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A coupled micromechanical model for triphasic granular system

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ABSTRACT: Modeling the mechanical behavior of partially wet granular materials are of major significance in many engineering applications encompassing soil mechanics, oil and gas extraction, pharmaceutical industries and among others. Since the pioneering work of Alonso et al. (1990) in development of a macro-continuum model for partially wet granular soils, considerable efforts have been made, extending the framework to consider many observed phenomena such as desiccation cracking, collapse on wetting and hydro-mechanical coupling. Despite its great success, such continuum based approaches have inherent limitations as they rely on the phenomenological relations including water retention behavior to model the macroscopic response of the multiphase granular system, and in such approaches the definition of a widely accepted effective stress is still missing. In recent years, significant developments have been made towards micro-mechanical modeling of wet granular materials (including studies based on discrete element method and lattice Boltzmann method (Scholtes et al. 2009a). Frequently, however, most micromechanical studies are limited to be applicable to the so-called pendular regime where the water phase exists in a highly-localized form of disconnected capillary bridges (Scholtes et al. 2009b). In this study, a pore network model is extended to overcome the imposed limitations of both macro-continuum and micro-mechanical models. In such methods, the pore spaces are discretized as set of pore bodies and throats, and local flow rules are introduced such that the movements of fluid phases are solved locally at the pore-scale level (Sweijen et al. 2017). The study is an extension of the dynamic two-phase pore-scale finite volume method coupled with discrete element model (2PFV-DEM) to simulate the isotropic compression behavior of the triphasic granular system using DEM.

1 INTRODUCTION

Modeling the mechanical behavior of wet granular materials is of great interest among many researchers across various disciplines of engineering and industry. In recent years, considerable efforts have been made for the development of a consistent continuum based framework for unsaturated soil mechanics, encompassing both volume change and shear strength behavior (Alonso et al. 1990, Zhou and Sheng 2009). But often such efforts involve many challenges and limitations due to the inherent dependence of continuum based models on the phenomenological relations and lack of experimental datasets for various soil types, required to calibrate such models. Furthermore, in continuum based model the definition of a widely accepted effective stress equation is still missing (Nuth and Laloui 2008). In an effort, to overcome these limitations of macro-continuum based models, considerable developments have been made towards micro-mechanical approaches to model the mechanical behavior of wet granular materials (including studies based on discrete element method and lattice Boltzmann method).

Discrete element method (DEM) simulations are widely used as a reliable experiment for idealized granular material and can be quantified for elasto-plastic deformations. As in lately, DEM has been extended to model the mechanical behavior of wet granular materials. In such methods, capillary bridges are introduced a priori to the particle contact area rather than as a consequence of fluid flow and the capillary pressure across the liquid-air interface is defined by the Young-Laplace equation (Scholtes et al. 2009a). However, these studies are limited to be applicable to the so-called pendular regime (degree of saturation ≤ 15%) where the water phase exists in a highly-localized form of disconnected capillary bridges (Scholtes et al. 2009b).

Recently, a new scheme pore finite volume (PFV) coupled with DEM was introduced by Chareyre et al. (2012) and Catalano et al. (2014), to simulate the hydro-mechanical behavior of a saturated granular medium. In PFV-DEM scheme, the DEM solver is used for the mechanical framework by considering the particle-particle interactions, whereas the PFV (i.e., a pore network based model) efficiently models the 3-dimensional fluid flow in the pore spaces of packing of spheres. The scheme is advantageous and efficient in a way that it considers, the two-way coupling between the solid and fluid phases at pore-scale level wherein the movement of the fluid phase (i.e., fluid flux) and the corresponding fluid forces are linked with the deformation of the solid skeleton (i.e., solid particles). Tong et al. (2012) reported that the predicted permeability values using PFV-DEM were in good agreement with the experiments. Lately, the single phase PFV-DEM has been extended to consider the two-phase fluid flow (2PFV-DEM) in a granular medium (Yuan and Chareyre 2017). Unlike, Yuan and Chareyre (2017), Sweijen et al. (2017) used a dynamic approach for solving the fluid pressure-saturation relationship during drainage for a non-deforming pore space. Sweijen (2017) further conceptualized the pore-scale version of dynamic flow for simulating the behavior of a deforming type of pore space for a bed of swelling particles. Therefore, based on the above discussion the pore-scale version for a dynamic two-phase flow in granular medium can be further used to study the hydro-mechanical behavior viz., volume change and shear strength of wet granular materials for a wide saturation range, unlike the previous DEM simulations where the degree of saturation was restricted to 15% and the capillary pressure across the liquid-air interface was introduced at priori rather than as a consequence of fluid flow.

