the CPA, flow through a soil is controlled by pore throats whose sizes are greater than some critical value (r_{c}; critical pore-throat radius), the smallest pore-throat radius required to form a conducting sample-spanning cluster (Hunt, 2001; Hunt et al., 2014; Skaggs, 2003). Within the CPA framework, pore throats with radii greater than the critical pore-throat radius should significantly contribute to fluid flow.

Katz and Thompson (1986, 1987) argued that, under full saturation conditions, the pore-throat size corresponding to the inflection point of mercury intrusion porosimetry curve would be the best approximation for the critical pore-throat radius, r_{c}. From a mathematical point of view, the mode of the logarithmic saturation distribution function $\{f_v[\ln(h)] = dS_{\text{w}}/d\ln(h)\}$; (see Equation 4.28 in [Sahimi, 2011]), corresponds to the inflection point on the water retention curve, and thus one can set $r_{\text{c}} = r_{\text{inf}}$. We demonstrate this in Figure 1, in which the water retention curve of a loamy sand soil with residual water saturation $S_{\text{wr}} = 0.14$, $a = 0.124$ (cm^{-1}), $n = 2.28$, $m = 0.56$ (Carsel & Parrish, 1988) and

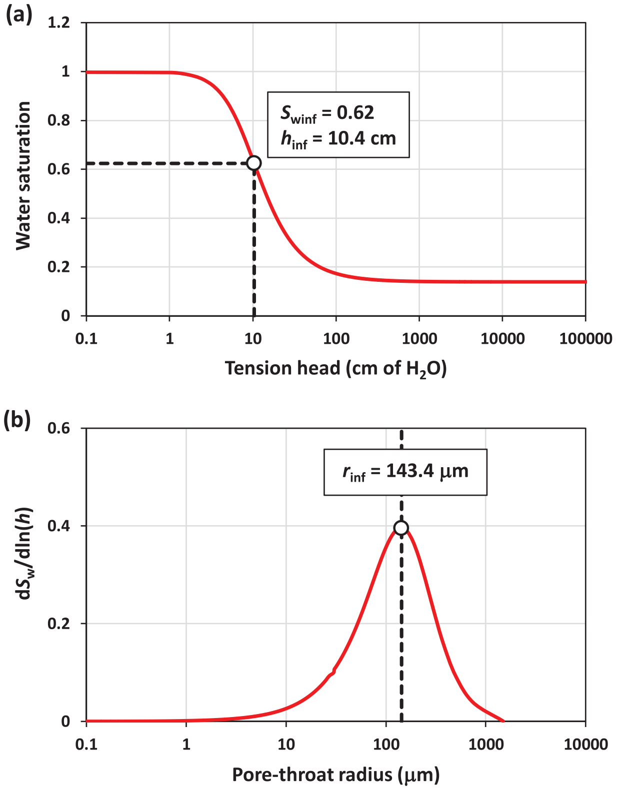

FIGURE 1 (a) The soil water retention curve of a loamy sand soil generated using the van Genuchten (1980) model with parameters S_{wr} = 0.14, $a = 0.124$ (cm^{-1}), $n = 2.28$, $m = 0.56$ (Carsel & Parrish, 1988); and (b) the corresponding logarithmic saturation distribution function, $f_v[\ln(h)]$. Water saturation and tension head at the inflection point determined from Equations 2 and 3 are equal to 0.62 and 10.4 cm H_2O, respectively. r_{inf} = 143.4 μm, determined from h_{inf} = 10.4 cm H_2O using the Young–Laplace equation, matches the mode of the pore-throat radius distribution. h_{inf}, suction head corresponding to the inflection point; $r_{\text{inf},}$ radius of the inflection point; S_{winf}, water saturation at the inflection point.

its inflection point as well as the corresponding logarithmic saturation distribution function and its mode. We should note that to be consistent with Dexter (2004), we determined the $f_v[\ln(h)]$ by plotting the $dS_w/d\ln(h)$ vs. the pore-throat radius (Figure 1b).

