Contents lists available at ScienceDirect

Computers and Geotechnics

journal homepage: www.elsevier.com/locate/compgeo

Obtaining soil-water characteristic curves by numerical modeling of drainage in particulate media

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ARTICLE INFO

Article history: Received 9 July 2015 Received in revised form 1 December 2015 Accepted 12 January 2016 Available online 4 February 2016

Keywords: Unsaturated soils Soil-water characteristic curve Packing algorithm Pore network Numerical modeling

ABSTRACT

Soil–water characteristic curve (SWCC) is widely used for obtaining mechanical and hydraulic properties of unsaturated soils, such as shear strength, deformation, permeability, and flow. An innovative approach, where a meso-scale medium is generated based on particle size distribution and void ratio of non-plastic soils, for estimating the drying SWCC is developed. With application of the finite difference and Newton-Raphson (Jacobian) approximations, the air-entry pressures of pore bodies in inter-particle medium (micro-scale) are determined and implemented in drainage simulation of the medium. The volumes of drained pore bodies and subsequently developed liquid bridges after each suction iteration are calculated and plotted. Eventually, homogeneity of the developed packing algorithm, parametric study, comparison of the simulated drying SWCC to experimental and estimation results as well as computational performance of the developed MATALB code is presented and discussed. It is shown that, the proposed methods (Arya and Paris, 1981; Fredlund and Wilson, 1997) and due to its accuracy and time efficiency, the algorithm can even be a viable option for replacing the tedious experimental methods.

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1. Introduction

The soil-water characteristic curve (SWCC) reflects fundamental drainage properties of unsaturated soils by revealing the relation between soil suction and water content. In order to determine the SWCC, various experimental tests, such as hanging column or pressure chamber (ASTM, D6836-02) [3], can be conducted. However, conducting these laboratory tests are generally time consuming, expensive and highly dependent on the operator skills. Therefore, a need for faster and inexpensive techniques has resulted in formation of various empirical methods. In these methods, the SWCCs are determined by fitting a curve into few experimental data [23,9,43,45,22,32]. In an alternative approach and in order to completely eliminate the cost and time required for conducting laboratory experiments, estimation techniques are emerged. These methods consider the physical properties of soils, such as particle size distribution (PSD) and void ratio data, to estimate the SWCC [5,44,19]. In these methods, pedo-transfer functions (PTF) [8] use the available soil survey data to predict the

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the SWCC is also estimated by training an artificial intelligence algorithm with available database [31,25,29]. However, limitations in available experimental data and dependency of SWCC on texture and density of soils yielded inaccurate results. In this research, while generating the meso-scale soil medium with consideration of the physical properties of non-plastic soils, such as PSD and void ratio, and determining the air-entry pressure (AEP) of individual pore bodies in micro-scale, an attempt toward better approximation of drying SWCC is taken. According to obtained results, which are provided in Section 3, the developed algorithm not only yields a better estimation of SWCC in comparison to the two main estimation techniques, but also decreases the required time in contrast to experimental tests.

SWCC of different types of soil. With implementation of genetic programming and neural networks into engineering problems,

2. Methodology

This study attempts to establish an accurate drainage simulation of the soil medium by a brute-force approach incorporating the physical properties of soils into a grain-by-grain simulation process. The MATLAB algorithm is developed in the following subroutine: (1) generating the solid phase of soil medium, (2)



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identification of pore bodies, (3) identification of pendular rings, (4) determining the air-entry pressures of pore bodies, and (5) simulation of drainage. In the proposed algorithm, few assumptions toward simplification of the problem are made. The particles are assumed to be spherical and immobile. So, there will be no void ratio changes during the drainage simulation. All forces applying on particles, such as gravity or inter-particle contact forces, are neglected. In the case of non-plastic soils, volume of adsorbed water is negligible [38]. Therefore, in drainage process of the simulated cubic medium, the volume of adsorbed water is neglected.

2.1. Generating the solid phase of soil medium

The solid phase of soil structure is generated in three steps: (1) generating the particles based on PSD, (2) packing the particles, and (3) validation of the simulated medium by comparison of its void ratio (e) to desired void ratio (e_d) of a soil. To begin with the particle generation, the necessity of a relation between PSD data and total number of particles leads to division of the PSD curve into small linear segments. By dividing the given PSD into "n" segments and assumption of the total number of particles in the coarsest segment (N_1), the total number of particles in each segment (N_i) with respect to previous segments is calculated. Note that the specific gravity (Gs) is considered to be constant.

$$N_{i} = N_{i-1} \frac{M_{i} - M_{i+1}}{M_{i-1} - M_{i}} \frac{\left(\frac{D_{i-1} - D_{i}}{2}\right)^{3}}{\left(\frac{D_{i} - D_{i+1}}{2}\right)^{3}}, \quad N = \sum_{j=1}^{n} N_{j}$$
(1)

where i = 2, ..., n (number of divided segments) and M_i is the mass percent of particles retained on sieve size D_i . With increasing the number of divided segments and assuming larger N_1 values the accuracy of representative elementary volume (REV) will increase (Section 3.4). Next, the diameter of each particle $(d_j, j = 1, ..., N)$ is determined as a uniformly distributed random variable within the diameter range of its segment.