The current paper presents an extension of the dynamic two-phase pore-scale finite volume method coupled with discrete element model to simulate the isotropic compression behavior of the triphasic granular system using DEM.

2 NUMERICAL MODEL

2.1 *Pore-scale network model*

For the numerical study, we consider a partially saturated system consisting of a perfectly wetting fluid (W), a non-wetting fluid (NW) and a solid phase (S). The S-phase is represented by a packing of monodispersed sphere, which is generated at a specified porosity using DEM solver, YADE (Smilauer et al. 2015). The coupled 2PFV-DEM method relies on the extraction of the pore-scale network model at two levels. At the first level, the pore spaces are discretized as set of pore bodies and throats using a regular triangulation, resulting in an assembly of tetrahedra (Yuan and Chareyre 2017). And, at the highest level a grain-based tetrahedra is replaced by a pore-unit assembly based on a regular geometry. For more details on the pore-unit assembly algorithm the readers may refer to Sweijen et al. (2017).

2.2 *Governing equations*

2.2.1 *Fluid phase*

For simulating the fluid flow in a pore-unit assembly, a finite difference scheme, IMPES is employed which implicitly solves for the water pressure (p^w), since air pressure (p^a) is considered zero and explicitly solves for the water saturation (S^w). For a given pore unit i, the capillary pressure p_i^c is defined as:

$$p_i^c = p_i^a - p_i^w \tag{1}$$

The volumetric flux (q_{ij}^w) across a pore throat ij is assumed to be linearly proportional to the pressure gradient.

$$q_{ij}^w = k_{ij}^w (p_i^w - p_j^w) \tag{2}$$

where k_{ij}^w is the hydraulic conductivity across the pore throat ij. Considering, the volume balance for partially saturated pore unit:

$$\sum_{j=1}^{N_i} k_{ij}^w (p_i^w - p_j^w) = -\frac{dV_i S_i^w}{dt} \tag{3}$$

where N_i is number of adjacent pores and V_i is the volume of the pore unit. Equation 3 is further discretized in form of linear set of equations and can be solved for water pressure. For more details pertaining to the IMPES scheme and critical time step for deforming pore-units, the readers may refer to Sweijen et al. (2017).

2.2.2 *Solid phase*

The total force $\vec{F}_k$ exerted on a particle k due to the two-phase fluid flow includes the pressure term $\vec{F}_k^f$ considering both W and NW phases and interfacial tension $\vec{F}_k^t$ for W-NW-S interface. After calculating the fluid force and interfacial tension forces on each particle, the new particle position is updated using the DEM solver. For brevity, the governing equations are not discussed here and further details on the calculation of these forces can be found in Yuan and Chareyre (2017).

2.3 *Numerical setup*

In the current study, we present a constant suction isotropic compression test, simulated for a monodispersed packing of spheres compacted at an initial porosity corresponding to 0.408. For our simulation, we prepared a partially saturated specimen by invoking primary drainage from a fully saturated condition. The specimen was drained under a capillary pressure of 4 kPa, which was kept constant throughout the simulation including both drainage and isotropic compression stage. It should be noted that, during the drainage process the pore topology remain unchanged. Figure 1 shows the initial condition of the unsaturated specimen and the corresponding boundary conditions. The choice of the boundary conditions depends on the type of the test to be simulated. As we intend to study the isotropic compression behavior for a compacted type of specimen under constant suction, so we have chosen the boundary conditions accordingly. The top boundary and the side boundaries are assumed to be an air reservoir having $p^a = 0$ and the bottom boundary is a water reservoir having $p^w = -4$ kPa. All the boundaries are assumed to be permeable. The material parameters and initial state of the specimen are given in Table 1. Figure 2 shows the pore size distribution for the monodispersed packing obtained from regular triangulation (Yuan and Chareyre 2017).

Table 1. Material parameters and initial state of the specimen.

Parameters	
Material parameters for DEM	
Radius (m)	0.0001
Number of spheres	2500
Elastic modulus (MPa)	20
Poisson's ratio	0.5
Density (kg/m^3)	2600
Friction angle (degree)	28
Damping	0.4
Initial condition of the specimen	
Porosity	0.408
Degree of saturation (%)	77.2
Capillary pressure (kPa)	4.0
Surface tension (N/m)	0.072

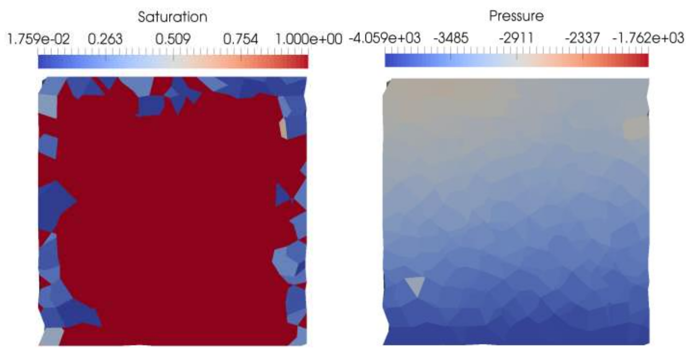

Figure 1. Water saturation and capillary pressure field across the domain (mid XY plane) before the initiation of isotropic compression stage.

