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Investigation of the packing structure of pebble beds by DEM for CFETR WCCB

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Li\(_2\)TiO\(_3\)/Be\(_{12}\)Ti mixed pebble beds with multi-sized particles are one of the potential candidates for the WCCB (water-cooled ceramic breeder blanket) of the CFETR (China Fusion Engineering Test Reactor). To meet the neutronics requirements of a WCCB, a study of the packing structure of the concerned pebble bed is necessary. In this paper, the discrete element method (DEM) is applied to produce a prototypical blanket pebble bed by directly simulating the contact state of each individual particle using basic interaction laws. According to the current simulation, the packing factor of a mono-sized pebble bed is 0.62–0.64, while the value will become more than 0.75 for Li\(_2\)TiO\(_3\)/Be\(_{12}\)Ti mixed breeding pebble bed with a diameter ratio of not less than 5 as well as an appropriate mixed volume ratio, and thus can meet the neutronics requirements.

Keywords: WCCB; pebble bed; packing structure; discrete element method; fusion blanket

1. Introduction

As one of the breeding blanket candidates for the CFETR (China Fusion Engineering Test Reactor), a design of the WCCB (water-cooled ceramic breeder blanket) is being performed [1–3]. One of the main functions of the WCCB is to produce enough tritium through the \(^{6}\)Li\((n,\alpha)\)T and \(^{7}\)Li\((n,\alpha)\)T reaction with a high tritium breeding ratio of not less than 1.2 [1]. To realize this function, Li\(_2\)TiO\(_3\) particles as primary tritium breeder and Be\(_{12}\)Ti particles as neutron multiplier are mixed together in a certain volume proportion to form a close-packed multi-sized pebble bed. According to the neutronics analysis of the WCCB [1], the packing factor of the mixed pebble beds should be not less than 0.75 and the optimal volume fraction of Be\(_{12}\)Ti to Li\(_2\)TiO\(_3\) is approximately 4. To improve the tritium breeding ratio and meet the neutronics requirements of the WCCB, it is necessary to study the packing structure of the Li\(_2\)TiO\(_3\)/Be\(_{12}\)Ti mixed pebble beds to obtain a feasible packed bed for the WCCB.

Previous studies of pebble bed structures have been reported in the literature. Du Toit [4,5] studied the radial and axial variation in porosity in annular and cylindrical packed beds. Van Antwerpen et al. [6] summarized a series of correlations to model the packing structure in packed beds of mono-sized spherical particles. KIT (Karlsruhe Institute of Technology, Germany) [7–9] and JAEA (Japan Atomic Energy Agency) [10,11] investigated the pebble bed structure experimentally. Besides, simulation work has been done in [4,12–14]. It is noted that Gan et al. [12] has performed a pioneer study of the multi-sized pebble bed structure for fusion blankets using a packing algorithm. However, all the mentioned studies had not considered multi-sized pebble bed consisting of different particle materials. Therefore, in this paper, the packing structure of a Li\(_2\)TiO\(_3\)/Be\(_{12}\)Ti mixed pebble bed with different particle sizes and materials for a WCCB is explored to meet the packing factor and material fraction required by the neutronics.

In this paper, the pebble bed considered is a porous medium involving particulate materials. It can be studied numerically using the discrete element method (DEM), which has been proved to be an effective numerical method particularly suitable for the simulation of particulate systems [15]. The description of the simulation of the bed is given in Section 2; and the following section discusses the exploration of the packing structure of the bed. Finally, the conclusions are summarized in Section 4.

