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Application of discrete element method to study mechanical behaviors of ceramic breeder pebble beds

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Abstract

In this paper, the discrete element method (DEM) approach has been applied to study mechanical behaviors of ceramic breeder pebble beds. Directly simulating the contact state of each individual particle by the physically based interaction laws, the DEM numerical program is capable of predicting the mechanical behaviors of non-standard packing structures. The program can also provide the data to trace the evolution of contact characteristics and forces as deformation proceeds, as well as the particle movement when the pebble bed is subjected to external loadings. Our numerical simulations focus on predicting the mechanical behaviors of ceramic breeder pebble beds, which include typical fusion breeder materials in solid breeder blankets. Current numerical results clearly show that the packing density and the bed geometry can have an impact on the mechanical stiffness of the pebble beds. Statistical data show that the contact forces are highly related to the contact status of the pebbles.

Keywords: Discrete element method; Breeding materials; Pebble beds

1. Introduction

In recent decades, substantial engineering problems involving particulate materials have been numerically studied by discrete element method (DEM), which was first developed and applied by Cundall and Strack [1] in 1979. DEM has proved to be a versatile numerical tool, particularly suitable for the simulation of granular or particulate systems, where the overall behaviors are determined by the movement of individual particles. Different from continuum solid materials, the particles involve interaction mainly through discrete contacts. The DEM model is based on the physical contact laws and can capture characteristics of particulate materials and remedy the deficiency when continuum mechanics methods are used to model discrete particulate materials. For example, evolution of the particle–particle contact characteristics under internal and external loadings can be monitored.

At the current stage of research, our DEM application is mainly used to offset the limit of the

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experimental results. Previous experimental studies [2–4] on thermo-mechanical behaviors of ceramic pebble beds have provided fundamental and important information about material properties, such as critical crush loads and the macroscopic stress–strain behaviors of tested pebble beds. Typically, the stress–strain relation of a pebble bed is nonlinear and the stiffness of the pebble bed is strongly dependent on the applied loadings. Also, in the HICU project, the information is particularly important for in-pile tests where the size of the pebble container is limited due to the available experimental rig sizes [5]. According to their results, the influence of boundary constraints on the thermo-mechanical behaviors of a ceramic breeder pebble bed has been revealed. Due to friction, the uniaxial compression tests (UCTs) can show distinct differences to those found in standard UCTs. However, current experiments are limited by the measurement technique and cannot provide detailed information, which are important to determine the mechanical state of a packed pebble bed and to quantify the appropriate limits on applied loadings. For example, there are limited results regarding the stress/force magnitude or force distribution in a ceramic pebble bed, especially under different loading conditions.

In this paper, we focus on recent discrete element modeling results, which are assessing the mechanical behaviors of ceramic breeder pebble beds related to the packing density and the bed geometry. Statistical data about the internal contact forces will help us to understand the overall behaviors of pebble beds.

2. Algorithm of the discrete element method

The discrete element method, which can be considered as a time-dependent finite difference scheme, is an effective numerical tool for investigating the micromechanics of granular materials [6]. The progressive movement of each constituent particle and incremental contact forces are cyclically calculated by Newton's second law of motion. During the simulation process, each particle is considered independently, and its movement and displacement are related to contact stresses with its neighbors. Any displacement of the neighboring contact particles would generates a new non-equilibrium situation of the pebble beds. An iterative calculation of the successive releasing of forces exerted on a single particle is then performed until the resultant force on each particle in the assembly is sufficiently small.

In our simulation, basic simplified assumptions are made as follows:

(1) all ceramic breeder pebbles are considered as one particle with perfect spherical shape, but the size can be different;
(2) at low stresses and low temperature, Hertz–9Mindlin contact theory is used to predict the contact forces and stiffness at each contact;
(3) Coulomb's law determines the friction at particle–particle or particle–wall interfaces.

3. Fundamental mechanical behavior

To extend the understanding about ceramic breeder pebble beds in fusion nuclear applications, mechanical behaviors of 3-D packed pebble beds under uniaxial compaction process have been simulated by our DEM program. The uniaxial compaction of granular material takes three basic steps: initial packing, loading and unloading. Initial packing is an important step to determine the parameters of the pebble beds. During this step, all the pebbles are randomly packed into a structure and the packing density of all studied pebble beds reaches $60 \pm 0.5\%$ after initial packing. Compared to the random packing experiments by Scott [7], where he defined the loose random density at approximately 60% and the dense random value at 63.7%, our initial packing density is relatively lower. It is partially due to the amount of particles used in the simulation.

