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Use of bimodal hydraulic property relationships to characterize soil physical quality

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ABSTRACT

Soil hydraulic properties have a predominating impact on soil physical quality (SPQ) because they directly or indirectly control air and water storage, infiltration and drainage, nutrient leaching, microbial activity, greenhouse gas generation, and carbon sequestration. The hydraulic properties of many soils are often better described using "bimodal" water content and hydraulic conductivity (θ-K-h) functions, where the θ-K-h of a large-pore "structure domain" is combined with the θ-K-h of a small-pore "matrix domain". This study uses closed-form bimodal van Genuchten θ-K-h functions to characterize SPQ from the perspective of storage and transmission of water and air in soils containing distinct structure and matrix domains. Consistently good fits were achieved between the soil water content function, θ(h), and water content data from intact soil, repacked diatomite pellets, and repacked soil aggregates ($R^2 \geq 0.9854$, RMSE ≤ 0.0223 m^3 m^{-3}), but variable fits were attained between the hydraulic conductivity function, K(h), and hydraulic conductivity data. It was found that even though the SPQ of bulk soil may be optimal or near-optimal, the SPQ of the corresponding structure and matrix domains could be limited or poor in one or more categories. The structure domain tended to be water-limited and potentially prone to leaching, while the matrix domain tended to be aeration-limited and potentially prone to greenhouse gas generation. It was concluded that maximizing the economic and environmental performance of field crop production would likely require selective improvement of structure or matrix SPQ, rather than bulk soil SPQ.

1. Introduction

Soil quality may be viewed as the "degree" or "level" of a soil's physical, chemical and biological suitability for particular functions or purposes (Carter et al., 1997). From crop production and environmental impact perspectives, the physical component of soil quality (often referred to as "soil physical quality", SPQ) relates to the soil's density and mechanical resistance to root growth, and the soil's ability to store and transmit air, water and nutrients (Reynolds et al., 2009, 2015). The SPQ of soil is usually assessed by comparing measured values of a set of "indicator parameters" to established optimal ranges and critical limits (e.g. Reynolds et al., 2009, 2015). Important SPQ indicators for air and water storage include porosity (P), air capacity (AC), plant-available water capacity (PAWC), pore size distribution (PSD), equivalent pore diameter (d_e), and relative field capacity (RFC) (Reynolds et al., 2009, 2015). Key indicators for water transmission include saturated hydraulic conductivity (K_{sat}), field capacity hydraulic conductivity (K_{FC}), and time for soil to gravity-drain from saturation to field capacity (t_{FC}) (Assouline and Or, 2014; Reynolds et al., 2015).

In rigid to moderately expansive soil, air and water storage indicators are obtained primarily from the soil's water content (i.e. sorption or desorption) relationship, θ(h), where θ [L^3 L^{-3}] is volumetric soil water content, and h [L] is pore water tension head. Water transmission indicators, on the other hand, are obtained mainly from the soil's hydraulic conductivity relationship, K(h), where K [LT^{-1}] is soil hydraulic conductivity. Because K(h) is known from first principles to be physically related to θ(h) (e.g. Burdine, 1953; Mualem, 1976; Brutsaert, 2000), functions and parameters describing the water content relationship are often also used to describe the hydraulic conductivity relationship (e.g. van Genuchten, 1980; Kutilek, 2004; Grant et al., 2010). As a result of this close connection, θ(h) and K(h) are often collectively referred to as the "soil hydraulic property relationships", θ-K-h.

Storage and transmission of soil water and air occurs in interconnected pore networks which are often self-organized into a bimodal (double peak) size distribution of small "matrix domain" pores and larger "structure domain" pores (e.g. Durner, 1994; Dexter et al., 2008). Matrix domain pores are principally the spaces within soil aggregates and between primary soil particles (e.g. mineral grains, organic materials), while structure domain pores are primarily inter-aggregate spaces, root channels, fauna burrows, and inter-pedal cracks (Durner, 1994; Kutilek, 2004; Dexter et al., 2008). The bimodal pore size distribution causes θ(h) and K(h) data curves to be sigmoidal in shape with two

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inflections, one inflection for the structure domain and one inflection for the matrix domain (Durner, 1994; Smettem and Kirkby, 1990; Dexter et al., 2008).

Characterizing the SPQ of soils with structure and matrix pore domains requires use of $\theta(h)$ and $K(h)$ functions that can be accurately fitted to bimodal $\theta(h)$ and $K(h)$ data. This can be achieved by fitting separate unimodal functions to pre-selected subsets of "structure domain" data and "matrix domain" data (e.g. Ross and Smettem, 1993; Kutilek et al., 2009; Mohanty et al., 1997), or by fitting a single bimodal function to the entire dataset (e.g. Priesack and Durner, 2006; Dexter et al., 2008). Although the literature contains many studies of fitting $\theta(h)$ and $K(h)$ functions to bimodal data, very few involve assessing the SPQ of soils with structure and matrix pore domains. Hence, the objectives of this investigation were to describe how closed-form bimodal van Genuchten (1980) $\theta(h)$ and $K(h)$ functions might be fitted to bimodal $\theta(h)$ and $K(h)$ data, and then used to characterize SPQ in soils containing distinct structure and matrix domains.