2. Simulation description

2.1. DEM model definition

In this paper, the DEM was applied to produce a prototypical blanket pebble bed. First, an initial loose
random packing of the pebble bed was built in a region far away from the base of a cubic container (see Figure 1(a)). After the application of gravity, the particles with an initial velocity $v_0$ fell from a height $h_0$ onto the base and finally reached a steady state. As a result, a final close-packed pebble bed was formed at the base of the container (see Figure 1(b)). In the current DEM simulation using PFC [16], the Hertz–Mindlin contact theory [17] was used to predict the contact force and stiffness at each contact area. In our model, friction at particle–particle and particle–wall interfaces was also considered. All the particles were assumed to be of a perfect spherical shape [17], but the size and material can be different. The mechanical physical properties of the particle materials were obtained from [18,19] and are listed in Table 1. The full-sized pebble bed (about 0.1 m in the radial direction and 1 m in the poloidal and toroidal directions) assembled in a box in the blanket is very large compared to the typical particle diameter (about 0.002 m). Simulating the full bed requires very large computer resources and computational time. Therefore, a scaled model of the box-shaped pebble bed is investigated in the following simulation and its scaling factors are about 0.1 in the radial direction and 0.01 in both the poloidal and toroidal directions.

2.2. Packing factor

The packing structure of a pebble bed, especially the packing factor $P_f$, is an important factor affecting the neutronics performance of the bed. Therefore, before any analysis, the structural arrangement of the packed bed should be thoroughly studied. The packing factor is defined by the solid particle volume ratio of the whole pebble bed. In our DEM model, a typical spherical representative elementary volume (REV) (see Figure 1(b)) with an appropriate diameter ($d_m$) is defined in the center of the bed. The packing factor of the bed is taken to be that of this REV which can be described by the following equation [16]

$$P_f = \frac{\sum V_p - V_{\text{overlap}}}{V_{\text{sphere}}}, \quad (1)$$

where $V_p$ is the volume of a particle in the REV; $V_{\text{overlap}}$ is the volume of particle overlaps contained within the REV. $V_{\text{sphere}}$ is the volume of the REV. It is noted that the partial volumes of particles that intersect the REV and the particle overlaps arising from compressive contact forces are accounted for in the PFC computation [16].

In order to determine an appropriate value of $d_m$ to obtain a high accuracy for $P_f$, the packing factor values of SC (simple cubic, see Figure 1(c)) and FCC (face-centered cubic, see Figure 1(d)) packed beds were measured by the above method and are listed in Table 2. It can be seen that when $d_m$ is five times larger than the particle diameter, the relative error (2.08%) between theoretical and numerical packing factor is less than 3%, which is roughly the same as the experimental error in the literature [20,21] and thus acceptable in our calculation. Therefore, it is necessary to ensure $d_m$ is within the range ($d_m \geq 5d_l \geq 5d_t$) in the following simulations. Besides, the REV diameter should be as large as possible to include as many particles as possible in the bed to represent the packing structure of the whole bed.

<table>
<thead>
<tr>
<th>Container size (mm)</th>
<th>Large particle diameter, $d_l$ (mm)</th>
<th>Young's modulus, $E$ (GPa)</th>
<th>Poisson rate, $\mu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X$</td>
<td>$y$</td>
<td>$d_l$</td>
<td>Li$_2$TiO$_3$</td>
</tr>
<tr>
<td>12.5</td>
<td>12.5</td>
<td>2.00**</td>
<td>185.95</td>
</tr>
</tbody>
</table>

Shear modulus ($G$) used in Hertz–Mindlin theory is obtained by $G = E/(2(1+\mu))$.

** For mono-sized pebble bed with Li$_2$TiO$_3$ and Be$_{12}$Ti particles, particle diameter is 1.5 mm; tiny particle diameter ($d_t$) in mixed pebble bed is $d_t = \epsilon d_l$, and $\epsilon$ is large-to-tiny diameter ratio.

*** An estimated value from Be–Ti alloy.
Table 2. Packing factor for SC and FCC packed bed.

<table>
<thead>
<tr>
<th>Theoretical</th>
<th>$d_m$ (mm)</th>
<th>Numerical</th>
<th>Relative error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5236</td>
<td>6</td>
<td>0.5158</td>
<td>-1.49</td>
</tr>
<tr>
<td>(SC)</td>
<td>5</td>
<td>0.5345</td>
<td>2.08</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>0.5012</td>
<td>-4.28</td>
</tr>
<tr>
<td>0.7405</td>
<td>6</td>
<td>0.7459</td>
<td>0.73</td>
</tr>
<tr>
<td>(FCC)</td>
<td>5</td>
<td>0.7391</td>
<td>-0.18</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>0.7421</td>
<td>0.21</td>
</tr>
</tbody>
</table>

*The particle diameter in the bed is 1 mm.