Katz and Thompson (1986, 1987) proposed that the K_{sat} is a power–law function of the critical pore-throat radius (= r_{inf}) as follows:

$$K_{\text{sat}} = \left(\sigma_b/\sigma_w\right)\left(r_{\text{inf}}^2/c\right) \propto r_{\text{inf}}^{\beta} \tag{4}$$

where σ_b and σ_w are bulk and water electrical conductivities, respectively, and c is a constant coefficient. For different values of c proposed in the literature, see Ghanbarian et al. (2016). The exponent β would be close to 2 if the effect of bulk electrical conductivity on the K_{sat} is negligible. Otherwise, its value can be determined from the pore space fractal dimension (Skaggs, 2011), as we explain in the following. Although the relationships $K_{\text{sat}} = (\sigma_b/\sigma_w)(r_{\text{inf}}^2/c)$ (Katz & Thompson, 1986) and $K_{\text{sat}} \propto r_{\text{inf}}^{\beta}$ (Skaggs, 2011) were previously proposed, in the latter the estimation of the exponent β has not been yet evaluated experimentally via soil samples.

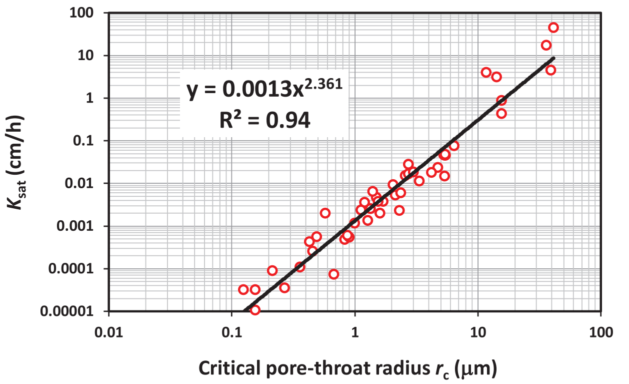

FIGURE 2 The saturated hydraulic conductivity against the critical pore-throat radius corresponding to the inflection point of mercury intrusion porosimetry curve. The Katz and Thompson (1986, 1987) dataset consists of 48 rock samples from different formations. The power law shows the fit to the rock samples. Note that $r_c = r_{\text{inf}}$. K_{sat}, saturated hydraulic conductivity

Using 48 rock samples collected from different formations, Katz and Thompson (1986, 1987) determined the inflection point from mercury intrusion porosimetry data and found that the K_{sat} was highly correlated to the critical pore-throat radius with $R^2 = .94$ (Figure 2). Recall that $r_c = r_{\text{inf}}$. Similar correlations were also reported by Ghanbarian et al. (2016) and Nishiyama and Yokoyama (2017) for rock samples. However, such a correlation is still required to be investigated for soils.

3 | COMPARISON WITH EXPERIMENTS

The GRIZZLY database consists of 660 soil samples from different parts of the world (e.g., the United States, Hungary, Spain, the Netherlands, France, Australia, and Senegal [Haverkamp et al., 1998]). For all samples, the water retention curves are available with at least eight retention points. Most samples within the GRIZZLY database are undisturbed and taken from the field. Part of the GRIZZLY database shared with us by Dr. Randel Haverkamp includes 59 samples from nine different soil textures (i.e., sand, sandy loam, loamy sand, loam, silty loam, silty clay loam, silty clay, clay loam, and clay). This dataset, as received, consisted of bulk density, particle density, organic matter, porosity, textural and water retention data, and K_{sat}. The textural data included the particle-size distribution (sand, silt, and clay contents) as well as the optimized parameters of the van Genuchten model adapted for particle size distribution (see Equation 4 in Haverkamp et al. [2005]). The water retention data were received as fitted

