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Research Paper

Modification of capillary pressure by considering pore throat geometry with the effects of particle shape and packing features on water retention curves for uniformly graded sands

Hyoung Suk Suh, Tae Sup Yun*

School of Civil and Environmental Engineering, Yonsei University, Seoul 03722, Republic of Korea

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ABSTRACT

Accurate estimation of capillary pressures at pore throats during pore network simulation is made by acquiring the effective distribution of non-wetting fluid and its effective shape factor. The suggested method is applied to authentic pore structures of synthetically assembled sphere packings and natural sands. Results highlight that the irregularity of pore throat tends to increase as particle shape becomes irregular while the effective shape factor of 0.8 can be consistently applicable regardless of particle shape. The modified water retention curve well captures experimental results. Packing density and gradation effects are less predominant compared with the effect of capillary pressure correction.

1. Introduction

Water flow in unsaturated soils, which is governed by the capillary force at pore spaces and the degree of saturation, is important in various applications such as stability analysis [1,2], hydraulic design of earth dam [3,4], groundwater remediation at contaminated sites [5,6], and vegetation and planting [7]. The water retention curve reflects the saturation dependent water-retaining capacity and flow velocity under a given capillary pressure, and is therefore considered to be the most essential soil property [8,9]. Conventional pore network model has been widely used to obtain water retention curves by assuming a randomly configured pore structure comprising pore chambers interconnected by pore channels modeled as inscribed spheres and cylindrical tubes. Iterative computation of sustained capillary pressure across the interface between two fluids allows calculating the evolution of capillary pressure with saturation [10,11]. Invading fluid is subjected to highest capillary pressure at the narrowest pore channels which is highly dependent on the radius of the idealized cylindrical tube representing the pore throats. Morphological extraction of a pore throat often fits the cylindrical tube whose cross-section closely inscribes [12,13] the irregularly shaped throat geometry; this therefore causes the computed capillary pressure to be overestimated [14]. For this reason, previous studies assigned angular pore throat cross-sections (e.g., polygonal cross-sections) to alleviate the problem [15–17], but their efforts still reside on idealized shapes, not the authentic geometries. The capillary pressure is primarily influenced by pore geometry (e.g., size and shape), which in turn is determined by the size, shape, gradation, and density of particles in soils [18]. Yet, recent studies of pore network modeling have rarely investigated the correlation between geometrical features of particles and the water retention curve. The Mayer and Stowe-Princen (MS–P) method [19–22] derives an analytical solution of capillary pressure at mathematically expressible (e.g., polygonal) cross-sections along the longitudinal direction, but may not be appropriate for randomly shaped pore structures in soils [23,24]. Alternative numerical model to simulate two-phase flow in authentic pore spaces such as lattice Boltzmann method can measure the capillary pressure at any geometry [25]; however, its high computational cost, complicated governing equations, and numerical sensitivity often hamper the methods' applicability. Therefore, it is desirable to explore the effects of soil density and particle features on the water retention curve when implementing a pore network model that consists of relatively simple and adoptable forms.

This study proposes a morphological analysis that not only quantitatively captures the effective pattern of non-wetting fluid at pore throat but also estimates the corresponding capillary pressure. The 3D pore structures for the sets of synthetically generated sphere packing and natural sands by X-ray computed tomography provide the simulation platform independently examine the effects of particle shape, packing density, and gradation on water retention curves for soils. The results are corroborated by experimental data.

* Corresponding author.
E-mail addresses: hssuh@yonsei.ac.kr (H.S. Suh), taesup@yonsei.ac.kr (T.S. Yun).

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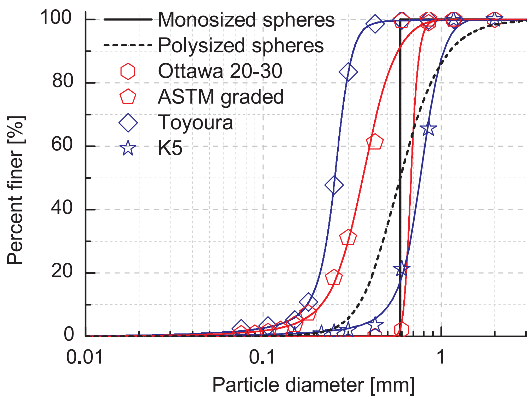

Fig. 1. Grain size distribution curves of granular assemblies used in this study. Symbols are fitted by Fredlund et al. [45].