2. Analysis

2.1. Bimodal soil water content function

Soil pore space can be segregated into "structure", "matrix" and "residual" domains, where the structure domain includes biopores, interpedal cracks and inter-aggregate voids, the matrix domain includes inter-grain and intra-aggregate spaces, and the residual domain includes all other pores (e.g. Kutilek, 2004; Dexter et al., 2008). Transmission and storage of plant-available soil water and soil air occurs in the structure and matrix pores, while the residual pores are effectively non-participatory due to small size and/or lack of interconnection with other pores (Jena and Gupta, 2003). By conservation of mass, water sorption and desorption in this type of three-domain system can be represented by an unweighted linear combination of component relationships:

$$\theta_B(h) = \theta_S(h) + \theta_M(h) + \theta_R; 0 \le h < \infty \quad (1)$$

where $\theta_B(h)$ [$L^3 L^{-3}$], $\theta_S(h)$ [$L^3 L^{-3}$], $\theta_M(h)$ [$L^3 L^{-3}$] and θ_R [$L^3 L^{-3}$] are the volumetric soil water content relationships of the bulk medium (e.g. bulk soil), structure domain, matrix domain and residual domain, respectively, and h [L] is the soil water tension head. In the special case of complete soil saturation (i.e. $h = 0$, no entrapped air), the terms in Eq. (1) collapse to:

$$\theta_B(h) = \theta_{BS} = P_B; h = 0 \quad (2.1)$$

$$\theta_S(h) = \theta_{SS} = P_S; h = 0 \quad (2.2)$$

$$\theta_M(h) = \theta_{MS} = P_M; h = 0 \quad (2.3)$$

$$\theta_R = P_R \quad (2.4)$$

where θ_{BS} [$L^3 L^{-3}$], θ_{SS} [$L^3 L^{-3}$], and θ_{MS} [$L^3 L^{-3}$] are the saturated volumetric soil water contents of the bulk medium, structure domain and matrix domain, respectively; and P_B [$L^3 L^{-3}$], P_S [$L^3 L^{-3}$], P_M [$L^3 L^{-3}$] and P_R [$L^3 L^{-3}$] are the bulk medium, structure, matrix and residual porosities, respectively, with $P_B = P_S + P_M + P_R$. In this system, $(P_S + P_M)$ might be viewed as "active" porosity with respect to the storage and transmission of plant-available soil water and air, while P_R is "inactive" porosity (although perhaps still available for microbial activity).

Building on McCoy and Stehouwer (1998) and Priesack and Durner (2006), Eq. (1) can be parameterized using:

$$\theta_B(h) = \frac{P_S}{\left[1 + (\alpha_S h)^{n_S}\right]^{m_S}} + \frac{P_M}{\left[1 + (\alpha_M h)^{n_M}\right]^{m_M}} + P_R; h \ge 0 \quad (3)$$

where the first two terms on the right are, respectively, van Genuchten (1980) $\theta(h)$ functions for the structure domain, $\theta_S(h)$, and matrix domain, $\theta_M(h)$. In Eq. (3), α_S [L^{-1}], n_S [−] and m_S [−] represent the van Genuchten (1980) curve fitting parameters for the structure domain, α_M [L^{-1}], n_M [−] and m_M [−] represent the corresponding parameters for the matrix domain, and parameter constraints include:

$$\alpha_S > 0; \alpha_M > 0 \quad (4)$$

$$0 < m_S < 1; 0 < m_M < 1 \quad (5)$$

$$n_S > q; n_M > q \quad (6)$$

where q [−] is defined in Eq. (7), and m_S and m_M can be independent or restricted to:

$$m_S = 1 - \frac{q}{n_S}; m_M = 1 - \frac{q}{n_M} \quad (7)$$

Comparing Eq. (3) above to Eq. (1) in McCoy and Stehouwer (1998) and Eqs. (1) and (2) in Priesack and Durner (2006) reveals that:

$$P_S = \omega_S(\theta_{BS} - \theta_R) = \theta_{BS} - \theta_{MS} \quad (8)$$

and

$$P_M = \omega_M(\theta_{BS} - \theta_R) = \theta_{MS} - \theta_R \quad (9)$$

where ω_S [−] and ω_M [−] are, respectively, the ratios of structure porosity and matrix porosity to the "active" bulk medium porosity (i.e. $P_S + P_M$) with the constraint, $\omega_S + \omega_M = 1$.

2.2. Bimodal pore size distribution function

Although there are several approaches for estimating the pore size distribution (PSD) of rigid to moderately expansive porous media (e.g. Meyer and Klobes, 1999), perhaps the most useful is given by:

$$PSD \rightarrow \frac{-d\theta(h)}{d\log_{10} h} \text{ versus equivalent pore diameter}, d_e[L], \text{on a } \log_{10} \text{ scale} \quad (10)$$

where it is recognized that (van Genuchten, 1980; Durner, 1994):

$$\frac{-d\theta(h)}{d\log_{10} h} = \ln(10) h \frac{-d\theta(h)}{dh} \quad (11)$$

and d_e is related to h via the capillary rise equation (Or and Wraith, 2002, p.80):

$$d_e = \frac{4\gamma \cos\mu}{\rho_W g h} \approx \frac{2977.4}{h}; h > 0 \text{ (cm)}; d_e(\mu m); 20\ ^\circ C \quad (12)$$

where $\gamma = 72.8$ g s^{-2} is pore water surface tension, $\rho_W = 0.998$ g cm^{-3} is water density, $g = 980$ cm s^{-2} is gravitational acceleration, and $\mu \approx 0$ is the assumed water-pore contact angle. Substituting Eq. (3) into (11) produces:

$$PSD_B = (PSD_S + PSD_M) \text{ versus } d_e \quad (13.1)$$

where

$$PSD_S \rightarrow \ln(10)\left\{\frac{m_S n_S P_S (\alpha_S h)^{n_S}}{\left[1 + (\alpha_S h)^{n_S}\right]^{(m_S+1)}}\right\} \text{versus } d_e \quad (13.2)$$