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Discrete element modelling of ellipsoidal particles using super-ellipsoids and multi-spheres: A comparative study

Ying You, Yonzhi Zhao *

Institute of Process Equipment, College of Energy Engineering, Zhejiang University, Hangzhou 310027, China

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ABSTRACT

Two discrete element models, super-ellipsoid model and multi-sphere model, are employed in this paper to describe the ellipsoidal particles. And the packing and flow behavior of ellipsoidal particles are investigated by the discrete element method (DEM) simulation and experiment. To compare the two models for ellipsoid, three tests are conducted: (i) the packing of ellipsoidal particles in a rectangular container, (ii) the flow of ellipsoidal particles in a horizontal rotating drum, and (iii) the discharge of ellipsoidal particles from a flat bottom hopper. Simulation results show that the super-ellipsoid model can accurately reproduce the packing and flow behavior of ellipsoidal particles. In the simulations using multi-spheres, when the spheres are more in a multi-sphere particle, the accuracy of simulation is acceptable while the computational time is much longer than the super-ellipsoid model. When fewer spheres are used to approximate the ellipsoidal particle, the computational time can be saved while the accuracy of the simulation decreases.

1. Introduction

Granular materials are commonly encountered in nature, industries and our daily life [1,2]. The dynamic behaviors of granular materials are complicated due to complex interactions between particles as well as their interactions with surroundings. Knowledge about the dynamic behaviors of granular systems is of major importance for related industrial applications. In recent years, the discrete element method (DEM), as pioneered by Cundall and Strack in 1979 [3], has been proven to be a capable tool for predicting the mechanical behaviors of granular systems in various application areas such as agriculture [4,5], mining [6–8], pharmaceutics [9–12], chemical engineering [13,14] and geological engineering [15,16], and it can provide much information of particle behaviors at both particle scale and granular system scale.

Numerous studies have shown that the representation of particle shape is one of the pivotal challenges for the development of DEM simulation [17–20] due to its significant effect on the mechanical properties of granular materials. However, most DEM studies published in literatures have been conducted using spherical particles due to the simplicity of contact detection between spheres [21–23]. Actually, most natural and industrial granular materials involved particles exhibit significant different shapes. The DEM based on spherical particle representation may predict a deviating mechanical behavior on the single particle level as well as in the larger particle assemblies, which leads to the simulation results may be questionable.

* Corresponding author.
E-mail address: yzzhao@zju.edu.cn (Y. Zhao).

To more accurately simulate the granular systems of real particles, various shape representation approaches of non-spherical particles have been proposed. The most commonly used approaches in literatures include: multi-sphere approaches [24–27], ellipsoid [28–30], super-ellipsoid approaches [31–35] and polyhedron [36–38]. These approaches are used to explicitly describe various shapes of the non-spherical particles such as cylinders, cubes, tablets and ellipsoids. A comprehensive overview of the possible particle shape representations in the DEM is given by Lu et al. [39]. In this study, the super-ellipsoid approach as well as the multi-sphere approach is adopted to model ellipsoidal particles.

Here we focus on the ellipsoidal particles because various types of granular matters are of this shape, which are widely used in the pharmaceutical, food, agricultural and other industries. In recent years, a number of researchers have contributed a lot of efforts in modelling of elliptical particles in DEM, including the development of two dimensional elliptical particles [40–42] as well as the three dimensional ellipsoids [43–47]. In particular, there have been several attempts to use ellipsoids [29], super-ellipsoids [33,48] and multi-spheres [49] to model ellipsoidal particles.

The super-ellipsoid method, which belongs to the larger class of super-quadric method [50], is extensively used to model and simulate symmetric particles with different aspect ratios, and the particle corners and edges range from rounded to spiky in shape. Super-ellipsoids was first introduced to DEM by Williams et al. [31] and used in two dimensional systems, which was extend to three dimensional systems by Cleary [51]. In the three dimensional systems, the super-ellipsoid method was used to simulate over one hundred thousand non-spherical particles, demonstrating the effectiveness of the approach [52,53]. The multi-

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sphere method is developed by Favier et al. [24] and Jensen et al. [54], of which the main advantages are the simplicity of implementation and the contact detection efficiency because it uses a sphere-sphere contact detection algorithm for irregular shape particles [25].