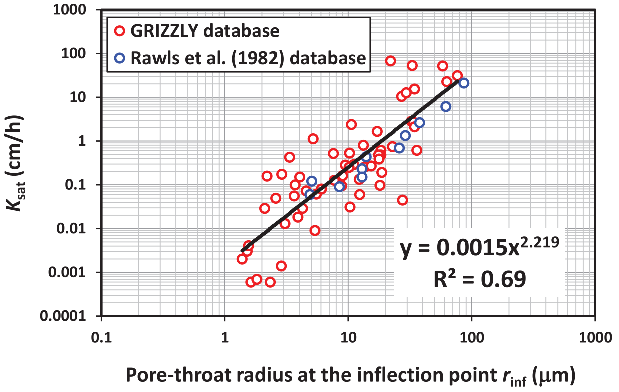

FIGURE 3 The saturated hydraulic conductivity against the pore-throat radius at the inflection point (r_{inf}). The GRIZZLY dataset consists of 59 soil samples from nine different soil textures. The power law shows the fit to the soil samples of GRIZZLY database. Note that $r_{\mathrm{c}} = r_{\mathrm{inf}}$. The data from Rawls et al. (1982) database analyzed by Ghanbarian et al. (2017) are also presented to show consistency in slopes. K_{sat}, saturated hydraulic conductivity; r_{inf}, pore-throat radius at the inflection point

Brooks and Corey (1964) and van Genuchten (1980) model parameters.

We used the optimized parameters of the van Genuchten (1980) water retention model to determine the tension head at the inflection point, h_{inf}, via Equation 3. We then calculated the value of the r_{inf} using the Young–Laplace equation with zero contact angle and 0.0728 N m^{-1} air–water interfacial tension (i.e., $r_{\mathrm{inf}} = 0.149/h_{\mathrm{inf}}$) (Brutsaert, 1966).

Figure 3 shows the K_{sat} vs. the r_{inf} ($r_{\mathrm{inf}} = r_{\mathrm{c}}$). We found that a power law with $R^2 = .69$ fitted the experimental data from the GRIZZLY dataset reasonably well. Figure 3 looks more scattered compared with Figure 2. This might be because the samples within the GRIZZLY dataset used here represent a wide range of soils of diverse properties from different areas under various conditions. Similar correlation between r_{inf} and K_{sat} was also reported by Ghanbarian et al. (2017) on soils. However, in that study, Ghanbarian et al. (2017) used the average K_{sat} values for 11 soil textures tabulated by Rawls et al. (1982). Ghanbarian et al. (2017) also estimated the value of r_{c} from the reported Brooks and Corey (1964) model parameters, because the original soil water retention data were not available. For the sake of comparison, we also show the K_{sat} and the critical pore-throat radius from Rawls et al. (1982) in Figure 3. As can be seen, the data of Rawls et al. (1982) are in good agreement with the GRIZZLY measurements.

Another reason for the scatter in the $K_{\mathrm{sat}} - r_{\mathrm{inf}}$ data shown in Figure 3 is that the relationship $K_{\mathrm{sat}} \propto r_{\mathrm{inf}}^{\beta}$ ignores the effect of the constant coefficient c and the electrical conductivity $\sigma_{\mathrm{b}}/\sigma_{\mathrm{w}}$ on the K_{sat}. Depending on pore geometry, the constant coefficient c may take a value between 32 and 226 spanning by a factor of 7 (see Table 1 in Ghanbarian et al. [2016]). Therefore, one should not expect one single value (e.g., $c = 32$) to be valid for all types of soils. The value of σ_b/σ_w may also vary over a relatively wide range depending on soil porosity and tortuosity (Ghanbarian et al., 2013, 2014); thus, its value changes from one soil sample to another.

As stated earlier, the exponent β in Equation 3 can be theoretically calculated from the pore space fractal dimension D. For hydraulic flow and cylindrical pore throats, Skaggs (2011) proposed (see his Equation 15):

$$\beta = 4 - \mathrm{y}D \tag{5}$$

where $y = 0.74$ in three dimensions is a universal exponent (Skaggs, 2011), and $-\infty < D < 3$ is the pore space fractal dimension (Ghanbarian-Alavijeh & Hunt, 2012a). The value of D can be determined from the water retention curve (Bird et al., 2000; Ghanbarian-Alavijeh & Hunt, 2012b) or approximated from the clay content (Ghanbarian-Alavijeh & Millán, 2009). Because the original water retention data from the GRIZZLY database are not available, we estimated D from the reported pore-size distribution index λ of the Brooks and Corey (1964) model using the relationship $D = 3 - \lambda$ (Tyler & Wheatcraft, 1990). We calculated the average λ value (i.e., 0.447) and found the average D value equal to 2.553. This D value led to $\beta = 2.111$, which is less than 5% smaller than the exponent 2.219 that was experimentally found by analyzing the GRIZZLY database (Figure 3).

