The gas-diffusivity-based Buckingham tortuosity factor from pF 1 to 6.91 as a soil structure fingerprint

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Abstract

Subsurface migration of greenhouse gases and other gaseous phase contaminants is predominantly controlled by soil gas diffusion coefficient (D_p) and its variations with soil-air content (ε) and soil moisture (or potential) status. Buckingham (1904) stated that D_p is proportional to ε^X with X characterizing the tortuosity and connectivity of air-filled pore space. In the Buckingham model, as well as many subsequent power-law models, the tortuosity factor, X, is assumed to be constant for a given soil irrespective of its soil potential status. This study shows a marked variation of X with soil matric potential (ψ) given by pF [= log (-ψ, cm H_2O)] ranging from 1 to 6.91 for a range of structureless and, in particular, aggregated/structured soils. The X-pF function for aggregated soils showed a monotonic decrease with increasing pF up to pF 3 near which inter-aggregate pores are completely drained, and an increase from pF 3 to pF 6.91 with the draining of intraaggregate pores. Two X(pF) expressions are proposed in order to independently describe the inter-aggregate tortuosity viz X, (for pF ≤ 3) and intra-aggregate tortuosity, X^*, (for 3 ≤ pF ≤ 6.91), These expressions not only yielded better predictions of D_p but also provided useful soil structure fingerprints across a wide range of soil types.

Key Words

Power-law model, pore tortuosity factor, soil matric potential and pF, aggregated soils.

Introduction

Growing concerns over the global, regional and local environmental problems such as global warming, climate shifts and indoor/outdoor air pollution emphasize the need of accurate prediction of gas transport parameters in soils. Gas diffusion coefficient in soil (D_p) is a key parameter controlling emission of greenhouse gases (Smith *et al.* 2003) and migration of volatile organic compounds from contaminated sites (Jury *et al.* 1990). Soil gas diffusivity (D_p/D_o, where D_o is the gas diffusion coefficient in free air), and its variation with air-filled porosity at differing soil moisture conditions, has been studied for more than a century after the pioneering work of Buckingham (1904). The aim is a universal expression for $D_p(\varepsilon)/D_o$. Buckingham (1904) suggested a power-law model to describe the relation between gas diffusivity (D_p/D_o) and air-filled porosity (ε) as follows:

$$D_p/D_o = \varepsilon^X \tag{1}$$

where X is the power-law exponent which can be calculated from measured $D_p(\varepsilon)/D_o$ values by

$$X = \frac{\log(D_p/D_o)}{\log(\varepsilon)} \tag{2}$$

Buckingham's model, as well as many similar power-law models subsequently developed for dry porous media, assumed X as a constant value, for example, $X = 2$ (Buckingham, 1904), $X = 1.5$ (Marshall 1959) , and $X = 1.33$ (Millington 1959). The idea of non constant X also emerged later, for example Currie (1960) interpreted X as a particle shape factor and material-dependent whereas Shimamura (1992) found X for repacked dry soils to vary with percentage of finer particles. Further, Moldrup *et al.* (1999; 2000) observed X to be soil water characteristic-dependant and proposed $X(b)$ functions in terms of a pore size distribution index ,b. In wet porous media, additional water-induced discontinuity due to water blockage effects further enhances tortuosity. Thorbjørn *et al.* (2008) considered solids-induced tortuosity and water-induced discontinuity separately to yield

$$X = X_{\mathrm{dry}} + f(\theta) \qquad (3)$$

where X_{dry} is solid-induced tortuosity and $f(\theta)$ is a function of volumetric water content (θ) to account for water-induced discontinuity.

Only few studies, however, have considered the variation of X with soil matric potential (ψ) or pF [= log ($-\psi$, cm H_2O)]. For example, for well-aggregated volcanic ash soils (Andisols), Resurreccion *et al.* (2008) proposed the following X–pF relationship:

$$X = \mathrm{B} + \mathrm{A}_1 \left| \mathrm{pF} - \mathrm{pF}^* \right|^{\mathrm{A}2} \qquad (4)$$

where A_1, A_2, B, and pF* are curve-fitting constants.

Our main objectives of this study were to (i) examine the variation of gas diffusivity-based Buckingham tortuosity factor, X, with soil water matric potential (given by pF) ranging from wet (pF 1) to completely dry (pF 6.91) conditions, particularly for aggregated soils, in order to derive simple and working expressions for X(pF) and (ii) observe the applicability of X-pF characteristics as soil functional structure fingerprints.