Fig. 1 shows the mechanical behaviors of the packed pebble beds during a loading/unloading cycle. In the numerical model, 5000 particles, all of the same size (diameter is 1.0 mm), are packed into a rectangular box, which is about 35 mm × 30 mm × 30 mm ($H \times L \times W$). The particles are Li_4SiO_4 ceramic pebbles. (At room temperature, Young's modulus $E \approx 101$ GPa, Poisson ratio $\nu = 0.24$.) The box is stainless steel (Young's modulus $E = 206$ GPa, Poisson ratio $\nu = 0.3$). The inset figure shows the modeling geometry. In the simulation process, there is assumed to be no friction

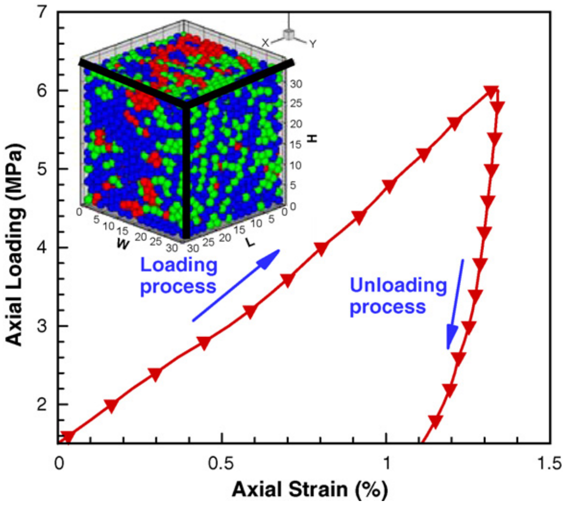

Fig. 1. Stress–strain behaviors of granular materials in a rectangular box under uniaxial compaction (initial packing density 60.3%; total particle number 5000; $H \times L \times W$ is $35 \times 30 \times 30$).

effect at either pebble/pebble or pebble/wall boundaries. Numerical results show that the stiffness of a packed pebble bed is highly dependent on the applied loading and packing density. Both loading and unloading process curves show that the stiffness of the pebble bed corresponds to the external loading magnitude. On the other hand, the numerical results show that an irreversible displacement is generated in the pebble bed during the loading-unloading cycle. This deformation behavior is similar to the plastic behavior of a solid material, which only appears when the loading exceeds the yield strength of the materials. For the pebble beds, experimental results showed that the plastic-like deformation can be removed after several loading cycles.

Uniaxial loading is only one typical loading for the pebble beds. Our numerical simulation is trying to study the mechanical behavior of the pebble bed under this simple loading condition, and provide information about the packing density and pebble bed geometry effects. Under 3-D loadings, the mechanical behaviors of the pebble beds should be different from uniaxial loading. However, the pebbles are different bulk material. Under uniaxial loading, they show more fluid type force transmits. The directions of force transferring from one pebble to others will also depend on the contact situation.

4. Special mechanics related to the pebble bed

Under solid blanket design of fusion reactor, packing density and bed geometry are two important characteristics for ceramic breeder pebble beds. In this section, numerical studies focus on the stress–strain deformation and the effective stiffness of the pebble beds during compaction processing.

4.1. Packing density

A rectangular pebble bed, identical to that used in Section 3, has been simulated with different packing densities.

Fig. 2 shows the stress–strain deformation behaviors of the pebble beds related to different packing densities. Each loading cycle starts with a different packing density. The results show that, under the same mechanical loading cycle (the maximal compaction loading is 6.0 MPa), the three pebble beds have significant differences in their deformation behaviors. First, the plastic-like deformation decreases with increased packing density; second, the effective stiffnesses of the pebble bed for the loading and unloading processes converge as the packing density increases.

Statistic mechanical data, i.e., packing density, average contact force and total contact number, which are included in Table 1, show that the total contact number of the pebble bed increases with the packing density. As a result, when the external loading force is held

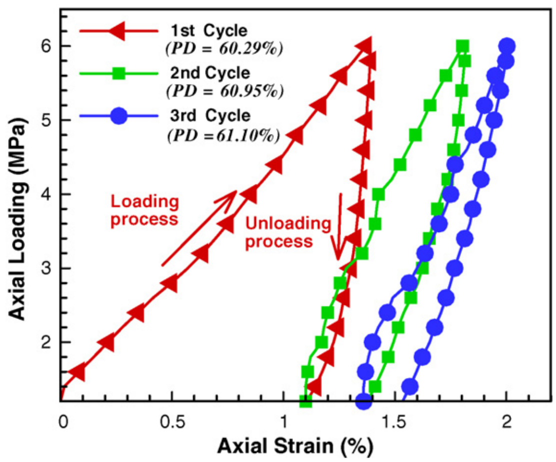

Fig. 2. Packing density effects on mechanical behaviors of the pebble beds.

