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Gas diffusion-derived tortuosity governs saturated hydraulic conductivity in sandy soils

Federico Masís-Meléndez [a,b,*], T.K.K. Chamindu Deepagoda [c], Lis Wollesen de Jonge [a], Markus Tuller [d], Per Moldrup [c]

[a] Aarhus University, Faculty of Science and Technology, Department of Agroecology, Blichers Alle 20, P.O. Box 50, DK-8830 Tjele, Denmark
[b] Costa Rica Institute of Technology (TEC), Cartago 30101, Costa Rica
[c] Aalborg University, Dept. of Civil Engineering, Sohngaardsholmsvej 57, DK-9000 Aalborg, Denmark
[d] The University of Arizona, Dept. of Soil, Water and Environmental Science, 1177 E. 4th Street, Tucson, AZ 85721, USA

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SUMMARY

The saturated hydraulic conductivity (K_{sat}) is an essential effective parameter for the development of improved distributed hydrological models and area-differentiated risk assessment of chemical leaching. Basic soil properties such as the particle size distribution or, more recently, air permeability are commonly used to estimate K_{sat}. Conversely, links to soil gas diffusivity (D_p/D_o) have not been fully explored even though gas diffusivity is intimately linked to the connectivity and tortuosity of the soil pore network. Based on measurements for a coarse sandy soil, potential relationships between K_{sat} and D_p/D_o were investigated. A total of 84 undisturbed soil cores were extracted from the topsoil of a field site, and D_p/D_o and K_{sat} were measured in the laboratory. Water-induced and solids-induced tortuosity factors were obtained by applying a two-parameter D_p/D_o model to measured data, and subsequently linked to the cementation exponent of the well-established Revil and Cathles predictive model for saturated hydraulic conductivity. Furthermore, a two-parameter model, analogue to the Kozeny–Carman equation, was developed for the $K_{sat} - D_p/D_o$ relationship. All analyses implied strong and fundamental relationships between K_{sat} and D_p/D_o.

1. Introduction

The saturated hydraulic conductivity (K_{sat}) is a measure for the maximum water transmission capacity of a saturated porous medium (Mallants et al., 1997). It has been widely used as a constant in hydrological transport models to assess the risk of chemical leaching, to characterize water infiltration, and to model surface runoff. However, a large number of samples is necessary to characterize the spatial and temporal variability of K_{sat} in natural soils (Amer et al., 2009). As a consequence, measurement of K_{sat} is expensive and labor intensive (Ahuja et al., 1989). Therefore, it is usually easier to estimate K_{sat} from easy-to-measure basic soil properties such as porosity (ϕ) or particle diameter (d_{10}, d_{50}, d_{80}), the latter being used in many recent studies (e.g., Rosas et al., 2013; Salarashayeri and Siosemarde, 2012). Efforts to predict saturated hydraulic conductivity based on basic soil structural properties date back many years. The idea is extremely attractive because of the obvious connection between water flow and the distribution of solids and pores in the soil medium. As a result, many theoretical and empirical predictive models linking K_{sat} to basic soil properties were developed over the last few decades. Among these, the generalized Kozeny–Carman (K–C) equation (Scheidegger, 1957) with its empirical parameters determined from measured data via nonlinear regression has proven useful for many applications. Improved K–C type models have been successfully applied to homogeneous porous media, for example shale sands, clay-free sands, and technosands (Arthur et al., 2012b; Arya et al., 2010; Revil and Cathles, 1999). Alternatively, the application of pedotransfer functions for estimating K_{sat} from available measured data (e.g., grain size distribution, texture, porosity, organic matter content, surface area, and fractals) has gained widespread interest in recent years (e.g., Gimenez et al., 1997; Nemes et al., 2005; Puckett et al., 1985).

While there is a difference between gas and liquid flow in porous media (i.e., gas is compressible and susceptible to the Klinkenberg gas slippage effect) (Wu et al., 1998), linking K_{sat} to

* Corresponding author at: Aarhus University, Faculty of Science and Technology, Department of Agroecology, Blichers Alle 20, P.O. Box 50, DK-8830 Tjele, Denmark. Tel.: +45 87154779.

E-mail address: Federico.Masis@agrsci.dk (F. Masís-Meléndez).

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other transport parameters seems to be a promising avenue because of the analogies between transmission of water, air, or electric current in porous media. For example, air permeability (k_a), which can be measured relatively fast and easy, is a key parameter representing soil structure and pore network characteristics in macropore-dominated flow domains and therefore exhibits a strong correlation to saturated and unsaturated hydraulic conductivities (Kawamoto et al., 2006). Evidence of this functional link between water and convective air flows was well documented during the last two decades (e.g., Blackwell et al., 1990; Iversen et al., 2001; Loll et al., 1999; Poulsen et al., 1999), especially for well-structured soils (e.g., Blackwell et al., 1990; Granovsky and McCoy, 1997; Millington and Quirk, 1961). However, caution is required when using k_a measurements for prediction of K_{sat} under varying field conditions. While air permeability is essentially a structure-dominated parameter, predominantly controlled by the largest structural pores present in the soil (e.g., earthworm burrows, freezing/thawing or shrinkage cracks), K_{sat} is additionally controlled by smaller and more abundant textural pores created by larger soil particles. This is particularly the case in sandy soils characterized by uniform, coarse-grained particles.

