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A Discrete Element Method to simulate the mechanical behavior of ellipsoidal particles for a fusion breeding blanket

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HIGHLIGHTS

- The influence of the particle shape on the bulk mechanical behavior of ceramic breeder was investigated.
- A DEM code was extended to analyse assemblies of ellipsoidal particles.
- A remarkable influence of the particles shape on the mechanical behavior of pebble beds was observed.
- A more compliant behavior was found in assemblies of particles with higher aspect ratios.

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ABSTRACT

The breeder materials proposed for the solid tritium breeding blanket concepts are ceramic lithium-based compounds in the form of pebble beds. Different fabrication processes have been developed to produce pebbles with a high sphericity. However, a small deviation from a perfectly spherical shape exists. In this paper the influence of non-sphericity on the mechanical behaviour of a pebble bed is assessed representing the currently produced pebbles by means of ellipsoidal particles. To this end, the in-house Discrete Element Method code KIT-DEM was further extended. The multi-sphere approach was implemented to generate the ellipsoidal particles while the existing random close packing algorithm was modified to create the assemblies. Uniaxial compression of the assemblies, under periodic boundary conditions, was simulated to investigate the bulk stress-strain behaviour of the bed. Sensitivity studies were carried out with different packing factors of the assembly and several aspect ratios of the particles. In agreement with previous studies carried on assemblies of spherical pebbles, the initial packing factor was found to noticeably affect the mechanical response of the investigated assemblies. Moreover, a remarkable influence of the shape on the mechanical behavior of the simulated assemblies was observed. Therefore it is concluded that for production techniques that result in poor sphericity, DEM simulations with non-spherical particles are necessary to reproduce realistic stress-strain behavior of pebble beds.

1. Introduction

The solid Breeding Blanket (BB) concepts make use of lithium-based ceramic pebble beds as tritium breeder. The pebbles are currently produced by different fabrication processes proposed by five members of the International Thermonuclear Experimental Reactor (ITER) agreement. The particles are characterized by a spheroidal shape with a maximum size around 1 mm to minimize volumetric swelling, thermal cracking as well as to ensure a homogeneous filling of the blanket [1–3]. The sphericity of the pebbles strongly depends on the fabrication method. Among the proposed processes both the sol-gel [4] and the melt-spraying [5] method show a high sphericity of 1.03 and 1.05, respectively.

The overall properties of pebble beds and their mechanical response depend strongly on the particle shape [6] as well as on the packing state [7,8]. A non-spherical particle shape could influence the bed response to external loads generating different stress levels, residual strains and micro response at the particle-scale compared to pebbles of a perfectly spherical shape. Moreover, the packing behavior as well as the packing structure could be affected by the particle shape, which in turn will further influence the mechanical response. All this, with regard to the breeder beds could have

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an impact on the configuration of the particles and the achievable packing factor, as well as on the occurrence of ratcheting, pebble breakage and gap formation between pebble bed and container wall. Consequently, understanding the effects of pebble shape is of significance with respect to pebble production and breeder zone design.

To model non-spherical particles, several numerical methods were proposed in the community of the Discrete Element Method (DEM). A brief overview of four main approaches is reported in the following: (1) The super quadratic method describes the shape of non-spherical particles mathematically. In particular one choice (1-a) is to discretize the surface of the particle by individual points meaning that a uniform discretization by equally spaced points is suitable for perfectly symmetrical particles while an adaptive discretization is used to represent particles with sharp vertices or edges for whom a large amount of points are required [9]. Another option (1-b) is a representation by a continuous function. The main weakness of the continuous function method is the use of an elaborate contact algorithm while the drawback of the particle surface discretization is the high computational time. (2) The polygons/polyhedrons methods allow generating shapes with sharp edges or flat surfaces. It has a very high stability however a very complex contact detection algorithm is needed [6]. (3) The Multi-Sphere (MS) method is a very robust approach and it was selected to represent the ellipsoidal particles in this work. It relies on representing different shapes by several overlapping primary spheres, such that the outer surface of the compound of the primary spheres represents the particle shape [6,10,11]. The main advantage of the MS method is that the robust contact algorithm developed for spherical particles is still applicable between the primary spheres of two non-spherical particles in contact. However, the computational time increases with the number of the primary spheres required to reach the desired level of smoothness of the particle surface. Furthermore, owing to the intrinsically non-convex surface of the particles, multiple contacts could occur overestimating the resulting contact forces. Höhner proposes in [12] a method to reduce the effect generated by Multi Contacts (MCs), introducing a "correction" by dividing, at each time step, the increment of the normal and tangential force by the number of the contact points between two particles.