Table 1
Detailed parameters and results of numerical simulations

Stages	Cycle	Packing density		Average contact force		Total contacts	
		Value (%)	Difference (%)	Value (N)	Difference (%)	Value (#)	Difference (%)
Initial stage ($P = 1.0$ MPa)	First	60.29	0.00	6.50	0.00	29,143	0.00
	Second	60.95	1.09	5.69	−12.5	29,538	1.36
	Third	61.10	1.34	5.76	−11.4	29,562	1.44
Top stage ($P = 6.0$ MPa)	First	61.13	0.00	18.86	0.00	30,593	0.00
	Second	61.38	0.416	18.69	−0.90	30,756	0.53
	Third	61.50	0.605	18.68	−0.95	30,972	1.24

constant, the average contact force is reduced, which means that, in some special loading conditions, a higher packing density can bring down the average contact forces of the pebble beds. Furthermore, from the table, it is found that the density effect is related to the force magnitude. When the external loading is small, the same change in the packing density can have a greater impact on the average contact force. For example, our numerical results show that, when the packing density is increased by only about 1%, the average contact force is decreased by more than 10% when the external loading is 1.0 MPa. When the external loading is 6.0 MPa, the change is not so significant.

4.2. Bed geometry

In fusion applications, to breed the maximum amount of tritium, it is important to determine the layout of the blankets, especially the layouts of breeder and neutron multiplier materials. On the other hand, different layouts or structures will have an impact on the mechanical behaviors of the pebble materials. In previous study [8], the effect of bed shape on the mechanical behaviors of the pebble beds has been found.

To study the effect of bed geometry, our simulations are based on two fundamental pebble bed shapes: cylindrical bed and rectangular bed, which can have different cross-sections and heights. The total numbers of pebbles are 2050 and 5000 for the cylinder bed and the rectangular bed, respectively. The same uniaxial compaction test is applied here.

Fig. 3(a and b) shows the uniaxial compaction behaviors of the different pebble beds. For both geometries, the plastic-like deformation, generated after the loading cycle, increases with the bed height. The difference is mostly generated during the loading process, especially for the cylinder pebble beds. When the height of the pebble bed is lower, its stiffness is stronger. However, the stiffness of the unloading processes does not change much. The reason for this is probably related to the packing density. When the packing densities are

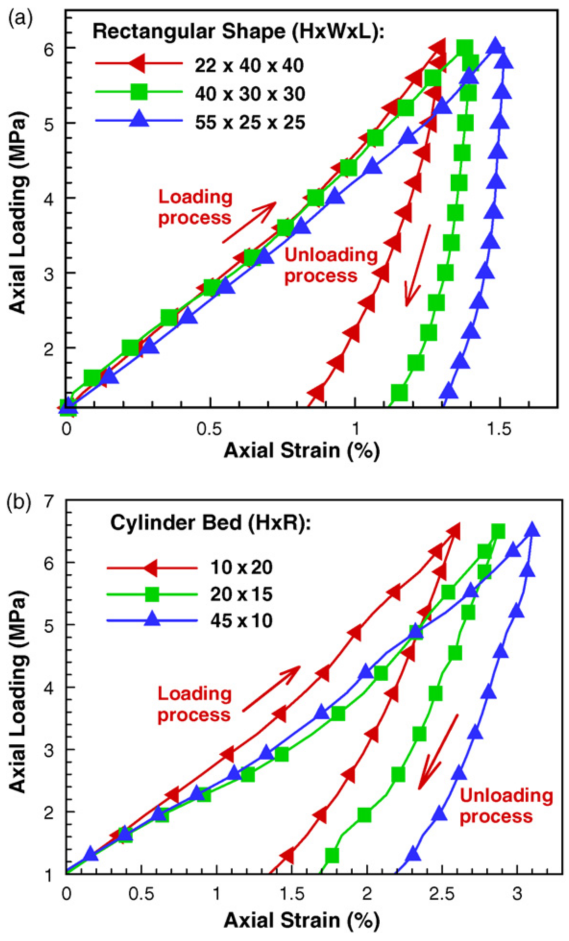

Fig. 3. Effect of bed geometry on the mechanical behaviors of the pebble beds. (a) rectangular pebble beds; (b) cylinder pebble beds.

high, the mechanical behaviors of the different pebble beds will be similar.

When comparing rectangular and cylinder pebble beds with each other, the numerical results show that the plastic-like deformation of the rectangular pebble bed is only about 2/3 of the cylinder pebble bed. According to our numerical simulation, the underlying reasons are still not clear. However, one of the reasons may relate to the different particle number and initial packing density.