Soil gas diffusivity (D_p/D_o), where D_p and D_o are the gas diffusion coefficients in soil and free air, respectively, is another important gas transport parameter representing pore tortuosity and connectivity, and hence has potential for prediction of soil hydraulic properties. Characteristically, D_p/D_o is not a strongly structure-dependent parameter like k_a, but it mainly depends on air-filled pores at a given matric potential. Therefore it is a useful parameter for predicting transport properties in uniform, coarse-grained sandy soils. Furthermore, accurate models are currently available for predicting D_p/D_o from basic soil physical properties, such as air-filled porosity (e.g., Moldrup et al., 2013, 2000), matric potential (ψ) (e.g., Chamindu Deepagoda et al., 2012), and bulk density (e.g., Chamindu Deepagoda et al., 2011, 2012).

The main objective of the present study was to examine potential relationships between D_p/D_o and K_{sat} based on measurements for a large number of intact soil samples extracted from a homogeneous coarse sandy field with a fine particle content (clay, silt, organic matter) of less than 10% on mass basis. Moreover, we evaluated the contribution of basic pore-network tortuosity (derived from D_p/D_o) to the overall cementation exponent used in Revil and Cathles (1999) type K_{sat} predictive models and applied the findings to formulate and calibrate a generalized two-parameter model for D_p/D_o predictions. Finally, we established more accurate capabilities for prediction of K_{sat} exploiting intimate links between D_p/D_o and K_{sat}.

2. Materials and methods

2.1. Sampling site, soils and particle size distribution

The sampling site located in Jyndevad (UTM 32U 507705mE 6082965mN) in southern Denmark (Fig. 1) covers a cultivated area of about 1.6 ha (150 × 105 m) and exhibits a slope of 0–1%. In this particular area, there are abundant Quaternary deposits of late glacial freshwater sands (Lindhardt et al., 2001). The soil at the site is classified as coarse-grained sand and has a natural organic matter gradient with organic matter content increasing from north to south.

To measure K_{sat} and D_p/D_o, undisturbed soil cores were extracted from 8 to 12 cm depth by gently tapping stainless steel sampling cylinders (6.05-cm I.D., 3.48-cm height, 100 cm^3 volume) into the soil on a grid of 15 × 15 m (in total 88 grid points; Fig. 1). The measured physical soil properties are listed in Table 1. Note that four of the core samples were damaged due to improper handling; hence we ended up with a total of 84 samples.

2.2. Texture and particle size distribution

In addition, bulk soil was collected at all grid points, air-dried, sieved through a 2-mm sieve, and then used for analysis of particle size distribution and texture. Soil texture was determined with a combination of wet-sieving and hydrometer methods (Arthur et al., 2012a).

To obtain characteristic particle size diameters (d_{50}, d_{63}) applied in the Revil and Cathles (R–C) and the modified R–C equations, samples of 200 g bulk soil were mechanically dispersed for 4 min at a speed setting of 100 in a Retsch KS 1000 sieve tower (Retsch GmbH, Haan, Germany) and further sieved using six size limits (90, 180, 250, 500, 1000 and 2000 μm). Data of cumulative mass of material passed at 4 min (g) and the respective size limits (μm) were plotted to find d and β parameters from the best-fit Rosin and Rammler (1933) cumulative particle size distribution curve (e.g., Fig. 1b). The d_{50} and d_{63} values were determined from the cumulative 50 and 63 percentiles, respectively.

2.3. Soil organic carbon content

Total organic carbon (TOC, kg kg^{-1}) was determined for ball-milled and previously air-dried subsamples with a FLASH 2000 organic elemental analyzer coupled to a thermal conductivity detector (Thermo Fisher Scientific, Waltham, MA, USA). Each sample was also tested for CO_3–C content (Arthur et al., 2012a).

Organic matter (OM) content was calculated by multiplying the soil total carbon content (kg kg^{-1}) with the conventional conversion factor 1.724 (Rasmussen and Collins, 1991).

2.4. Volumetric water content and air filled porosity

For soil water characteristic measurements the soil cores were slowly saturated with tap water from the bottom and subsequently drained to the intended matric potentials utilizing a sand box (−30 and −100 cm H_2O), hanging water column (−300 cm H_2O) and the Richards pressure plate apparatus (ψ = −1000 cm H_2O) (Tuller and Or, 2004). At each measurement step, the volumetric water content (θ, $cm^3\ cm^{-3}$) was calculated by multiplying gravimetric water content with soil bulk density and dividing by the density of the tap water. Subsequently, the air filled porosity (ε, $cm^3\ cm^{-3}$) was calculated by subtracting the volumetric water content equivalent to the water-filled void space from the total porosity (ϕ, $cm^3\ cm^{-3}$) at each given matric potential. The corresponding data for total porosity were derived from soil bulk density measurements (g cm^{-3}), determined by oven-drying the soil cores for 24 h at 105 °C, to obtain the total dry matter content.

2.5. Gas diffusivity

The gas diffusivity (D_p/D_o) was measured on the same cores that were used for the soil water characteristic and K_{sat} measurements, at the same four matric potentials (ψ = −30, −100, −300 and −1000 cm H_2O). Soil gas diffusivity was measured at 20 °C by means of a non-steady-state method first proposed by Taylor (1949) and further developed by Schjønning (1985). The soil cores were first attached to the gas-tight chamber and then purged with nitrogen to remove all oxygen from the chamber. A Figaro KE-12 oxygen sensor (Figaro Engineering Inc., Osaka, Japan) mounted at the top of the chamber was employed to continuously (2 min intervals) monitor changes in oxygen concentration. The soil oxygen diffusion coefficient (D_p) was calculated following the Currie (1960) method. The oxygen diffusion coefficient in free air (D_o) is 0.205 cm^2 air s^{-1} at 20 °C. For a detailed description of applied measurement procedure readers are referred to Schjønning et al. (2013).