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A physical–chemical model for the static water retention characteristic of unsaturated porous media

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Abstract

Water retention characteristic or water retention curve (WRC) is an important constitutive feature of porous media, and also meanwhile is an indispensable requirement in hydraulic transport modelling. Previous experiments have indicated that the specific surface area of porous media has effects on the WRC. It has also been observed that a linear relationship generally exists between the air–water interface area and the water saturation within unsaturated porous media. However it seems that no detailed study on their internal linkage with the WRC has been reported yet. This paper, at first gives a review of the development of WRC modelling, then it tries to explain the water retention characteristic according to the physical and chemical behaviours of the phases involved in unsaturated porous media. Using the traditional capillary theory, the volume averaging theorem and the advances in physical chemistry of interfacial surfaces, this paper then derives out a formula which represents the water retention characteristic of porous media. This formula demonstrates the internal linkage of the WRC to the specific surface area of porosities. It also shows agreements with the experimental observations mathematically. Based on this formula, a fitting model is proposed for the static WRC of porous media. Finally, this model is tested to fit the WRC measurements of a wide range of porous materials. Comparison with other main models is presented.

Keywords: Unsaturated porous media; Capillary pressure; Water retention curve; Multi-phase interaction; Specific surface area

1. Introduction

Water flow in unsaturated (or partially saturated) porous media is a subject of concern in a wide range of sciences and engineering, such as hydrology [35], soil physics [26] and building materials [24]. Water retention characteristic or water retention curve (WRC), which defines the relationship between the water saturation and water pressure head, is an important constitutive feature of the porosity of porous media [16], and meanwhile is an indispensable requirement in hydraulic transport modelling [3,36]. Due to its great interest, a large number of researches have been conducted since the middle of last century. Many models using different theories and methods were proposed for the WRC of soils.

In general, all of these models could be classified into two groups, i.e. the phenomenological or empirical models, and the conceptual or physical models. Among the first group, the power function proposed by Brooks and Corey [10] and the formula by van Genuchten [47] could be the two most popular ones. But previous practices showed that the former one was not good in accuracy [47] and the later one usually failed at low water content [5,29]. Among the second group, most conceptual models use a bundle of cylindrical capillaries (BCC) to represent the real pore configuration and assume that the soil particle size distribution (PSD) due to the fragmentation processes derives the void/pore size distribution (VSD) [4]. It is the pore size distribution that decides the WRC accord-

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Nomenclature

A, B	constants
h	thickness (m)
P	pressure (Pa)
P_c	capillary pressure (Pa)
P_w	absolute pressure of water phase in unsaturated porous media (Pa)
P_v	absolute pressure of vapour phase in unsaturated porous media (Pa)
σ_{wv}	surface tension on the water–vapour interface (N/m)
σ_{vs}	surface tension between vapour and solid phase (N/m)
σ_{ws}	surface tension between water and solid phase (N/m)
θ	contact angle
r_m	radius of meniscus interface (m)
r	local pore radius at the position of meniscus (m)
u	chemical potential (J/mol)
$\bar{s}$	specific surface (1/m)
S	water saturation
S_A	surface area (m^2)
V	molar volume (m^3/mol), volume (m^3)

Subscripts

w	water phase
v	vapour phase
s	solid phase
f	fluid

ing to the capillary law. For certain type of soils, previous experiments showed that PSD could be described using a power-law function of water saturation [4], and the power-law PSD assumption has been backed by single fractal models. Because soil structure is hierarchical with organizational levels ranging from a microscale to macroscale, a structure similar to a fractal object which has a hierarchical infrastructure with larger units containing smaller units and smaller units enclosing even smaller units and so on ad infinitum, fractal modelling was employed to predict soil hydraulic properties [19]. However the single fractal models usually failed to represent the inflection points [48] which generally present in the WRC of porous media. The inflection points are very important, because they decide the shape and slope of the WRC, and these characters usually indicate the physical quality of soils [16]. The failure of single fractal model could be related to the fact that a fractal function could be fitted to the WRC does not prove that the soil is fractal [15]. Another conceptual model which is based on the probability of fragmentation assumes the PSD of a lognormal form. The lognormal PSD leads to a lognormal VSD as a result [4,27,28,34,44]. A key issue for all PSD models is that the relationship between the PSD and VSD is far from deterministic, which could be linear (representing the similarity between VSD and PSD) [2], or nonlinear [4]. On another hand, the lognormal PSD hasn't been verified for other different texture porous materials, for example, previous researches indicated that the WRC of continuous polyester fibre geotextiles which were manufactured by needle punching had the same basic shape as that of coarse-grained soils [8]. Precisely, all of these preceding models were proposed to model the WRC under static conditions, which do not take into account of dynamic effects, such as the fluid in flowing processes, the viscous and/or gravity effects [7]. The dynamic effects on WRC are very important. Hassanizadeh and Gray [25] ever studied the dynamic capillary pressure according to the thermodynamic behaviour of the fluids in multi-phase flowing processes within porous media [21]. In this paper, however, we'll still only discuss the WRC under static conditions.

Intensive studies on the WRC of soils indicated that water retention characteristic is not only closely related to the pore size distribution, but also to the solid phase and/or the solid-pore interfaces [19]. Bachmann and van der Ploeg [5] reviewed that the involved effects include such as adsorption, wettability and temperature. The previous 'experimental and theoretical evidence suggest a radically different liquid configuration in unsaturated porous media···. Because of the relative large surface area in most porous media, interfacial forces are likely to play a larger role' [46]. 'In the absence of consensus regarding the special scales, flow behaviour, and types of pore space heterogeneity amenable to continuum representation, there is a clear need for physically sound constitutive relationships between matric potential, liquid retention, and hydraulic conductivity' [45]. Recently, a liquid configuration-based model using a representative unit cell which has an angular pore space with two slits attached was proposed and developed [39,46]. In this model, the angular pore space was used to evaluate the capillary component while the surfaces of the two slits were used to evaluate the effect of the adsorbed water film. However, it has already been pointed out that such model cannot generally represent the irregular pore space in actual soils [13]. On the other hand, the physical model that was employed to evaluate the adsorption effect of the slit surfaces in this model was not quantitatively satisfactory when compared with experimental data because it ignored the long range interactions [30]. In fact, the chemical potential of the adsorbed fluids not only depends on the fluid thickness on the adsorption surface but also on the total surface area of the solid substrate [1].