In general, the bed geometry effect can be related to two aspects: boundary effect and inner pebble chains. Seidler et al. [9] studied a 3-D sandpile of spherical granules with synchrotron X-ray microtomography. They found that the strong boundary effect decays fully when the pebble centers are 5.0 diameters away from the container wall. Anthony and Marone [10] showed the deformation effect of the pebble force chain structure. They argued that chains consisting of fewer grains are less brittle, and chains consisting of more grains are more brittle and will undergo more deformation before failure. In our pebble beds, which have the almost same bed volume, more pebbles will interact with the boundary walls when the bed height is larger. Theoretically, these interactions can diminish the deformation of a pebble bed in the bed height direction. On the other hand, a thicker pebble bed will have more long chains, which will increase the flexibility of the pebble bed. Therefore, based on our numerical results, the conclusion is that, for the uniaxial compaction process, the inner structures of the pebble force chains have greater influence than the boundary effect.

5. Statistical results

When considering the intrinsic mechanics of each pebble, those with fewer contacts must react differently

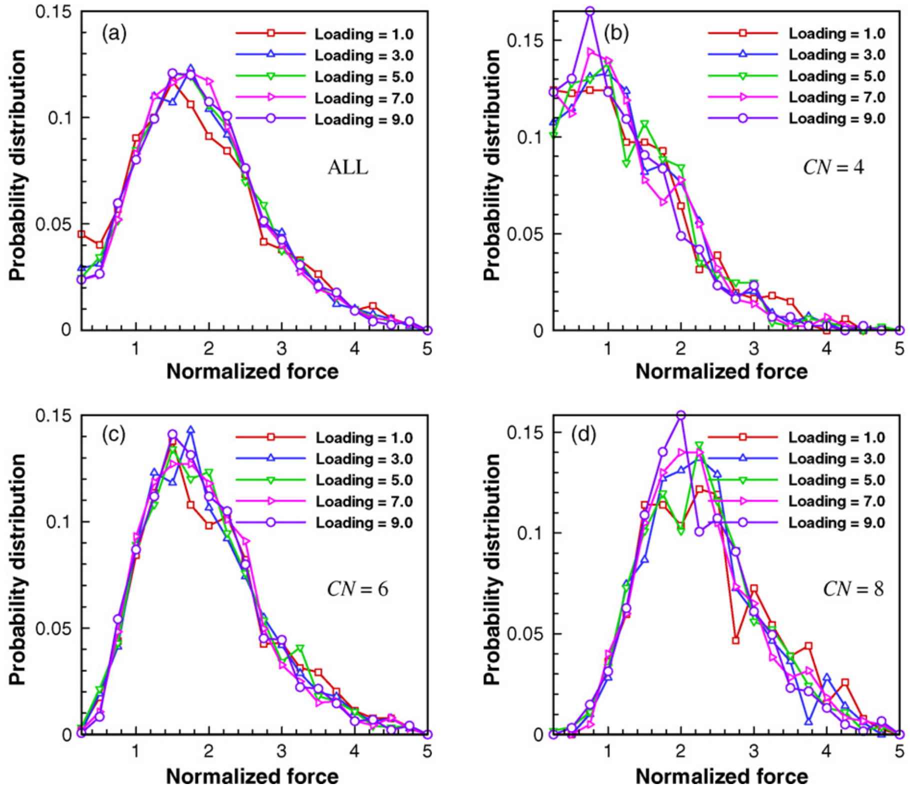

Fig. 4. Probability distribution of the maximal contact forces under different compaction loading (loading unit: MPa). (a) All together; (b) CN = 4; (c) CN = 6; (d) CN = 8.

from pebbles with more contacts. Therefore, the particles inside the pebble bed need to be cataloged and studied as different groups based on their coordination numbers. One result to be shown here is the relationship between the maximal contact force on each pebble and the coordination number. According to the numerical simulation, the maximal contact force on each particle can be obtained. Then the DEM program can give the probability distribution of these largest contact forces, $P_C(f)$, which is different from the probability distribution of all contact forces, $P_C(f)$. Fig. 4(a) shows the normalized maximal contact force probability distribution of all particles. Fig. 4(b–d) shows the probability distribution of pebbles whose coordination numbers (CN) are 4, 6 and 8, respectively. First, the results show that the probability distributions are independent of the external loadings. Second, the maximal contact force on the particle increases with the coordination number. The average maximal contact force inside the pebble bed is about two times the average value of all contact forces, and some particles' contact forces can be more than four times the average contact force.

6. Conclusion

In general, with further refinements of material properties characterizations and particle contact laws, our discrete element program interprets well the global behaviors found in the experiments. In this paper, our numerical simulations have studied the uniaxial compaction behaviors of typical fusion breeder materials of solid breeder blankets. Our numerical results clearly show that the packing density and the bed geometry can have an impact on the mechanical stiffness of the pebble beds. According to current study, the inner structures of the pebble force chains have greater influence than the boundary effect on the mechanical behaviors of the pebble beds. With the help of statistical data about the internal contact forces, it is found that the coordination numbers of the pebbles is related to the overall behaviors of the pebble beds.

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