2. Materials and methods

2.1. Granular domain

To investigate the effects of particle shape and packing features on water retention curves, total eight types of uniformly graded granular assemblies are subjected to pore network simulation; four synthetic sphere packings by PFC^{3D} to explore the effect of packing features [26] and four natural sands of different shapes (Ottawa 20-30, ASTM graded, Toyoura and K5) with medium relative densities (i.e., D_r = 50–60%) to investigate the particle shape effect. Synthetic packings with mean particle size of 0.59 mm are generated by the radius expansion method. Three uniformly sized assemblies [monosized loose (MS-L), medium (MS-M), and dense (MS-D)], as well as polysized packing (PS), are made by controlling the inter-particle friction coefficient [27,28]. Synthetic sphere packings and natural sands are classified as SP by the unified soil classification system (USCS) with uniform gradation (Fig. 1). The 3D pore structures of the granular packings used here are formed by discretizing the synthetic packings into 3D binary images of 400 × 400 × 400 voxels with 18.00 μm and 9.83 μm voxel size for monosized and polysized packings, respectively. Each natural sand is packed in a glass cylinder of 10 mm diameter and is subjected to 3D X-ray computed tomographic imaging (PCT-G3; 150 kV and 100 μA with CCD camera as a flat-panel detector, SEC Ltd.). The 8-bit 2D sliced images are stacked and segmented into a 400 × 400 × 400 voxel structure to obtain a binarized pore structure by using the Otsu's method [29]. The resolution is 17.54, 9.93, 5.84 and 17.54 μm for Ottawa 20-30, ASTM graded, Toyoura and K5 sands, respectively. Two shape parameters for the natural sand grains are selected: sphericity Ψ_S for bulk form and roundness Ψ_R for small-scale smoothness. Sphericity Ψ_S refers to the degree of resemblance of a particle to a circle and is defined as the ratio of the diameter of a circle having equivalent area to the diameter of a particle's circumscribing circle. Roundness Ψ_R describes the surface features, defined as the ratio of average radius of curvature in particle corners to the radius of particle's inscribing circle. Determination of each shape parameter follows the analytical solution and numerical implementation validated by Suh et al. [30]. Note that Ψ_S and Ψ_R are equal to unity for a sphere (e.g., synthetic packing cases). Table 1 and Fig. 2 present the index properties, shape parameters, and 3D pore structure for each assembly.

2.2. Pore network modeling

Pore network structure comprises spherical pore chambers (pore volume segments) connected to each other by cylindrical pore throats (capillary tubes) and is directly extracted from the 3D image [31]. This study initially defines the pore throat by adopting the maximal ball theory proposed by Silin and Patzek [13], but simultaneously captures the authentic pore throat cross-section to further modify the imposed capillary pressure. The overall procedure is illustrated in Fig. 3. The pore skeleton of the 3D pore volume is first obtained by a thinning algorithm [32,33]. Junctions and dead ends in the pore skeleton are initially defined as potential pore chambers, and the remaining skeletal segments connecting two neighboring prospective chambers are regarded as pore channels (Fig. 3). A voxel in the pore channel skeleton having a local minimum Euclidean distance value (i.e., center of minimum inscribing sphere) then becomes the center of the pore throat, and its inscribing radius r_{ins} is defined as the radius of the pore throat. Note that the determined r_{ins} for each pore throat is then inversely proportional to the capillary pressure. A 2D cross-sectional image of each pore throat is acquired by inserting a virtual plane with 200 × 200 pixels (AA′ in Fig. 3) through the center of the pore throat perpendicular to the polynomial curve fitted to the skeleton. Cubic interpolation enables to fully capture the irregularity of the pore throats by attaining sufficient image resolution (i.e., at least 20 pixels per r_{ins}). The pore throats are assumed to be volume-negligible, and the potential pore chambers are dilated until they reach the inserted planes to represent the entire pore volume. The radius of each pore chamber is regarded as the radius of a sphere of equivalent volume. This process quantifies the pore structure into an idealized web of pores and a 2D geometry of real pore throats (Table 2).

Table 1
Basic properties of granular assemblies used in this study.

Granular assemblies		Size distribution		Packing		Particle shape	
		D_{50} [mm]	C_u	n	D_r [%]	Ψ_S	Ψ_R
Synthetic sphere packings	MS-L	0.59	1	0.33	28.1	1	1
	MS-M	0.59	1	0.37	54.5	1	1
	MS-D	0.59	1	0.42	73.9	1	1
	PS	0.59	1.92	0.35	–	1	1
Natural sands	Ottawa 20-30	0.68	1.12	0.37	57.5	0.94	0.72
	ASTM graded	0.36	1.86	0.39	53.9	0.88	0.57
	Toyoura	0.25	1.49	0.44	50.9	0.83	0.47
	K5	0.76	1.59	0.45	59.7	0.80	0.27

Note: D_{50} = mean particle diameter, C_u = uniformity coefficient, n = porosity, D_r = relative density, Ψ_S = particle sphericity, Ψ_R = particle roundness.

The drainage water retention curve (i.e., for the invasion of non-wetting fluid into a water-saturated pore network) is constructed by iteratively computing the saturation values S_w of the participating fluids (e.g., air and water) under sustained capillary pressures p_c at each pore throat. The simulation uses the method proposed by Joekar-Niasar et al. [11]. Interfacial tension T_s is 72.86 mN/m with zero-contact angle to represent the high surface energy of soil minerals [34]. The obtained water retention curves are then parameterized (using air entry value p_0, fitting parameter m and residual saturation S_{wr}) by fitting the van Genuchten equation [35]:

$$p_c = p_0\left[\left(\frac{S_w - S_{wr}}{1 - S_{wr}}\right)^{-\frac{1}{m}} - 1\right]^{1-m} \tag{1}$$

2.3. Quantification of pore throat shape

The possible geometrical configuration of non-wetting fluid at irregularly shaped pore throat determines its sustained capillary pressure. The use of an inscribing circle to represent a pore throat (Fig. 3) undermines the actual shape of pore throat and thus results in an overestimate of the capillary pressure [14]. We therefore introduce a new, simple and approachable morphological method to accurately evaluate the effective cross-sectional area (i.e., the expected area occupied by the non-wetting fluid after drainage) [24]. This is correlated