In this study, DEM simulation and experimental study on the packing and flow behavior of ellipsoidal particles with different aspect ratios were carried out. In order to evaluate the adequacy of the super-ellipsoid method and multi-sphere method for modelling ellipsoidal particles, we conducted three tests: packing of ellipsoidal particles in a rectangular container, flow of ellipsoidal particles in a rotating drum, and discharge of ellipsoidal particles from a flat bottom hopper. Besides, in order to compare the computational efficiency between the super-ellipsoid method and multi-sphere method, the computational time of these three tests was also recorded, respectively.

2. Mathematical model

2.1. Representation of ellipsoidal particles and contact detection

2.1.1. Super-ellipsoid model

According to Barr [50] the surface of a super-ellipsoid can be described by the so-called inside-outside function:

$$f(x,y,z) = \left(\left|\frac{x}{a}\right|^{s_2} + \left|\frac{y}{b}\right|^{s_2}\right)^{\frac{s_1}{s_2}} + \left|\frac{z}{c}\right|^{s_1} - 1 = 0, \tag{1}$$

where a, b and c are referred to be the half-lengths of the particle along the particle's principle axes, and s_1 and s_2 (written as $2/\varepsilon_1$ and $2/\varepsilon_2$ in [50]) control the sharpness of the particle edges and are called the shape indices in this paper. In this function, s_1 determines the shape of the cross section in the y-z and x-z planes, and s_2 relates to the shape in the x-y plane. Fig. 1 shows four different non-spherical particles with different shape indices or half-lengths. When $a = b = c$ and $s_1 = s_2 = 2$, the particle is spherical. When $a = b = c$ and $s_1 = s_2 > 2$, the particle looks more like a cube with the increase of s_1 and s_2. When $s_1 = s_2 = 2$, a wide range of shapes of ellipsoid from platy to elongated can be represented by changing the value of a, b and c, respectively.

It should be clearly that only when the center and principle axes of the particle coincides with that of the global coordinate system can Eq. (1) be used to describe the particle. Thus, when a particle is at optional position in the global coordinate system, the local coordinate system should be introduced, in which the center and principle axes of the particle must coincide with that of the local coordinate system. Then using a matrix $\boldsymbol{A}$ to perform the coordinate transformation of Eq. (1), and the function can be written as:

$$\boldsymbol{x} = \boldsymbol{A}\,\boldsymbol{x}' + \boldsymbol{P}, \tag{2}$$

$$\boldsymbol{A} = \begin{bmatrix} \cos\psi\cos\varphi - \sin\psi\cos\theta\sin\varphi & -\cos\psi\sin\varphi - \sin\psi\cos\theta\cos\varphi & \sin\psi\sin\theta \\ \sin\psi\cos\varphi + \cos\psi\cos\theta\sin\varphi & -\sin\psi\sin\varphi + \cos\psi\cos\theta\cos\varphi & -\cos\psi\sin\theta \\ \sin\theta\sin\varphi & \sin\theta\cos\varphi & \cos\theta \end{bmatrix}, \tag{3}$$

where $\boldsymbol{x} = (x,y,z)^T$ is the position vector in the global coordinate system, $\boldsymbol{P} = (x_0,y_0,z_0)^T$ is the position vector of the particle centroid in the global coordinate system, $\boldsymbol{x}' = (x',y',z')^T$ is the position vector in the local coordinate system, and (ψ, θ, φ) are the Euler angles.