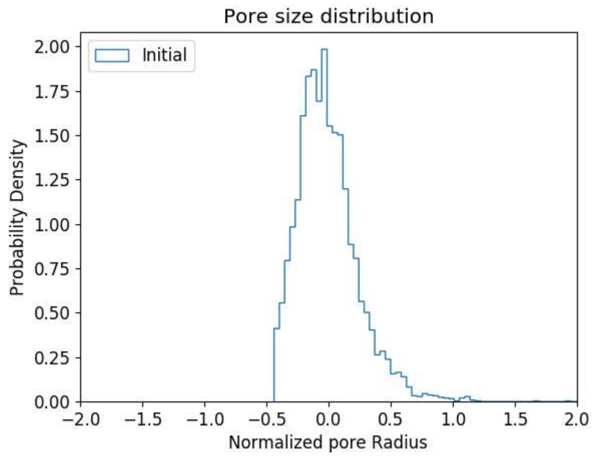

Figure 2. Pore size distribution for the packing of spheres.

3 RESULTS AND DISCUSSION

For the unsaturated soils mechanics loading-collapse yield curve (LC) represents an important relationship between the yield stress and capillary pressure (i.e., matric suction). But, often the existence of this unique relationship is questioned due to the lack of proper understanding about how an unsaturated soil specimen prepared from slurry state yields differently from an unsaturated compacted specimen (Sheng et al. 2008, Zhou and Sheng 2009). Even though many experimental studies in recent years have tried to focus on understanding this plastic yielding based on the pore size distribution, but they certainly lack in establishing a clear basis for a wide range of soil types having unimodal and bimodal pore size distributions, due to the imposed limitations on conducting experiments (Mountassir et al. 2014, Thyagaraj and Das 2017). For such shortcomings, micromechanical approach indeed can be a helpful tool in analyzing such contrasting behavior. In an effort, to understand the isotropic compression behavior of wet granular materials, we used the dynamic 2PFV-DEM method. Figure 3, shows the isotropic compression behavior of an unsaturated compacted specimen. Based on the definition of the net stress, $\sigma_{net} = \sigma - p^a$, σ_{net} is measured as an external stress at the moving boundaries during the compression stage. In a recent study, Yuan et al. (2017) stated and evidenced that the average micro-mechanical contact stress $\langle \sigma_c \rangle$ can indeed be considered as an alternative definition for the effective stress in a partially saturated system. From the Figure 3, it can be seen that the net mean stress and mean effective stress (i.e., average contact stress obtained from Love-Weber's homogenization formula) definitions follow the Bishop's type of single effective stress equation (equation 4). Although, during the compression stage the degree of saturation keeps on reducing with an increase in the net stress and then becomes constant at higher net stress, but at the pore-unit level a local imbibition was also observed where a contracting pore-unit takes in water to maintain the pressure equilibrium across the neighboring pores. The overall decrease in the water saturation is attributed due to a unimodal pore size distribution (Figure 2), where the capillary pressure across the pore throat is greater than entry capillary pressure invoking a drainage of pore-unit during compression, Figure 4. Figure 5 shows the water saturation and capillary pressure across the domain at different net mean stress.

$$\sigma_{effective} = \sigma_{net} + \chi\ (p^a - p^w) \tag{4}$$

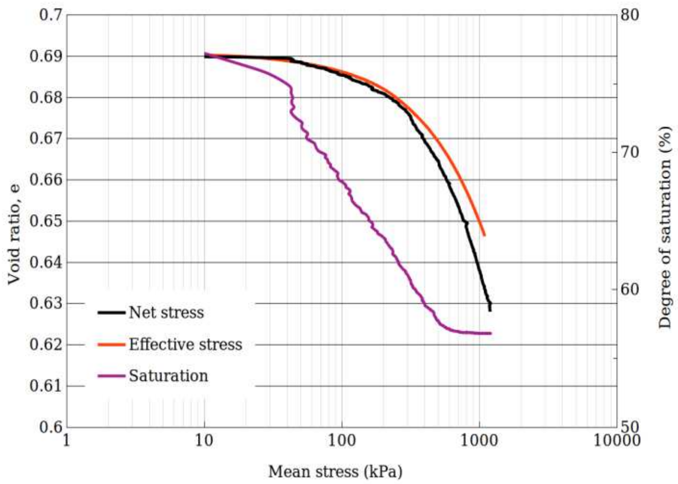

Figure 3. Isotropic compression curves showing the variation of void ratio (e) with net mean and mean effective stress, as well as change in degree of saturation (S^w) with net mean stress during the isotropic compression loading.

