Particle shape effect on the mechanical properties of the granular material using novel 3D angular ellipsoid

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Abstract. Particle shape has long been a key issue for engineering. However, the underlying microscopic mechanism of this effect is not well understood, and thus the connection between the particle shape and mechanical behaviour of the particulate system remains empirical and qualitative. This study intends to obtain desired shape descriptors that govern the mechanical behaviour of a granular material at the particulate level and deduce a possible underlying micro-macro relationship between the particle shape parameters and the mechanical characteristics of the assembly of the particles. A modified open-source 3D discrete element code, Yade is used to simulate a series of tri-axial compression tests on specimens composed of angular ellipsoids. The mechanical behaviour such as the shear strength, the anti-deformation ability are obtained. The results show that the shear strength increases with the angularity. However it first increases then drops with the increase of the aspect ratio. The anti-deformation ability decreases with the increase of the aspect ratio and angularity. This study provides insight into the micro-macro relationship between mechanical properties and particle shape parameters.

1. Introduction
Granular materials are commonly used in man-made earthworks such as rockfill dams, of which the mechanical behaviour including the strength and the deformation variables has to be reasonably predicted and cautiously controlled so as to ensure safe operations. Most granular materials in engineering scenarios exhibit a wide range of particle shapes, which justifiably and significantly affects mechanical behaviour of the structure. A long range of shape parameters are available such as aspect ratio, angularity and roughness. It has always been an aspiration to discover a simple yet concise way to describe the shape characteristics and link them with the bulk mechanical behaviour. With the advanced imaging technologies such as X-ray and computed tomography scan (CT scan), it is possible to obtain the shape characteristics of a real material and conduct corresponding analysis [1–4]. For understanding the underlying mechanism, it is, however, more advisable to model particles with different shapes and implement analysis via numerical simulation. Such practices have been surging recently. Different shapes are modelled and investigated ranging from bonded particles simulating shapes of triangle, square and hexagon, clumped balls, ellipses, polygons, ellipsoids, polyhedrons to super ellipsoids [5-7]. With quantified and different shape polydispersity, a number of behaviours at different scales including the fabric of granular packing patterns [8], friction and dilation angle[9], basic shear strength and dilatancy properties[10], shear modulus and damping
ratio[11], particle orientation distribution[12] and fabric and force distribution and anisotropies[13]. Besides activities at micro and macro level, phenomenon at meso-scale are observed as well [14]. To interpret these phenomena, various variables or activities are examined to formulate relationships between micro or meso-scale and the macro behaviour of granular material. Force chains and contact network topology [15], coordination number [16], the probability distributions of friction mobilization [17] are explored. However, it is still quite open in terms of the particle shape effects on granular material mechanical behaviour, which is of strong practical significance and will be the focus of this study. Furthermore, while it is true that the two-dimensional (2D) model works better in terms of calculation efficiency, but it is weak in capturing shape features and far from the realistic scenario. With the development, it is easy to conduct 3D simulations tough it may require longer time.

2. Methodology

2.1 DEM contact model

Yade is an open-source DEM (Discrete Element Method) simulation tool [14]. In this study, a modified version is used where the particle shape is generated using several planes. The particle is enclosed by numerous infinite planes as predefined so that the ellipsoid tends to be angular.

As for the contact model, the linear contact model is used, combined with the Coulomb’s law. The normal contact force $f_n$ is calculated as follows:

$$f_n = k_n A_n n_n$$  \hspace{1cm} (1)

where $A_n$ is the overlapping volume of two particles in contact, $n_n$ represents the normal direction vector, and $k_n$ is the normal stiffness given by:

$$k_n = \frac{2E r_a r_b}{(r_a + r_b)}$$ \hspace{1cm} (2)

where $E$ is the Young’s modulus of the two contacting particles with radius $r_a$ and $r_b$. The tangential stiffness $k_t$ equals the normal stiffness multiplied by the Poisson’s ratio. The tangential contact force $f_t$ is calculated in an incremental manner as follows:

$$f_t = \begin{cases} (f_t)_0 - k_t \Delta u, & \text{if } |f_t| \leq \mu |f_n| \\ -\mu |f_n| n_t, & \text{otherwise} \end{cases}$$ \hspace{1cm} (3)

where $(f_t)_0$ is the shear(tangential) contact force acquired from the previous time step, $\Delta u$ is the increment of the relative tangential displacement, $n_t$ denotes the direction vector of $u$, $\mu$ is the inter-particle friction coefficient, $|\cdot|$ returns the magnitude of a vector.

In addition, a local viscous damper is introduced to dissipate kinematic energy and take into account the quasi-static condition. The damping force is defined as:

$$f_{\text{damping}} = 2\alpha \sqrt{mk_n V}$$ \hspace{1cm} (4)

where $\alpha$ represents the damping coefficient, and $m$ is the equivalent mass of the two contacting particles. $V$ is the relative velocity of the two contacting particles. It should be noted that the direction of the damping force is opposite to the relative velocity of the particle.
2.2 Particle shape

Fig. 1. The close-up of the angular ellipsoid employed in this study with (a) 20 and (b) 100 vertices.