In the DEM simulation, a key step of the algorithm is the contact detection. For non-spherical particles, the contacts between them are difficult to calculate. Various analytical approaches have been proposed to detect the contacts between ellipsoidal particles including intersection algorithm [40], geometric potential algorithm [41,43,44], and common normal algorithm [43,55]. In the current work, the geometric potential algorithm is used. To determine the overlap of two contacting non-spherical particles, a "deepest point method" [33,34,39] is adopted. In the global coordinate system, there are two ellipsoidal particles, Particle 1 and Particle 2, satisfying the $F_1(x,y,z) = 0$ and $F_2(x,y,z) = 0$, respectively, which are shown in Fig. 2a. Suppose that $P_1(x_1,y_1,z_1)$ is any point on the surface of Particle 1, then $F_1(x_1,y_1,z_1) = 0$. If $P_1(x_1,y_1,z_1)$ is inside the Particle 2 and it satisfies the relation of $F_2(x_1,y_1,z_1) < 0$, then we consider that Particle 1 is in contact with Particle 2. If two particles are in contact, there must be a point $P_1(x_1,y_1,z_1)$ meets the condition that $F_2(x_1,y_1,z_1)$ is the minimum of all $F_2(x,y,z)$. Therefore, the problem of calculating the contact detection is transformed into calculating the minimum value of the equations below:

Objective function:

$$\min F_2(x,y,z) \tag{4}$$

Constraint equation:

$$F_1(x,y,z) = 0 \tag{5}$$

In this study, an efficient Lagrange multiplier approach based on the CFR method [56] is employed to solve the optimization numerically, of which the tolerance of error is the minimum half length of the principle axes of the particle multiplied by 10^{-6}, i.e. min $\{a, b, c\} \times 10^{-6}$. The Lagrangian can be expressed as follows:

$$L(x,y,z,\lambda) = F_2(x,y,z) + \lambda[F_1(x,y,z)], \tag{6}$$

where λ is the Lagrange multiplier, and L is minimized with respect to the variables x, y, z, and λ. The Newton-Raphson approach is used to solve the Eq. (6). Starting with an initial guess for x, y, z, and λ, the first deepest point $P_1(x_1, y_1, z_1)$ on the surface of Particle 1 is obtained. Repeating the process can also obtain the deepest point $P_2(x_2, y_2, z_2)$ on the surface of Particle 2. The overlap between the two particles can be represented by a line segment that joining the two deepest points, and the midpoint of the line segment represents the contact point P_c. For the contact detection between an ellipsoidal particle and the wall, as shown in Fig. 2b, the overlap between the particle and the wall is represented by the line P_1P_3 rather than the line P_1P_2, as well as the effective contact point is the point P_1 rather than the midpoint of the line segment P_1P_3, and the action direction is perpendicular to the wall. Except

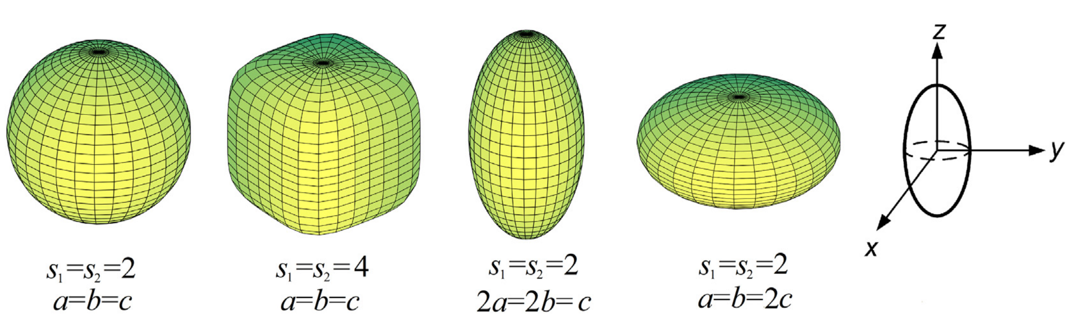

Fig. 1. Spherical and non-spherical particles described by super-ellipsoids.