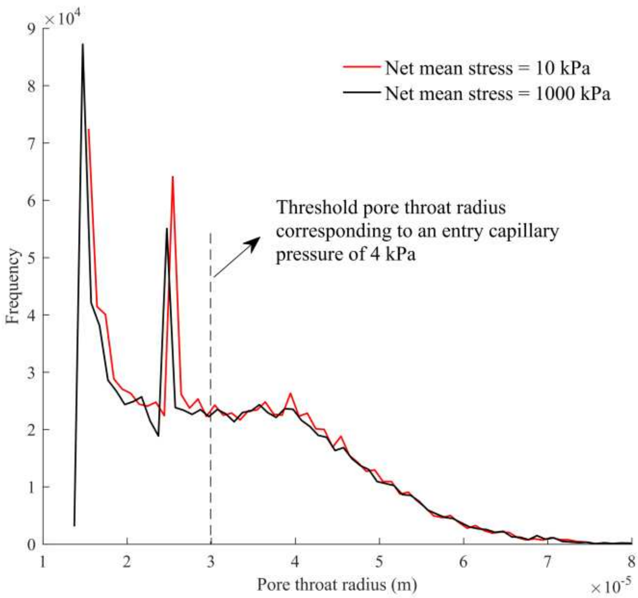

Figure 4. Pore throat radius distribution.

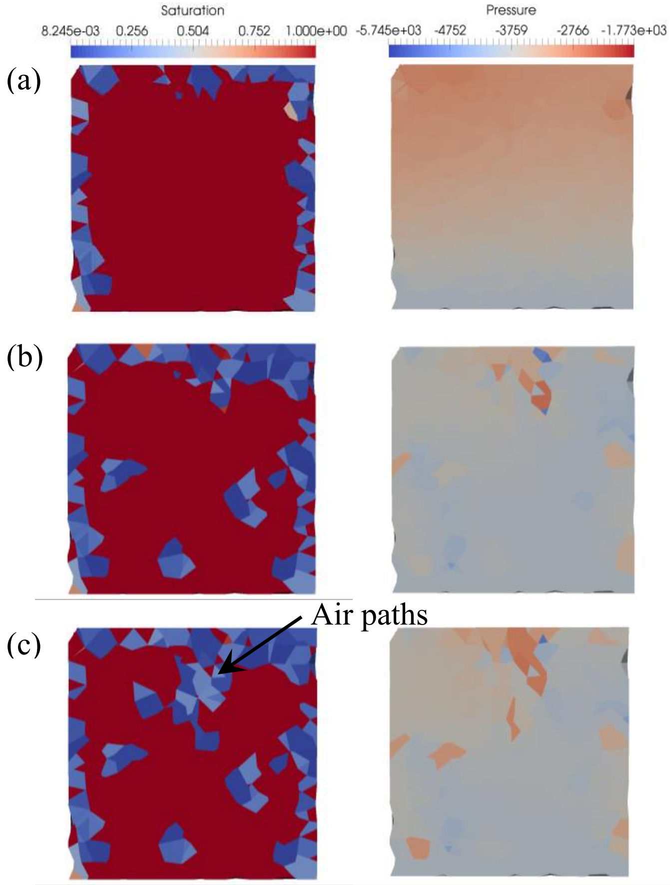

Figure 5. Saturation and capillary pressure field across the domain (XY plane) at net mean stress of (a) 10 kPa (b) 347 kPa (c) 478 kPa.

4 CONCLUSIONS

The paper briefly discussed about the dynamic two-phase pore-finite volume method coupled with discrete element method and presented a case simulating the isotropic compression behavior of a partially saturated granular medium. The paper clearly highlighted the distinction between the measured net mean stress and mean effective stress for a partially saturated granular system loaded under constant suction condition. The net mean and mean effective stress are related through a Bishop's type of single effective stress equation.

A future step towards such investigation would be to understand the underlying phenomenon of hydro-mechanical behavior of partially saturated granular system and subsequent studies (i.e., simulating different stress paths) to highlight the influence of pore size distribution on the hydro-mechanical behavior.

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