Influence of Particle Shape on Mechanical Behavior of Granular Materials

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Abstract The purpose of this paper is to explore the influence of particle shape on the mechanical behaviors of granular materials using the discrete element method (DEM). Particles with random polygonal shapes were generated using 'clumps' (groups of circular particles). The relationships between the particle-scale parameters and the macroscopic responses of granular materials were identified by simulating the biaxial compression tests on numerical samples. The effects of particle shape on the shear strength and deformation of granular materials were analyzed. The micromechanics of the macroscopic responses were investigated through a variety of mechanism demonstrations and micromechanical analysis.

1 Introduction

Granular materials such as sand, gravel, ballast, rockfill, consist of a mixture particles with different sizes and different shapes. Previous studies [1, 4, 10, 16, 20] have shown that particle shape has significant influences on the macro-mechanical behavior of granular materials. The underlying mechanism results from the particle level interactions which are mainly affected by particle shape.

The discrete element method (DEM), which was pioneered by Cundall and Strack [6], has been applied in the research fields of granular materials and accepted as an excellent approach to investigate both the macro-mechanical behavior and the

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underlying micro-mechanism of granular materials. However, the particle shape cannot be reproduced in DEM environment directly as the base element is disk (2D situation) or sphere (3D situation) in the early DEM models. In order to investigate the particle shape effect on the constitutive behaviors of granular materials using DEM, several methods have been proposed to approximate the real particle shapes. An agglomerate of discs or spheres (overlapping and non-overlapping) was introduced to model the irregular particle shapes [5, 7, 8, 12, 13, 17, 18, 19]. In addition, non-spherical base elements such as polygon-shaped elements [2, 3], ellipse-shaped elements [9, 14, 15] were developed to introduce the particle shape effect. However, the simulation of real particle shapes requires a mass of discs or spheres, which may significantly decrease the computation efficiency. The irregular particle shapes are also hard to be considered in large scale analysis, at least with present available computational facility. In addition, ellipse-shaped elements and polygonal elements used in previous literatures cannot reflect the randomness of the real particle shapes.

In this paper, a novel method is proposed to simulate the complex shape of granular materials in the frame of polygonal shape under DEM environment. The generation of random polygon-shaped particle is first briefly introduced. Then a series of biaxial compression tests are conducted. The particle shape effects on the mechanical behaviors of granular materials, including the shear strength, volume strain, and peak friction angle are discussed. Lastly, conclusions and remarks are provided to guide further studies.

2 Modeling Method of Particle Shape

In previous studies the particle shape was generally simulated by polygonal or elliptical elements, which can represent the real particle shape on some degree (e.g. [2, 3, 14]). In this paper the particle shape is generated under the frame of polygonal shape.

The polygonal shape is generated by randomly selecting points on the circle before lining the adjacent two points along a counter-clockwise direction (see Fig. 1). This process abides by an algorithm that forms a convex polygon from the randomly selected points. Polar coordinate is used to determine the position of each vertex based on the local coordinate of the circle as follows:

$$\theta_k = 2\pi[1 + (2b_k - 1)\delta]/n \tag{1}$$

where θ_k is the angle corresponding to the kth edge, b_k and δ are random number in the interval [0, 1], n is the total number of edges of a polygon. As the introduction of b_k and δ, the sum of θ_k may not equal to 2π, θ_k should be corrected to make the polygon closed. The correction equation is described as follows:

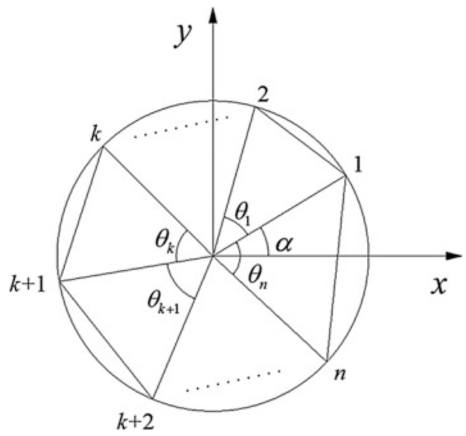

Fig. 1 Random polygonal particle shape

$$\bar{\theta}_k = \theta_k \left(2\pi / \sum_{j=1}^{n} \theta_j \right) \tag{2}$$

The coordinate of polygon vertex is determined as follows:

$$\begin{aligned} x_k &= x_0 + r\cos(\alpha + \theta') \\ y_k &= y_0 + r\sin(\alpha + \theta') \\ \theta' &= \sum_{i=1}^{k} \bar{\theta}_i \end{aligned} \tag{3}$$

where (x_0, y_0) is the center coordinate of the circle in global Cartesian Coordinate System, r is the radius of the circle, α is an original phase angle which can be described as $(\frac{\pi}{2} \times rand)$, where *rand* is a random value in the range of [0, 1].

