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Influence of particle shape on the microstructure evolution and the mechanical properties of granular materials

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ABSTRACT

In order to study the influence of particle shape on the microstructure evolution and the mechanical properties of granular materials, a two-dimensional DEM analysis of samples with three particle shapes, including circular particles, triangular particles, and elongated particles, is proposed here to simulate the direct shear tests of coarse-grained soils. For the numerical test results, analyses are conducted in terms of particle rotations, fabric evolution, and average path length evolution. A modified Rowe's stress–dilatancy equation is also proposed and successfully fitted onto simulation data.

1. Introduction

Granular materials exist in nature and human activities extensively, such as debris-flow in nature and rockfill materials in civil engineering. Their strength and deformation vary with the different particle shapes. The physical mechanisms responsible for these differences are a question often raised by many researchers [1–5], from which we can see that the mechanisms also need to be explored through different perspectives and methods. Therefore, the particle shape is still worth noting, and its influence on the mechanical behaviour of granular materials remains an open topic.

Laboratory experiments have been carried out to explore the influence of particle shape on the mechanical properties of granular assemblies by many researchers, such as Shinohara et al. [6], Cho et al. [7], and Yang et al. [8]. However, these traditional laboratory experiments (such as direct shear tests, simple shear tests, and triaxial tests) only provide limited macroscopic strength and deformation. To collect microscopic information about the specimens, X-rays [9], CT scan [10], photoelasticity [11] and so on were employed in laboratory tests. But these methods are extremely expensive. Therefore, a cheaper technique, discrete element method (DEM), was employed by many researchers [12]; it has also other advantages, such as having access to any microscopic data including contact forces and controlling different loading-paths easier. DEM could also be used to investigate the relationship between microscopic information and the macromechanical properties of granular assemblies [13]. With the help of DEM, the microscopic information of a specimen is collected more easily than

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before. At the same time, with an improved computational efficiency, the non-circular and non-spherical shapes can be considered in the DEM. Hence, many numerical simulations for researching the role of particle shape in granular materials were performed. For instance, Nouguier-Lehon et al. [14], using biaxial numerical simulation to explore different shapes (i.e. circular, isotropic polygonal, and elongated polygonal shapes) showed that the behaviour of samples with isotropic particles can be dissociated from that of samples with anisotropic particles. Zhao et al. [15] developed four categories of assemblies with different angularities to investigate the evolution of coordination number, contact force distribution, and anisotropies of particle orientation and contact normal by the YADE DEM code. Yang et al. [5] performed undrained numerical simulation to study the differences between three types of non-convex grains (i.e. disk, ellipse, and triangle) without rolling resistance and disks with rolling resistance, demonstrating that the influence of the shape irregularity of particles is much different from that of the rolling resistance at the particle contact. In previous works [16–18], some other characters of particle shape have been studied by using DEM. From these references, particle shape was systematically accounted for through anisotropy and coordination numbers. This is however too rough in some cases and more information can be recovered for instance by considering particle rotation and complex networks. Complex network has been used in the analysis of granular materials [19,20]; nevertheless, only one shape of particles was used in numerical simulations with circular or spherical particles. Hence, using a complex network to analyse the role of particle shape in granular materials is a new way.

There is an increasing interest in quantifying the interactions between particles, as evidenced by publications, including those by Thornton et al. [21], Kuhn [22], and Wang et al. [23]. Furthermore, information about particle contact in connection with the macromechanical properties of granular materials has been studied by researchers in many ways. For instance, Kruyt [24] investigated the relations between macro-level, continuum characteristics and micro-level, particle characteristics, and an evolution relation was proposed for the changes in the fabric tensor as a function of the fabric tensor and the strain increment tensor, which agreed well with the simulations. Nicot et al. [25] proposed two micromechanical models that agree well with the results from numerical simulations containing 10,000 spherical particles. Other researchers, including Chang et al. [26] and Zhao et al. [27], also tried to establish the relationship between fabric evolution and the macro mechanical behaviour of granular materials. There were few non-circular particles considered in the existing researches to establish the bridge between micro-information and the macrobehaviour of granular materials. Hence, in this paper we will propose a two-dimensional DEM analysis of different particle shapes and try to establish a bridge between the micro and macro property.

In recent researches [14–18], most of them have been focused on investigating the influence of particle shape on the micro-scale information through a traditional method (i.e. fabric evolution). The influence of particle shape on granular materials explored from other perspectives and methods is relatively lacking. On the other hand, establishing the bridge between micro-analysis and macrobehaviour just considers the circular or spherical particles in major related references. Particle shape received little attention in most analyses aimed at establishing the bridge between micro- and macroproperties. It is obvious that the influence of particle shape on the microstructure evolution and the mechanical properties of granular materials is still an open topic, and many works can be done on this. In this paper, we propose a two-dimensional DEM analysis of different granular materials: circular particles, triangular particles, and elongated particles. Firstly, the particle shape measurement is introduced to identify the particles used in numerical simulations. Secondly, the simulated method of direct shear tests is proposed to do the numerical simulations. Then, influences of particle shape on macromechanical properties, particle rotation, fabric and average path length are analysed, respectively. Finally, the Rowe's stress–dilatancy relation is modified according to particle shape and fabric, and this modified equation is compared with the numerical results.

2. Particle shape measurement and structural characteristics

2.1. Particle shape measurement

The aspect ratio (AR), convexity (C) and sphericity (S) proposed by Yang and Altuhafi [1,28] are adopted to measure the particle shape, referring to Fig. 1a. The aspect ratio is defined as the ratio between the minimum and maximum Feret diameters, where the Feret diameter of the particle is defined as the measured distance between parallel lines tangent to an object's outline; the convexity is the area of the particle (A) divided by its area if any concavity within its perimeter is filled ($A + B$); the sphericity is defined as the ratio of the perimeter of a circle with the same area as the area of the particle to its actual perimeter. From the definitions of the aspect ratio, convexity and sphericity [28], we know that the three methods consider the influence of different factors on the shape. AR is sensitive to the elongation of the particle; C controls the concavity of the particle; S is a parameter comparing particles with circles. The whole information about particle shape cannot be described using one or two of them [28], and the weighted coefficients of these three parameters are still not clear. Therefore, by combining AR, C, and S, a new shape measurement, the overall regularity (OR), is defined as the average of the three shape parameters proposed as [1]:

$$OR = (AR + C + S)/3 \tag{1}$$

Using this method to calculate the three types of particle, the OR values for circular, triangular and elongated particles are determined as 1.0, 0.96, and 0.79, respectively. Such process is illustrated in Fig. 1b.

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