Methods

We used soil gas diffusivity data from Ozosawa (1998) for ten repacked soils, with varying bulk densities/total porosities: three Andisols, four lysimeter soils, and three Gray-Lowland soils. With the exception of one lysimeter soil (Lysimeter 4), all have aggregated soil structures. Gas diffusivity measurements were carried out at different matric potentials ranging from pF 1 to pF 6.91 (oven dry). 100-cm^3 repacked samples were first saturated and drained stepwise to desired matric potentials. For gas diffusivity measurements, the experimental set-up and procedure outlined by Schjønning (1985) was used. For sampling, preparation and soil characteristics, we refer to Ozosawa (1998).

Results

Figure 1a shows the variation of tortuosity factor (X), Eq. (2), as a function of pF for the selected soils. The X values initially showed monotonic decrease with increasing pF due to draining of inter-aggregate pores reaching a minimum value at around pF 3.0 (shown by dotted line) near which inter-aggregate pores were assumed to have completely drained (Resurreccion *et al.* 2008). During subsequent draining from pF 3 to 6.91, when the aggregates themselves were draining, all soils (except for lysimeter 4 soil) showed an increase in X because the diffusion now also occurred in more tortuous air-filled pores within the aggregates which were remote and separate from main diffusion pathways. These observations are in good agreement with the results of previous studies (eg., Resurreccion *et al.* 2008; Currie 1961) and further support the concept that the transition from inter- to intra-aggregate pores occur around -1000 cm H_2O (pF 3) for aggregated porous media. Lysimeter 4 soil, on the other hand, consisted mainly of non-aggregated dune sand with uniform coarse sand particles which probably explain its different behaviour compared to the other aggregated soils.

Note here that for pF > 3, the tortuosity factor (X) shown in Figure 1a is a lump factor representing both inter- and intra-aggregate tortuosity. For the purpose of analysis, we separated the inter-aggregate tortuosity, X, as described by Eq.(2), from intra-aggregate tortuosity, denoted by X^*, which can be written as,

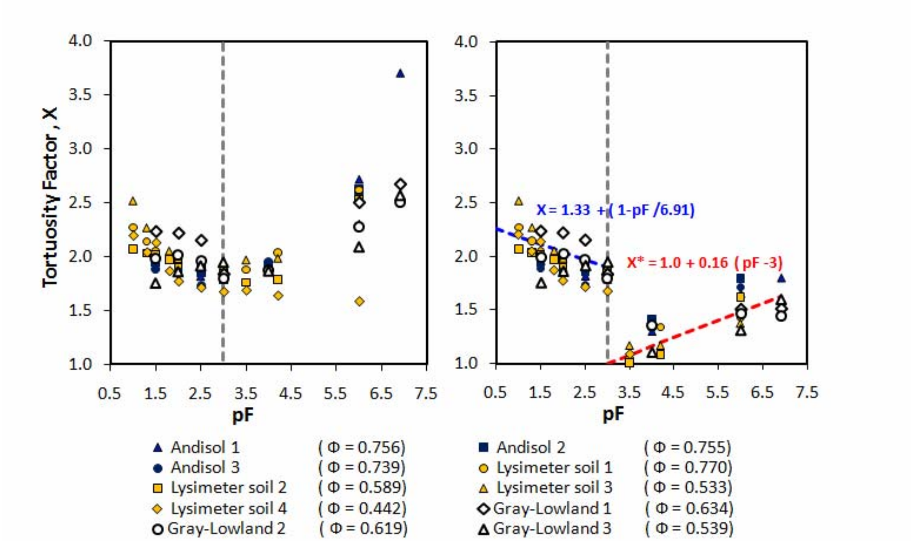

Figure 1. *X*-pF variations for aggregated soils. The proposed X(pF) expressions are shown in dotted line in (b).

$$X^* = \frac{\log\left(D_p/D_o - D_p/D_o\big|_{pF=3}\right)}{\log\left(\varepsilon - \varepsilon\big|_{pF=3}\right)} \tag{5}$$

Figure 1b illustrates the variation of X ($\text{pF} \le 3$) and X^* ($\text{pF} \ge 3$) as a function of pF. We observed that an X-pF expression, previously proposed for structureless soils for the entire range of pF values ($1 \le \text{pF} \le 6.91$), is also applicable for aggregated soils in the range of $\text{pF} \le 3$:

$$X = 1.33 + (1 - \text{pF}/6.91) \tag{6}$$

Note that at completely dry conditions (i.e., pF = 6.91), X reduced to 1.33, a constant suggested by Millington (1959) for dry porous media.