2.3. Packing for WCCB mixed pebble bed

The mixed pebble bed with particles of lithium titanate (Li$_2$TiO$_3$) and beryllium titanium alloy (Be$_{12}$Ti) is the main candidate breeder zone for the WCCB of the CFETR. According to the neutronics analysis of the WCCB [1], the $P_f$ of the mixed pebble beds and the optimal volume fraction ($v_m$) of Be$_{12}$Ti to Li$_2$TiO$_3$ were determined to be $P_f \geq 0.75$, $v_m \approx 4$. Therefore, it is necessary to find the applicable packing of the pebble beds case by case in order to satisfy the neutronics requirements. Since the large-to-tiny particle diameter ratio ($\varepsilon$) and the large-to-total particle volume ratio ($\nu$) can be important parameters affecting the neutronics requirements. Since the large-to-tiny particle diameter ratio ($\varepsilon$) and the large-to-total particle volume ratio ($\nu$) can be important parameters affecting the neutronics requirements.

According to the above formula, $N_0$ can be determined by $L_x$, $L_y$, $P_f$, $\varepsilon$, $\nu$ and $d_i$. After that, $N_i$, $N_t$ and $d_3$ can be solved at different values of $\varepsilon$ and $\nu$. Finally, the required material volume ratio of Be$_{12}$Ti to Li$_2$TiO$_3$ is considered as a parameter to determine the number of the Be$_{12}$Ti and Li$_2$TiO$_3$ particles according to the equation

$$v_m = \frac{N_{be} \varepsilon^3 + N_{tb}}{N_{tb} \varepsilon^3 + N_t}.$$  (4)

Here, $N_{be}$, $N_{tb}$, $N_{tb}$ and $N_t$ are the number of large Be$_{12}$Ti particles, number of tiny Be$_{12}$Ti particles, number of large Li$_2$TiO$_3$ particles and number of tiny Li$_2$TiO$_3$ particles, respectively. It is noted that these four variables are integers. When $L_x$ and $L_y$ equal 15 mm, $d_i$ is set to be 2 mm, and $P_f$ is taken to be an estimated value of 0.8, a possible solution of $N_{be}$, $N_{tb}$, $N_{tb}$ and $N_t$ to the above problem is listed in Table 3. It can be seen that all the large particles are Be$_{12}$Ti while all the Li$_2$TiO$_3$ particles are the tiny ones. Besides, there are also some tiny Be$_{12}$Ti particles mixed among them to meet the material fraction required by the neutronics. Above all, three types of particles are included in the mixed pebble bed for the WCCB. The next step is to judge from the DEM
Figure 2. Packing results of mono-sized pebble bed with the same material (for these cases of mono-sized beds, $L_x \times L_y = 30 \times 30$ mm).

3. Packing results and discussion

In this section, the DEM simulation cases for a mono-sized Li$_2$TiO$_3$ pebble bed and a Li$_2$TiO$_3$/Be$_{12}$Ti mixed pebble bed with different diameter ratios were calculated and the packing factors were measured using the method mentioned above.

3.1. Mono-sized pebble bed with one particle material

The Li$_2$TiO$_3$ pebble bed is widely used in fusion solid blanket as tritium breeder [22,23]. An example case of a mono-sized Li$_2$TiO$_3$ pebble bed was selected and the geometry is shown in Figure 1(b). The total number of the particles in this case is 5000; the particle diameter is 2 mm; the base size of the box container is 30 $\times$ 30 mm.