The shape parameters we choose are listed in this section. The baseline shape we choose is an angular ellipsoid which is shown in Fig. 1. Ellipsoid is prevalent in research, however, in reality, particles are angular. Therefore, we define an angular ellipsoid in Yade using Python script.

The angularity $\delta$ is described as the number of the vertices of the ellipsoid. More vertices contribute to a rounder shape and is therefore corresponding to a larger angularity. The angularity we have defined is directly related to the change of the shape form and will significantly influence other shape metrics. Therefore, we define the angularity as one of the primary shape parameter. The angularity is normalized as 0 (corresponds to 20 vertices) to 1 (corresponds to 100 vertices) with an interval of 0.25. Other shape parameters are calculated as follows. Another primary shape parameter is the aspect ratio which is defined as the ratio of the longest diameter of the particle to the smallest one. We carefully control both the aspect ratio and the angularity to explore the shape effect on the mechanical behavior. We have generated 3 different levels of aspect ratio ranging from 1 to 3. Therefore, we have obtained in total 15 samples with different levels of shape parameters.

2.3 Simulation setup

In our simulation, 15,000 particles with the same shape parameters are used to generate the dense sample where the friction angle of inter-particle and particle-wall is both set to zero followed by a minor vibration of the wall to further compact the sample. It is noted that every particle is identical in terms of shape but differs in size within one sample. The equivalent diameter of the particle, which is the diameter of a sphere with the same volume of one particle ranges from 1 mm to 3 mm.

Then, the drained biaxial compression simulation is conducted, which includes two steps, namely an isotropic compression stage and a shear loading stage. At first, every sample is isotropically compressed using a servo-control mechanism under several different levels of confining ranging from 100 kPa to 500 kPa with an interval of 100. The compression will not stop until the kinetic energy of the whole system is smaller than $10^{-15}$ J, which manifests a desired stable state. Afterwards, the sample is vertically compressed by moving the top rigid wall downward at a constant velocity of 0.01 m/s. This loading rate is cautiously chosen to be small enough to satisfy a quasi-static condition. As shearing starts, the confining pressure on the lateral walls remains constant by the servo-control. All samples are sheared to an axial strain of 30%, when a critical state is reached and the re-organization of the internal texture becomes nearly steady. The major simulation parameters are listed below. To guarantee the accuracy, all the samples are sheared for three times independently and the results shown below are averaged as well.

| Table 1. DEM simulation parameters. |
|-------------------------------------|
| Parameter                            | Value        |
| Young’s modulus $E$ (GPa)            | 10           |
| Poisson’s ratio                      | 0.3          |
| Density (kg/m$^3$)                   | 2650         |
| Particle number                      | 15000        |
| Circumscribed diameter range (mm)    | 1 mm–3 mm    |
| Inter-particle friction angle (°)    | 35           |
3. Results

3.1 Strength

The critical internal friction angle is plotted against different levels of angularity and aspect ratio, as shown in Fig.2. It could be reached that the shear strength goes up with the angularity, as proven by plenty of previous research. The increase in the angularity intensifies the interlocking between contacting particles, resulting in larger shear strength. As for the aspect ratio, it could be found that when aspect ratio changes from one to two, the increase of the shear strength is obvious. However, as the aspect ratio goes even larger, the tendency becomes somehow vague. Although the shear strength still goes up with the angularity, sample with aspect ratio equaling three demonstrates smaller shear strength than that with aspect ratio equaling two.

3.2 Deformation

Deformation has long been crucial to engineering safety. The slope of the $e$-$p$ curve is a strong indicator for the deformation capability. We have presented the $e$-$p$ curves for two sets of samples as...
shown in Fig.3. In Fig.3 (a), the sample with aspect ratio equalling two is shown. It could be reached that the slope of larger angularity becomes steeper, indicating weaker anti-deformation capability. In Fig.3 (b), the sample with angularity equalling zero is shown. The effect of aspect ratio on the deformation ability is not as strong as that of the angularity. However, it is still evident that particles with larger aspect ratio tend to form a sample equipped with larger $e$-$p$ curve slope, denoting the weaker anti-deformation capability. The reason could be that with more angular and elongated shape, the rotation and rolling of an individual particle will induce larger deformation of its adjacent particles.

4. Conclusions
This study puts forward a novel approach for generating angular ellipsoids and have conducted a series of tri-axial compression tests on dense samples composed of particles with different levels of angularity and aspect ratio. Five different confining pressures are selected. The results concerning both the strength and the deformation properties are discussed. The shear strength goes up with the angularity. However, the shear strength goes up at first then drops when the aspect ratio changes from one to three. As for the deformation ability, the slope of the $e$-$p$ curve is chosen as the index. It is found that particles with smaller aspect ratio and angularity will form a packing with stronger anti-deformation capability. And the effect of the angularity is larger than that of the aspect ratio. This study focuses on a brand new type of shape and reaches several interesting conclusions regarding the mechanical behavior of the granular material.

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