Starting from the in-house code KIT-DEM [7], several modifications have been implemented to generate assemblies of ellipsoidal particles in oder to study their mechanical behavior. In the next section the algorithm implemented to create the assemblies of ellipsoidal particles is described. Section 3 explains in detail the DEM code used to simulate the compression of the assemblies. The numerical results are reported in Section 4 while the conclusions are drawn in Section 5.

2. Generation of assemblies of ellipsoidal particles

This section presents the developed algorithm to generate assemblies consisting of composite ellipsoidal particles. It consists of two subsections. The first subsection provides a detailed overview of the MS method while in the second subsection the modifications of the existing Random Close Packing (RCP) algorithm are described.

2.1. Multi-sphere approach

In the MS approach several primary spheres in overlap are clustered to form approximately the desired geometry. The size, the number and the overlap of the primary spheres can be tailored to obtain the desired shape. To maintain the geometry the relative position between the primary spheres of a single particle must not change. For an ellipsoidal shape an odd number of primary spheres is suggested to simplify the implementation of the equations of motion. The studies reported in this paper were performed on assemblies consisting of mono-sized ellipsoidal particles. The implementation of the MS method in this code was limited to clustering three mono-sized spheres to create each ellipsoidal particle. This limitation was sufficient to represents the pebbles currently produced and, more important, developing an understanding of some basic effects of non-spherical particles. The number of the particles in a bed and the aspect ratio are set as input parameters. The aspect ratio a_r is defined as the ratio between the major axis of the ellipsoidal particle generated and the diameter of the primary spheres. Furthermore, the overlap (δ_s) is related to the aspect ratio, to the number of the clustered primary spheres (N_s) and to their radius (R) as

$$\delta_s = \delta R\,, \tag{1}$$

where

$$\delta = 2\frac{N_s - a_r}{N_s - 1} \tag{2}$$

is the fraction of the radius in overlap.

Initially all spheres required to create the ellipsoidal particles are randomly generated in a cubic box with an edge length L (Fig. 1a). In this work 15,000 spheres are generated to create 5000 ellipsoidal particles. Each ellipsoidal particle and each sphere is numbered sequentially. According to the assigned number the spheres are then classified in three groups, namely spheres "a" (from 1 to 5000), spheres "b" (from 5001 to 10,000) and spheres "c" (from 10,001 to 15,000). Each ellipsoidal particle is formed by aligning three spheres belonging to the groups "a", "b" and "c" with a fixed distance and overlap depending on the desired aspect ratio. The spheres "a" and "b" become the external primary spheres of the ellipsoidal particle while the sphere "c" is placed in the middle of the line joining centers of "a" and "b" to complete the formation of an ellipsoidal particle (Fig. 1b). In particular the ellipsoidal particle number 1 is created moving the sphere "b" 5001 in the direction of the sphere "a" 1, thereafter the sphere "c" 10,001 is moved in the middle (Fig. 1a). With the same method the other ellipsoidal particles are generated (e.g., the ellipsoidal particle number i is composed by the spheres i, $5000+i$ and $10{,}000+i$ belonging to the groups "a", "b" and "c", respectively). The coordinates of the motion of a sphere "b" along the line showed in Fig. 1a are given by:

$$\begin{cases} x\left(t_f\right) = x_\mathrm{a} + t_f\left(x_\mathrm{b} - x_\mathrm{a}\right) \\ y\left(t_f\right) = y_\mathrm{a} + t_f\left(y_\mathrm{b} - y_\mathrm{a}\right)\;, \\ z\left(t_f\right) = z_\mathrm{a} + t_f\left(z_\mathrm{b} - z_\mathrm{a}\right) \end{cases} \tag{3}$$

where subscript a indicates the position of sphere "a", while subscript b indicates the initial position of sphere "b". The value t_f for the final position $(x(t_f), y(t_f), z(t_f))$ of sphere "b" is chosen such that a given aspect ratio a_r is obtained. For the composite particle, the aspect ratio is given by:

$$a_r = \frac{d + 2R}{2R}, \tag{4}$$

where R is the radius of a primary sphere and

$$d = \sqrt{\left(x\left(t_f\right) - x_\mathrm{a}\right)^2 + \left(y\left(t_f\right) - y_\mathrm{a}\right)^2 + \left(z\left(t_f\right) - z_\mathrm{a}\right)^2}, \tag{5}$$

is the distance between the two external spheres in the final configuration. Plugging $x(t_f)$, $y(t_f)$, $z(t_f)$ into Eq. (5) and defining the