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Pore orientation of granular materials during biaxial compression

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ABSTRACT

The local pore spaces in granular materials tend to be aligned parallel to the major principal stress direction upon particle mobilization. Manifestation of this response has been numerically validated in our previous studies with the aid of discrete element method modeling and image processing techniques during creep and shearing. We now extend the modeling of pore geometry, constructed with spherical particles, to assemblies of particle clumps. Two-dimensional simulations are performed for both loose and dense assemblies of spherical particles and particle clumps. Each particle packing is bound by rigid or flexible walls and subjected to biaxial compression and the particle mobilization effect on the evolution of pore orientation is explored. Randomly shaped pores surrounded by adjacent particles are geometrically quantified by Delaunay tessellation and fitted with ellipses. Results show that localization is apparent in dense assemblies, in particular for clumped particle packing, while loose assemblies exhibit diffusive failure. Small pores within well-defined shear bands tend to align either parallel to the direction of the shear band or perpendicular to the major principal stress. On the other hand, small pores within the blocks and large pores have a tendency to become elongate towards the major principal stress direction. This study reveals for the first time that pore orientation is dependent upon particle shape, pore size, and assembly conditions on the pore and global scales.

1. Introduction

The geometry and characteristics of pores play a significant role in physical and geomechanical behaviors during consolidation, and in response to fluid and heat flow, and bio-activity [1–4]. The evolution of pore shapes and orientations when granular materials are subjected to shearing has been explored by physical experimentation and numerical simulation using the discrete element method [5–8]. The salient observations are that the orientations of particles and pores in cohesive soils tend to develop parallel to the shear failure plane, although the consequence of pore orientation is simply attributed to the systematic alignment of elongated particles rather than the unique formation of a skeletal structure [5,6]. Our previous research has shown numerically that particle mobilization induced by shearing and creep tends to form an arching structure that leads to an elongated pore space parallel to the major principal stress direction in 2D and 3D spaces, with the initial void ratio being a dominant factor [7–9]. It has also been suggested that the pore space becomes either collapsed or merged during particle mobilization, and that the resultant orientations of large and small pores are perpendicular to each other due to different mechanisms (e.g., alignment of large pores parallel to σ_1 and small pores normal to σ_3) [7]. However, strain localization, which takes place in a shear zone defined by a region of high void ratio and the relative motion of facing blocks on either side of the shear zone, and its relevance to pore geometry, have not been studied extensively. Many previous studies have focused on the stress–strain responses predicted by continuum numerical analyses and constitutive relationships that can be used to explain the mechanism of shear banding [10–12]. The most basic implementation of the discrete element method (DEM) involves spherical particles within a sample space defined by rigid walls, which makes it challenging to closely examine natural granular materials. Clumped particle assemblies and flexible membrane wall boundaries are alternatives when modeling irregularly shaped particles and mobilization in the fields of soil and rock mechanics [13]. Pore orientation can be assessed quantitatively using a series of image processing techniques such as Delaunay tessellation, the iterative identification of particle groupings for defining unit pores, and regression-based fitting of irregularly shaped pore spaces with ellipses. However,

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numerical assemblies subjected to pore orientation analyses in previous studies involved spherical particles in rigid walls, which circumvent insightful observation within the geometry-based framework. Moreover, little attention has been given to pore orientation within the shear-induced localization zone.

This study aims to extend the observation of stress-induced evolution of pore orientation to include a consideration of both particle shapes and boundary effects. We implemented a DEM for numerically synthesized two-dimensional packed assemblies with different initial void ratios. Subsequently, we analyzed the consequences of global and local pore orientations related to localization.

2. DEM simulation

The pore structure analyses presented below are based on the results of numerical experiments performed using the discrete element method software PFC^{2D} [14]. A total of eight particle assemblies were constructed to investigate the effects of boundary conditions, particle shape, and initial void ratio on global and local pore orientation induced by compression. The simulated cases are summarized in Table 1. All assemblies are generated using explosive repulsion followed by forced dissipation of kinetic energy and isotropic consolidation. Each numerical assembly is generated within a rectangular container with a height-to-width ratio of 2:1.

