Powder Technology 323 (2018) 323–336

Contents lists available at ScienceDirect

Powder Technology

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

Three-dimensional Voronoi analysis of monodisperse ellipsoids during triaxial shear

Shiwei Zhao [a,b], T. Matthew Evans [b], Xiaowen Zhou [a,c,*]

[a] State Key Laboratory of Subtropical Building Science, South China University of Technology, Guangzhou 510641, China
[b] School of Civil and Construction Engineering, Oregon State University, Corvallis, OR 97331, USA
[c] Powerchina Huadong Engineering Corporation Limited, Hangzhou 310014, China

ARTICLE INFO

Article history:
Received 19 April 2017
Received in revised form 15 September 2017
Accepted 8 October 2017
Available online 12 October 2017

Keywords:
Discrete element
Granular structure
Ellipsoid packings
Set Voronoi
Triaxial compression

ABSTRACT

The internal structure of a sheared assembly of monodisperse ellipsoids is investigated using three-dimensional Voronoi analysis. The discrete element method is employed to simulate isotropic and triaxial compression tests of ellipsoidal particles. A recently developed Voronoi tessellation technique, i.e., Set Voronoi tessellation, is applied to constructing Voronoi cells of assemblies at a series of shearing states. Several quantities are provided to quantify the properties of Voronoi cells, including local porosity, reduced surface area, sphericity, and a modified Minkowski tensor. We show that average local porosity, average reduced surface area, and average sphericity are functions of global porosity and mean coordination number during shearing, suggesting a relationship between void and particle networks. Moreover, local porosity and reduced surface area statistically comply with a modified lognormal distribution regardless of particle shape for a similar global porosity. However, the shape of a Voronoi cell is significantly dependent on the particle it encloses. Shear-induced inhomogeneity and anisotropy measured by Voronoi-based quantities are also examined. Increasing shear-induced entropy is observed, which means a more disordered void network during shearing. Furthermore, anisotropy of Voronoi cell orientations shows a comparable trend with anisotropy of contact normals. These findings are useful for developing a better understanding of void networks and their relationship with particle networks for non-spherical assemblies.

1. Introduction

Granular materials are complex non-linear systems comprised of interacting discrete particles and exhibiting complex physical properties and mechanical behaviors varying from solid-like to fluid-like. Extensive experimental and numerical investigations, e.g., [1–3], have been conducted, with the conclusion that macroscopic physical and mechanical properties are strongly related to internal packing structure (or fabric). For example, effective thermal conductivity can be estimated based on particle networks [4] and shear strength can be linked to the anisotropy of angular dependences (e.g., contact directions and contact forces) via the so-called stress-force-fabric relationship [5]. Therefore, a deeper understanding of granular structure is of great importance for better applications in industry (e.g., powder handling and granulates in pharmacy) and engineering (e.g., soil mechanics and additive manufacturing). However, quantitatively characterizing internal structure of a packing is still challenging due to disordered particle and void networks.

Particle shape has been regarded as one of the key factors affecting a packing structure [1,6]. In recent years, there has been a growing interest in packing structure of non-spherical particles in different disciplines, especially using numerical methods, e.g., the discrete element method (DEM) [7–9]. A broad range of particle shapes has been investigated, such as ellipsoids/super-ellipsoids [10,11], polyhedrons/sphero-polyhedrons [12,13] and cylinders/sphero-cylinders [14,15], where packing structure is characterized with several parameters including packing density, coordination number, and the radial distribution function. In addition to these commonly used parameters, packing structure can be charaterized in terms of fabric vectors, such as particle orientation, contact orientation, branch vector, normal and tangential contact forces. For example, Zhao et al. [6] found that particle shape has a significant effect on the anisotropy of fabric vectors by using DEM simulations of super-ellipsoid packings.

In addition to particle networks, void networks also play an important role in internal structural inhomogeneity and anisotropy of a packing, which however, receives limited attention due to the

* Corresponding author at: State Key Laboratory of Subtropical Building Science, South China University of Technology, Guangzhou 510640, China.
E-mail address: xwzhou@scut.edu.cn (X. Zhou).

https://doi.org/10.1016/j.powtec.2017.10.023
0032-5910/

difficulties in characterizing. Porosity, for example, provides an important macroscopic measure of assembly state, but does not elucidate particle-scale details such as void shape and distribution. Previous studies have shown that the particle-scale information of void space is related to deformation behavior, stress state, and conduction phenomena in granular materials [16–20]. Hence, it is necessary to investigate the particle-scale void space for a better understanding of packing structure.

Several schemes have been employed to quantify void space within a granular material to date. A direct approach is to extract the void network from the matrix. However, it is difficult to quantify the entire void network. For simplicity, individual voids are often approximated by using ellipses or ellipsoids, e.g., [18,19]. However, this method might be not applicable for complex void shapes. Another approach is to enclose a void unit with part of its surrounding solid. For example, Oda [21] connected the mass centers of particles surrounding a void to define a polygonal cell (i.e., a void unit) to quantify the local porosity for sands in 2D. An alternative to Oda's void-centric approach is a granocentric tessellation [22,23] which captures local void space surrounding individual particles. One typical approach is the Voronoi tessellation, which has been widely applied to sphere packings, e.g. [24–27], whereas just a few for non-spherical particles [28–31] due to the complication of construction of Voronoi cells. Three-dimensional Voronoi analysis of sheared assemblies of non-spherical particles is even less.