A Fish code is written to realize this process based on the initial sample generated in PFC2D. The data of polygonal vertexes is saved as a text file to produce the areas of polygons in Finite Element (FE) environment. After generating the areas of polygons, the meshing technique embedded in ANSYS is applied to mesh the areas with a desired element size. Then the area and the central coordinate of each element are calculated and the information of the corresponding disk with the same area and central coordinate is outputted to a text file. Lastly, the text file is inputted into PFC2D and the clumps composed of overlapping discs are created by grouping the balls within the same surface of the irregularly shaped particle. The generation process is shown as Fig. 2. Figure 3 shows the randomly generated polygon with different number of edges. It is obvious that polygonal particle with more edges is much closer to a disk.

As the center of each disk is seated on the mass centroid of each corresponding element and the disk has same area with the replaced element, the total mass is

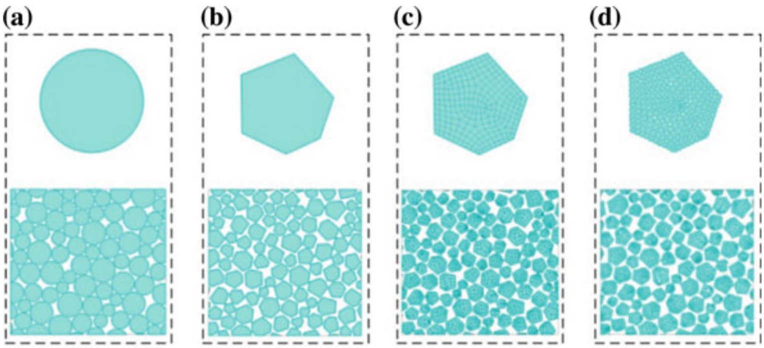

Fig. 2 Illustration of the generation process of random polygonal particle assembly. **a** Original particle assembly generated in PFC2D environment; **b** areas of random polygonal particles generated in ANSYS; **c** random polygonal particles after meshing with a desired element size; **d** particle assembly composed of clumps with overlapping discs generated in PFC2D environment

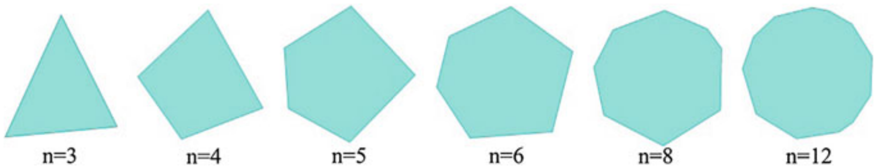

Fig. 3 Randomly generated polygonal particle with different number of edges

unchanged after the replacement as well as the particle inertia. This method can avoid the particle inertia problem mentioned by Ferellec and McDowell [7].

3 Biaxial Compression Simulation Tests

3.1 Generation of Samples

A series of biaxial compression simulations were implemented in PFC2D environment. The polygonal particle generating method mentioned above was used to generate particles with different shapes. Samples with a desired porosity were generated in a space with 600 mm height and 300 mm width. All samples were isotropically compressed with a servomechanism to a confining pressure of 0.8 MPa before biaxial shearing. All the compression tests were carried out under a gravity-free environment. The input parameters are listed in Table 1. A uniform particle size distribution was used with the particle diameter ranges from 10 to 20 mm. The number of polygon edges, *n*, was used as a shape descriptor (as shown in Fig. 3) and the element size used was 0.003 m.

Table 1 Set of parameters used in the simulations

	Particle density (kg/m^3)	2650
Disk	Normal stiffness, k_n (N/m)	1.0e^8
	Shear stiffness, k_s (N/m)	1.0e^8
	Friction coefficient	0.5
Wall	Normal stiffness of top and bottom walls (N/m)	3.0e^8
	Normal stiffness of lateral walls (N/m)	3.0e^7
	Friction coefficient	0.0

Three kinds of polygon with different edges (i.e., n = 4, 6, 8) and a perfect disk were used to generate four different samples with an initial porosity of 17 % (Fig. 4). The area conversion ratio $\alpha = A_{aim}/A_{orig}$, was introduced to describe the overall sphericity of the desired sample (e.g. Figure 2d) compared with that of the original sample (e.g. Figure 2a). A_{aim} and A_{orig} are the total area of the particles of desired sample and the total area of the particles of original sample, respectively. Apparently, α increases with the increasing number of polygon edges. The maxima of α, i.e. 1, can be obtained when the sample is composed of ideal circular particle (see Fig. 4d). The parameters of numerical samples with different-shaped particles were shown in Table 2.