The initial density of the specimen was controlled by varying the initial coefficients of friction of the particles during generation and consolidation. Specifically, higher coefficients of friction result in assemblies that are stable at higher porosities. After consolidation, the contact coefficient of friction for all particles in all assemblies was set to a uniform value of 0.31 (the coefficient of static friction for planar quartz-on-quartz sliding [15]) while all boundaries remain frictionless. For some of the simulations, non-spherical particles are generated using the 'clump logic' inherent to PFC^{2D}. This allows particles to be fixed together to form arbitrary shapes but is computationally very efficient because internal contacts (i.e., overlaps) are ignored in subsequent calculations, and the same contact detection scheme that is used for particles may be exploited. The clumped particles considered in the current work consisted of identical spheres overlapped to create a 1.5:1 aspect ratio (note that these clumps have the same sieve diameter as their constituent spheres). Fig. 1 shows the clumped particle and the particle size distribution curves for both sphere and clump packings (the equivalent diameter is used for clumped particles). Particle interactions were modeled as linear elastic springs in the normal direction, and elastic and perfectly plastic spring–slider combinations in the shear direction. The associated mechanical properties were selected to be generally consistent with quartz sand (normal stiffness $k_n = 10^8$ N/m, shear stiffness $k_s = 10^7$ N/m, coefficient of friction $\mu = 0.31$, specific gravity $G_s = 2.65$; e.g., [12,16]).

The biaxial compression test was performed by applying a constant rate of axial compression on the specimen using upper and lower 'platens' while maintaining constant lateral stress conditions using either a rigid or a flexible boundary. Lateral stresses were servo-controlled by adjusting boundary velocities in response to global deviations from the desired stress conditions. The flexible membrane algorithm was used to apply a constant lateral stress to the sides of the assembly by measuring the out-of-balance force on each membrane particle and constantly adjusting the velocity of the membrane particles such that the sum of the out-of-balance forces on the membrane, divided by the current height of the specimen, was equal to the specified confining stress per unit depth into the page (100 kPa in the current work). In our simulations the flexible confinement algorithm was accurate to within ±1 kPa compared to ±0.1 kPa for rigid confinement.

The stress–strain–volume responses of tested specimens are presented in Fig. 2. The observed substantial decreases in deviatoric stress in the flexible cases (resulting in a negative deviatoric stress in one case) are due to the absence of any boundary effects at the top and bottom loading platens. The end platens are truly frictionless, and it is therefore possible for the specimen to 'collapse' diagonally after the onset of localization due to the significant heterogeneities in local stresses and strains across the regions of localization. Because the behavior of the assembly is no longer constitutive and the stresses and strains vary spatially within the specimen, there is no real 'correct' measure of stress and strain for the entire assembly. Accordingly, we elected to continue using boundary measurements for the global stress and strain of the assemblies so that the values reported are consistent across simulations.

On the macro-scale, the differences in the responses between rigid and flexible confinement are generally minor, particularly in the elastic regime, consistent with [13]. Notably, in rigid lateral confinement, a greater dilation is predicted for dense specimens because the rigid boundaries do not conform to the irregularly shaped particle assemblies. Due to increasing rotational frustration resulting in volume increases during shear, dense assemblies of clumps dilate more than dense assemblies of spheres; conversely, loose assemblies of clumps are more contractive than loose assemblies of spheres because the loose fabrics generated in assemblies of clumps tend to be metastable. The increased rotational frustration that is manifest in the clump assemblies results in higher shear strengths relative to sphere assemblies. The critical state is also a function of particle shape [17,18]. Particle information was extracted at every 1% global axial strain in order to further analyze the pore geometry.

3. Characterization of pore space

We defined the unit pore surrounded by adjacent particles on the basis of particle separation, and the orientation of the randomly shaped unit pore is analyzed by an ellipse-fitting before evaluating the global and local orientations.

3.1. Defining the unit pore

Pore geometry depends on the ensembles of neighboring particles. The identification of unit pores is a prerequisite to evaluating

Table 1
Assembly information.

Packing	Boundary wall	Particle shape	Initial void ratio	State	Number of particles
RCD	Rigid	Clump	0.1564	Dense	4665
RCL			0.2389	Loose	4665
RSD		Sphere	0.2551	Dense	7507
RSL			0.3069	Loose	7507
FCD	Flexible	Clump	0.1576	Dense	4665
FCL			0.2372	Loose	4665
FSD		Sphere	0.2537	Dense	7507
FSL			0.3131	Loose	7507