This paper investigates Voronoi cell properties of sheared assemblies of ellipsoids with particle shape effect during shearing. An in-house DEM code [6] is used to conduct isotropic consolidation and triaxial compression simulations for mono-disperse ellipsoid assemblies with different aspect ratios. The recently-developed Set Voronoi tessellation method [32] is applied to tessellate assemblies. The evolution of local porosity, reduced surface area, and Voronoi cell sphericity are investigated during shearing, followed by a preliminary study on their relationships with coordination number. Then, inhomogeneity and anisotropy are investigated from both particle and void networks.

2. Method description

2.1. Discrete element model

The discrete element method [7] is one of the most efficient and powerful numerical tools for modelling granular assemblies. Particle motion is governed by the following Newton's and Euler's equations:

$$F_i^{(b)} + f_i^{(d)} + \sum_{c=1}^{N} F_i^{(c)} = m\frac{\mathrm{d}v_i}{\mathrm{d}t} \tag{1a}$$

$$T_i^{(d)} + \sum_{c=1}^{N} M_i^{(c)} = I_i\frac{\mathrm{d}\omega_i}{\mathrm{d}t} - (I_j - I_k)\omega_j\omega_k \tag{1b}$$

where i, j, k are subsequent indexes; m is particle mass; v_i and ω_i are the translational and angular velocities, respectively; N is the number of contacts; $F_i^{(c)}$ is the contact force at contact c; $F_i^{(b)}$ is the body force; I_i is the principal moment of inertia; $M_i^{(c)}$ is the torque around the mass center at contact c; $f_i^{(d)}$ and $T_i^{(d)}$ are damping force and damping torque, respectively, which are artificially introduced to facilitate the dissipation of kinetic energy in the system. A linear-spring contact model and the Coulomb friction model are applied at each contact. Note that the computation of contact force involves a procedure of contact detection which is more complicated for non-spherical particles than spherical particles. All algorithms are implemented in an in-house DEM code, *SudoDEM*, developed by the authors [6].

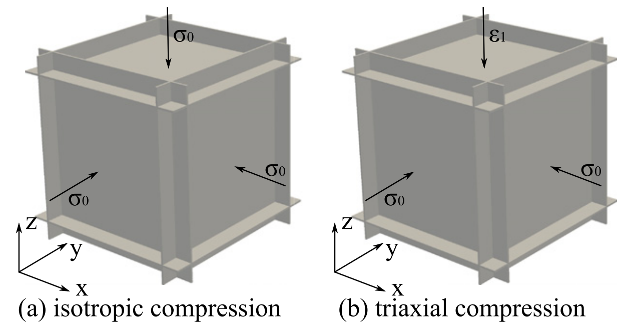

Fig. 1. Loading schemes of (a) isotropic compression and (b) triaxial compression. Note: the two parallel walls have the same boundary condition.

2.2. Isotropic consolidation

Prior to being subjected to isotropic consolidation, five groups of monodisperse assemblies with different aspect ratios η are generated in a cubic container with six frictionless rigid walls. Each assembly is comprised of 5000 monodisperse ellipsoidal particles. Specimens are prepared for consolidation using the procedure described below. First, particles are randomly generated without consideration of the induced particle overlap. Second, the system is allowed to cycle to equilibrium as excess kinetic energy is dissipated. Energy is dissipated by periodically setting the velocities of all particles to zero while the container walls remain fixed.

The consolidation procedure is implemented via a numerical stress-control servo [33] to keep a constant stress σ_0 of 100 kPa on each wall, referring to Fig. 1 (a). Accordingly, each assembly reaches an isotropic stress state with an unspecified porosity after consolidation. Varying the inter-particle coefficient of friction μ between 0.1 and 0.5 yields consolidated specimens with a range of porosities. Specimens with porosities close to the target (i.e., 0.394) are selected for triaxial compression tests. Such a trial and error procedure for obtaining consolidated specimens with similar porosities is also adopted in the literature [34,35]. The inter-particle coefficient of friction is set to 0.5 after consolidation, while the other basic material properties are kept constant (Table 1).

2.3. Triaxial compression

Five consolidated specimens with a target porosity of 0.394, denoted as S10, S12, S15, S17, and S20, are selected for the triaxial compression tests. Their corresponding characteristics are listed in Table 2. Fig. 2 shows snapshots of initial configuration of these specimens.

During triaxial compression, the top and bottom walls move towards one another at a constant velocity, while the other four side walls move individually to maintain a constant confining stress σ_0 of 100 kPa with the stress-control servo (Fig. 1 (b)). To ensure quasi-static behavior during shear, the shear strain rate should be

Table 1
Material properties used in the DEM simulation.

Parameter	Value
Particle density, ρ (kg/m^3)	2650
Particle coefficient of friction, μ	0.5
Damping coefficient, α	0.3
Particle/wall normal stiffness, K_n (N/m)	1×10^8
Particle/wall tangential stiffness, K_t (N/m)	7×10^7