Recently, Armindo and Wendroth (2016) evaluated various soil quality indices such as mean, median and mode pore diameters, macroporosity, field capacity, absolute water retention energy, and absolute aeration energy. Interestingly, they reported that r_{inf} (denoted by d_{mode} in their study) was not correlated to bulk density or total porosity and stated that this soil quality index provides valuable information about soil physical quality that is not revealed through bulk density or total porosity. Evidence from Armindo and Wendroth (2016) and Dexter (2004) along with theoretical insights from percolation theory clearly indicate that the inflection point on the water retention curve represents a key parameter to quantify soil structures.

In Equation 4, K_{sat} is substantially influenced by the soil structure (Eck et al., 2016; Logsdon et al., 1990). Not only is r_{inf} linked to the soil structure as recommended (Armindo & Wendroth, 2016; Dexter, 2004), but also D captures the heterogeneity of pore space. Ghanbarian-Alavijeh and Millán (2009) analyzed 172 soil samples from five different databases including the GRIZZLY dataset used here and found an inverse relationship between the fractal dimension, D, and the slope at the inflection point of the water retention curve, s_{inf}, with $R^2 = .83$ (i.e., $s_{\mathrm{inf}} = 1.054{-}0.349D$). The value $s_{\mathrm{inf}} = 0.035$ proposed by Dexter (2004) as the threshold corresponds to $D = 2.92$. Dexter (2004) also claimed that $s_{\mathrm{inf}} = 0.02$ represents very poor soil structural quality, which corresponds to soils with $D \geq 2.96$ near the space filling conditions ($D \rightarrow 3$). $D = 3$ represents the dimension (Euclidean dimension) of a solid cube. Because β is a function of fractal dimension D (Equation 4) and D is experimentally linked to s_{inf} (Ghanbarian-Alavijeh & Millan, 2009), one should expect a relationship between β and s_{inf}.

We should point out that the r_{inf} should be determined using the mercury intrusion porosimetry method. Although mercury injection tests were previously used to capture pore sizes and their distribution in soils (Nagpal et al., 1972; Olson, 1985; Pagliai et al., 2004), the soil water retention method is still routinely utilized to find the distribution of pore throats in soil science. Bartoli et al. (1999) measured mercury intrusion porosimetry curve on six silty soils and linked it to soil structure quantified by image analysis. They found that mercury porosimetry data provided a useful link between microscale soil structure and macroscale transport in soils and resulted in new interpretations beyond traditional approaches of characterizing soil structures.

4 | CONCLUSION

In the literature, various parameters and indices have been proposed to quantify the structure of soils. Although the slope of soil water retention at the inflection point has been widely used as a soil structure indicator in literature, there is no unique revealing quantity for its full evaluation. In this short communication, we provided theoretical insights from percolation theory and critical path analysis about the inflection point of water retention curve and its link to the K_{sat}, one of the soil hydraulic properties substantially influenced by the soil structure. By analyzing 59 soil samples from the GRIZZLY database, we showed that the K_{sat} was correlated to the pore-throat radius corresponding to the inflection point ($K_{\mathrm{sat}} \propto r_{\mathrm{inf}}^{2.219}$ with $R^2 = .69$). We argued that the scatter in the K_{sat} and r_{inf} data was probably because the analyzed samples represented a wide range of soils. We also showed that the experimental exponent 2.219 could be theoretically estimated from the fractal dimension D, if measured. We found a reasonable agreement between the experimental and theoretical exponents (2.219 vs. 2.111). Our theoretical insights indicated that the inflection point of water retention curve can be used to quantify the structure of soils.

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AUTHOR CONTRIBUTIONS

Behzad Ghanbarian: Conceptualization; Data curation; Formal analysis; Investigation; Methodology; Validation; Visualization; Writing – original draft. Todd H. Skaggs: Conceptualization; Methodology; Validation; Writing – original draft.

CONFLICT OF INTEREST

Authors declare no conflicts of interest.

DATA AVAILABILITY STATEMENT

The data used in this study are available at: http://www.hydroshare.org/resource/8577a98022c4414ca0404ffcafbe0c3a

ORCID

Behzad Ghanbarian https://orcid.org/0000-0002-7002-4193

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