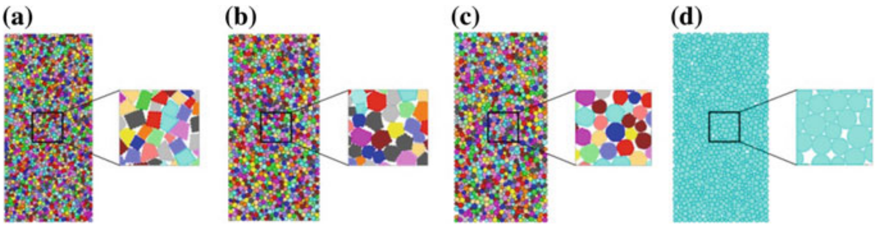

Fig. 4 Numerical samples with differently shaped particles: **a** sample 1; **b** sample 2; **c** sample 3; **d** sample 4

Table 2 Parameters of numerical samples

Numerical sample	n	Initial porosity	Particle counts	Clump counts	Disk counts	α	Sample no.
Sample 1	4	0.170	1470	1470	24,707	0.575	S-1
Sample 2	6	0.171	1083	1083	23,196	0.780	S-2
Sample 3	8	0.170	980	980	34,137	0.862	S-3
Sample 4	–	0.170	845	–	845	1	S-4

3.2 Results and Discussions

The deviatoric stress versus axial strain and volumetric strain versus axial strain curves of different samples were monitored during the tests and shown in Fig. 5.

The peak deviatoric stress decreased with the increasing number of polygonal edges (see Fig. 5a). This was consistent with the conclusion of [11] that particles with more angular shape cause an increase in shear strength. The peak deviatoric stresses and peak friction angles of different samples obtained from the simulation results were shown in Fig. 6. The volumetric stain variation of different samples (see Fig. 5b) reflected the particle shape effect as well. For S-4, the sample behaved a strong shear contraction as the circular particles have no rolling resistance. For samples with shaped particles, the more angular the particle shape was, the larger shear contraction and shear dilatancy can be mobilized.

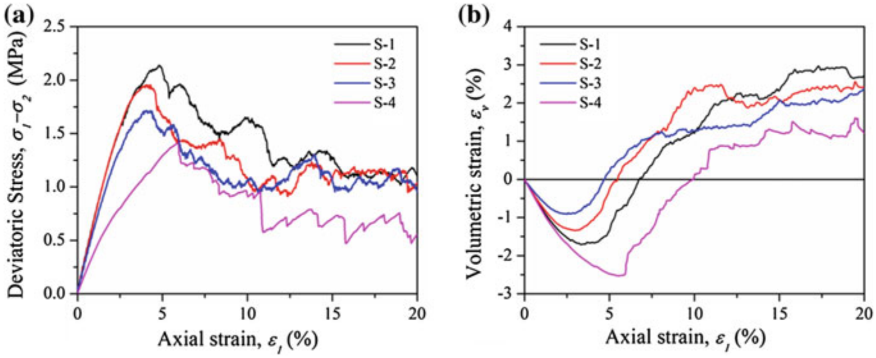

Fig. 5 **a** Deviatoric stress-axial strain relationships of different samples; **b** volumetric strain-axial strain relationships of different samples

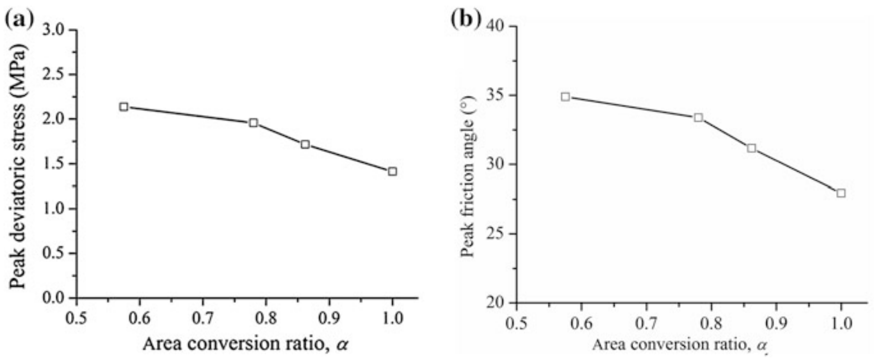

Fig. 6 **a** Peak deviatoric stress variation of different samples; **b** peak friction angle variation of different samples

4 Conclusions

A novel polygonal particle shape generating method for DEM using the meshing technique embedded in ANSYS and overlapping discs has been developed. The method can produce irregular particle shape randomly under the frame of polygonal shape. The particle inertia of irregularly shaped particles generated in DEM environment is same as original particle inertia. Particle shape effects on the mechanical behavior of granular materials were investigated based on this method. The numerical results match the finding of Matsushima and Saomoto [11] very well. This method provides a feasible way to study the particle shape effects on granular materials. In the proposed numerical simulation, complex particle shape was not considered as well as the particle breakage. The other kind of simplified particle shape and particle breakage will be discussed in subsequent papers.

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