On the other hand, the intraaggregate tortuosity factor, X^*, showed a linear increase with increasing pF which can be expressed by,

$$X^* = 1.0 + 0.16(\text{pF} - 3) \tag{7}$$

Figure 2 illustrates the observed gas diffusivities (D_p/D_o) as a function of air-filled porosity (ε) for some selected soils.

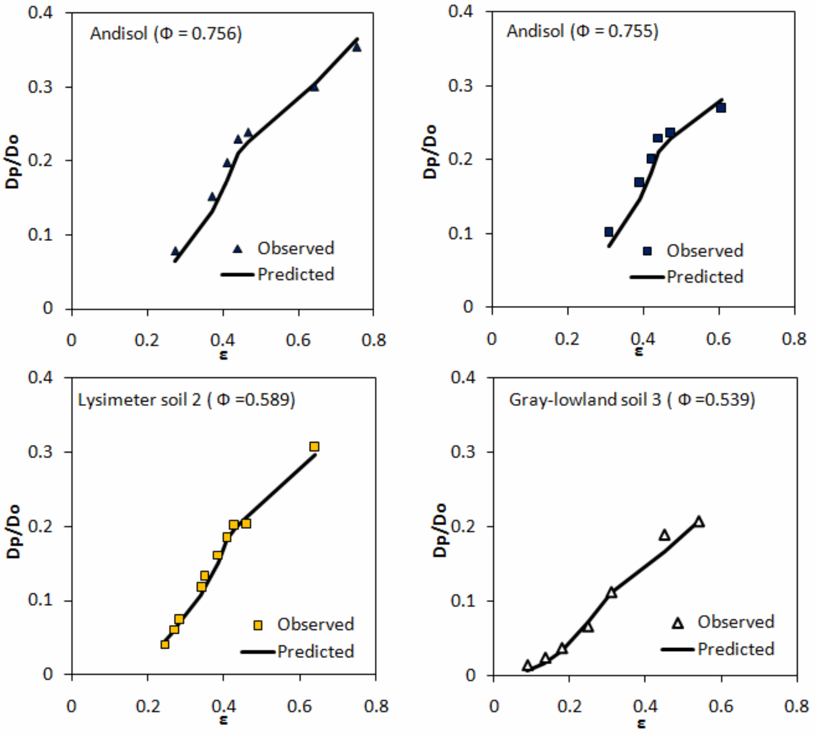

Figure 2. Observed and predicted gas diffusivities (D_p/D_o) as a function of air-filled porosity (ε) for selected soils.

The model predictions using Eq. (6) and Eq. (7) in combination with Eq. (1) are also illustrated. The predictions are in good agreement with the measured data suggesting that the two proposed X-pF expressions can be successfully used to describe gas diffusivity in aggregated soils throughout the entire range of matric potentials. Similarly, the X-pF relationship (Eq. (6)) was tested for structureless and weakly-structured soils with promising results (not shown) hence proved its usefulness across wide range of soil types. Moreover, the X-pF function exhibited unique behaviour for differently-structured soils thereby giving a valuable insight into the soil inner space. These unique X-pF relations are a promising tool for fingerprinting soil functional architecture (Moldrup *et al.* 2009).

Conclusions

The classical Buckingham-based power-law exponent, tortuosity factor X, was reintroduced as a function of soil matric potential (ψ), expressed by pF (= log [$-\psi$, cm H_2O]) ranging from 1 to 6.91, for both structureless as well as structured/aggregated porous media. For aggregated soils, X monotonically decreased with increasing pF reaching a minimum at pF 3 and increased again at higher pF values. The proposed linear X-pF expression for structureless soils for the entire range of pF values was also applicable for aggregated soils to describe inter-aggregate tortuosity in the range of $\text{pF} \le 3$. A different X (pF) expression was proposed for $\text{pF} \ge 3$ to account for intra-aggregate tortuosity. X-pF behaviour has a unique relationship to soil functional structure and hence provides useful soil architecture fingerprints.

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