After generating the particles, the packing subroutine of the algorithm arranges the generated particles inside a medium in a geometry that satisfies the desired void ratio of soil. The packing procedure of particles is developed in following order: (1) arrangement of the particles inside a medium, (2) stability control to form a realistic and dense medium, and (3) application of the periodic boundary condition (PBC). For each packing particle, P_i (i = 1, ...,N), these steps are considered simultaneously. Initially, a cubic medium is considered in a way that its volume is equal to the total volume of all particles. With satiation of the medium, the medium is expanded in Z direction. The cubic medium will eventually be considered as the simulated sample (in Section 3.1, the repeatability and homogeneity of the particle packing is reported). While arranging the particles inside the medium, particles can encounter different arrangement conditions according to number of contacts at the moment of placement (0, 1, 2 and 3 contacts). For each P_i , the motion of particle falling from upper boundary of the medium is simulated (assigning a random *x* and *y* coordinates to the center of the spherical particles within the boundaries of cubic medium while changing the z coordinates in a small steps toward lower boundary of the medium). When a P_i collides with another particle (the Euclidean distance between the surface of particles becomes negative) the contacted particle is considered to be the first contact point. Then, the algorithm searches for a new contact possibilities while keeping its initial contact point. Eventually, the algorithm relocates the P_i in a way that it forms tangent points with contacted particles.

A packing particle is considered to be stable when it forms three contacts with other particles or is located in lower boundary of the medium. If P_i does not collide with any particle throughout its

falling simulation, it will be located at lower boundary of the medium. Forming three contacts does not always lead to stable condition. In the case of three contacts, by projecting the centers of the all contacted particles to the horizontal X-Y plane the stability of P_i is controlled. If the projection of center of P_i is inside the triangle formed by the projections of centers of the contacted particles, the new particle is considered to be stable. When a particle is not stable (contacts <3 or unstable in 3 contact condition) it will move deeper to the medium as if by gravity (changing the *z* coordinates toward lower boundary). This step is known as stability control. The stability control not only provides denser and realistic medium, but also will be used to match the void ratio of simulated cubic medium to the desired void ratio of a soil.

Modeling individual particles of a real-scale or even a lab-scale soil body would require an immense power that is currently not feasible. Results of a meso-scale might be affected by boundaries if they are defined as simple borders of geometry. Hence, in this research, application of the periodic boundary condition (PBC) is considered. In order to form PBC, the particles, which are located adjacent to the borders of the medium, are replicated in X, Y or XY directions. A schematic 2D representation of the packed (white) and duplicated particles (gray) is illustrated in Fig. 1. The packed particles, whose centers are located inside the mirroring range of M_R (= d_{max}) are replicated. For example, the P_i is replicated in X, Y and XY directions. Therefore, the porous connectivity has been extended beyond the limitation of the cubic medium boundaries. This property is deployed in the drainage simulation of medium (Section 2.5). Application of the PBC also eliminates the need for defining boundary-air-water interfaces.

After packing the medium, validation of the generated medium is carried out. If the void ratio of simulated medium is outside of the acceptable tolerance (± 0.02) of desired void ratio (e_d) , the particles packing procedure will be repeated. In this matter, a new parameter known as density factor (D_f) is defined and considered to be one of the few inputs of the algorithm. If a dense medium is an object of the simulation, the value of D_f should be set to 1. For loose packing, the value of D_f is gradually increased. With increasing its value more particles will skip the stability control (a packing particle will be considered as stable regardless of its number of contacts) and a looser sample will be simulated. While the algorithm changes the value of D_f in the beginning of each packing iteration, if after 10 iterations the void ratio of generated medium cannot satisfy the acceptable tolerance of target void ratio, the process will stop and previously packed medium with the closest void ratio to e_d will be chosen. The value of 10 is found sufficient for the developed algorithm to reach any target void ratio. While simulating a super dense medium, the algorithm may not be able to reach the desired tolerance. However, a small amount of error in void ratio does not affect the simulated SWCC significantly (Section 3.2).

2.2. Identification of pore bodies

During the past decades, in order to obtain the mechanical properties of soils, various methods for representing the porous medium have been developed [42]. The earlier theories were assuming the pores as bundle of tubes [15,21,11]. The main idea was to relate the properties of porous media to tube radius frequency distribution but they all fail to represent porous media accurately. The need of accurate description of porous media leads to development of regular network approaches. In regular network approach, the group of spheres representing the particles is packed in various shapes, such as cubic, hexagonal and rhombohedral packings [20,4]. Chatzis and Dullien [13] compared the experimental data with regular network results and observed unrealistic results according to regular networks. For better reflection of

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