Predicting Gas Diffusivity for Undisturbed Volcanic Ash Soils: A New Linear Model

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1. Introduction:

Accurate prediction of soil-gas diffusivity (D_p/D_o) , as a function of soil-air content ε , is needed in describing the transport and emission of volatile organic compound and the release of greenhouse gases in soils. Volcanic ash soils (Andisols) typically exhibit a well-developed soil structure with high total porosity, and it has been known that previous models for soil-gas diffusivity could not give a good prediction of D_p/D_o for the entire range of soil-water content from saturation to fully dried condition. In this study, we propose a new linear model based upon the Buckingham-Burdine-Campbell (BBC, Moldrup et al., 1999) model, and tested it against measured D_p/D_o data for undisturbed volcanic ash soils.

2. Measurement of Soil-Gas Diffusivity:

A total of 48 undisturbed soil cores (100-cm^3) were collected from a forested site at Fukushima and a pasture field at Nishi-Tokyo. The soil-gas diffusion, D_p, at different matric potentials (pF = 1.0, 1.8, 2.0, 3.0 and 4.1) including air- and oven-dry conditions were measured according to the method of Rolston and Moldrup (2002).

3. A New Linear Model:

Measured D_p/D_o showed a good linear relationship between D_p/D_o and ϵ . The Penman-Call linear model (Moldrup et al., 2005) described well the linearity of D_p/D_o data (Fig. 1). The Penman-Call linear model, based on the findings of Call (1957), is given by

$$\frac{\mathbf{D}_{p}}{\mathbf{D}_{o}} = \begin{cases} \mathbf{C}(\varepsilon - \varepsilon_{th}) & \text{if } \varepsilon \ge \varepsilon_{th} \\ 0 & \text{if } \varepsilon < \varepsilon_{th} \end{cases}$$
[1]

where ε_{th} is the threshold air content below which soil-gas diffusion is considered negligible. However, no knowledge on the slope C and intercept ε_{th} linked to basic soil physical parameters has been established. In this study, the C and ε_{th} were estimated based on the assumption that the BBC model intersects the best fitted linear regression at pF 1.8 and at pF 4.1. This new model uses only two points of the water retention curve (at pF 1.8 and pF 4.1 of soil-water matric potentials) in addition to saturation (soil total porosity) and in-situ soil-moisture contents. The slope C, Eq. [2], and the intercept ε_{th} , Eq. [3], are estimated as

$$C = \left(\frac{D_{p,4,1}}{D_o} - \frac{D_{p,1,8}}{D_o}\right) / (\varepsilon_{4,1} - \varepsilon_{1,8})$$

$$(2)$$

$$\varepsilon_{th} = \left(C\varepsilon_{1.8} - \frac{D_{p,1.8}}{D_o} \right) / C$$
(3)
The $D_{p,1.8} / D_o$ and $D_{p,4.1} / D_o$ are estimated using the BBC mode





Fig. 1 Variation of D_p/D_o with soil-air content ϵ . Best fitted linear regression and the BBC model (using average pore-size distribution index b and soil total porosity) are also shown.



Fig.2a Comparison of slope C obtained using Eq. [6] and from the fitted linear regression on all measurements.



Fig.2b. Comparison of threshold soil-air content obtained using Eq. [7] and from the fitted linear regression on all

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Furthermore, the Campbell (1974) pore-size distribution index b is estimated as b' using the soil-water retention data at pF 1.8 and at pF 4.1 and is given as

$$b' = -\frac{\log(-\psi_{4,1}) - \log(-\psi_{1,8})}{\log(\theta_{4,1}) - \log(\theta_{1,8})}.$$
[5]

It is noted that soil air content (ϵ) and soil-water content θ add up to the soil total porosity Φ . Substituting Eq. [4] and Eq. [5] into Eq. [2], the slope C becomes

$$\mathbf{C} = \left(\Phi^2 \left[\left(\frac{\varepsilon_{4,1}}{\Phi} \right)^{2+\frac{3}{b'}} - \left(\frac{\varepsilon_{1,8}}{\Phi} \right)^{2+\frac{3}{b'}} \right] \right) / \left(\varepsilon_{4,1} - \varepsilon_{1,8} \right)$$
[6]

and substituting Eq. [6] into Eq. [3], the threshold air content ϵ_{th} becomes

$$\varepsilon_{\rm th} = \varepsilon_{1.8} - \left(\varepsilon_{4.1} - \varepsilon_{1.8}\right) \left(\frac{\varepsilon_{1.8}}{\Phi}\right)^{2+\frac{3}{b'}} / \left(\left(\frac{\varepsilon_{4.1}}{\Phi}\right)^{2+\frac{3}{b'}} - \left(\frac{\varepsilon_{1.8}}{\Phi}\right)^{2+\frac{3}{b'}}\right)$$
[7]

Eq. [1] with Eq. [6] and Eq. [7] is hereafter labeled as the two-point BBC-linear model.

4. Results and Discussion:

For most samples, the estimated C and ε_{th} compared reasonably with the observed values from linear regression (Fig. 2). It was observed that the C and ε_{th} depend mainly on the prediction of the BBC model at pF 4.1. The two-point BBC linear model evidently performed better than the BBC model for samples in this study and for independent tests on Japanese Andisols from literature (Fig. 3). Large reduction of prediction error for measurements at the air- and oven-dry D_p/D_o data and a slight improvement in prediction performance on D_p/D_o data at wet conditions were observed. This resulted to the alignment of air-and oven-dry data within the 1:1 line of the scatter plot comparison between predicted and measured values (Fig. 4). Overall, the root-mean-squareerror (RMSE) of the two-point BBC linear model (RMSE = 0.033) is less than half of the RMSE of the BBC model (RMSE = 0.07) on data including dry data; and slightly lower than that of BBC model for data excluding air- and oven-dry conditions. This was expected since the observed linearity of D_p/D_o was captured by the estimated slope and intercept of the Penman-Call linear model. Thus, soil-gas diffusivity for humic Andisols can now be accurately predicted when we know the soil-water content at the following conditions: saturation, field capacity, wilting point, and in-situ conditions.

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Fig. 3. Test of the two-point BBC linear model on selected samples from a) this study and b) data from literature (Moldrup et al., 2003; Osozawa, 1998). The BBC model and the best linear fit are also shown.



Fig. 4. Scatterplot comparison showing the performance of the two-point BBC linear model on gas diffusivity measurements from this study.