At the initial state of the DEM packing, the initial velocity and height of the particles were set to be $v_0$ and $h_0$, respectively. The particle centers of this bed at the final state was projected onto $xy$ plane on the base of the bed and plotted in Figure 2(a). It can be seen that in the near-wall region, most particle centers are located at some regular layers, which will lead to a peak value in the local packing factor. While in the region between adjacent layers, the local packing factor will reach a minimum value. It is the so-called wall effect reported by previous researchers [4,6,14]. This layered distribution of particles accounts for the oscillatory behavior of the local packing factor in the near-wall region. However, in the bulk region, it seems that the regular layers disappear gradually and the particles distribute randomly, which will result in a stable value for the local packing factor in the corresponding region. These characteristics of the cubic packed bed are very similar to those of cylindrical packed beds in [12], which indicates that the simulation whether the packing factor of these cases can reach 0.75.

Figure 3. Geometry for Li$_2$TiO$_3$/Be$_{12}$Ti mixed pebble bed (for these cases of multi-sized pebble beds, $L_x = 12.5$ mm and $L_y = 12.5$ mm are fixed).
bed obtained by the current DEM model has a typical packing structure of a prototypical pebble bed.

A REV with a diameter of 30 mm (Sphere 1 in Figure 1(b)) located at the center of the bed was defined to calculate the packing factor of the Li$_2$TiO$_3$ pebble bed. Figure 2(b) gives the results for different packing parameters. It can be seen that $P_f$ is 0.6235 for Case 1, of which $h_0$ equals 0.1 m and $v_0$ is 1 m/s. When $h_0$ is increased to 1.0 m (Case 2), $P_f$ has a slightly higher value. A similar phenomenon can be observed by increasing $v_0$ (Case 3) or reducing the particle diameter (Case 4). Besides, a higher particle density will also lead to a larger value of the packing factor (Case 5). For Case 2, 3 and 5, the variation compared with Case 1 may be explained by the initial unbalanced force between particles. Increasing $h_0$, $v_0$ and the particle density will introduce a relative large unbalanced force at the initial stage. Hence, the motion of the particles will be enhanced and the particles will have enough energy to fill more space before they become static, which will be helpful to obtain a higher value of $P_f$. For Case 4, since the layers of the near-wall region are thinner than the layers for the other cases, the negative effect on the packing factor will be smaller than that of Case 1. As a result, a higher packing factor can be achieved by the case. But in all the cases, the packing factor varies within a small range from 0.62 to 0.64, which agrees well with the typical experimental value of a prototypical pebble bed in the literature [20,24]. In other words, it seems that the influences of the initial parameters, particle size as well as density are limited and the packing factor of a mono-sized bed tends to be a stable value at about 0.63. Therefore, for a mono-sized pebble bed with the same material, it is difficult to obtain a packing factor of 0.75 and thus such beds cannot meet the $P_f$ required by the neutronics. One way to increase the packing factor is to fill the spaces between particles with smaller ones, i.e. to use a multi-sized bed.

3.2. Mixed pebble bed for WCCB

Similar to the simulation of the mono-sized pebble bed with the same material, all the Li$_2$TiO$_3$ and Be$_{12}$Ti particles were generated and mixed loosely by a random program in a box over the base of the bed. Then they were released and fell freely by gravity. Finally, a steady-state pebble bed was obtained to study the packing structure and thereby measure the packing factor. When $\varepsilon$ equals 1, all the particle diameters of the Li$_2$TiO$_3$/Be$_{12}$Ti mixed pebble bed was set to be 1.5 mm. For DEM cases at other values of $\varepsilon$, the simulation parameters are listed in Table 1. Figure 3 shows several geometries for these cases. Among these three cases, when the diameter ratio $\varepsilon$ increases from 1 to 5, the space between particles seems to be smaller. Therefore, the packing factor will become larger.

Figure 4(a) shows the particle center distribution on $xy$ plane for the Li$_2$TiO$_3$/Be$_{12}$Ti mixed pebble bed with $\varepsilon = 5$ and $v = 0.6$. The tiny particles form some layers in the near-wall region, and the layered region is much smaller compared to that of a mono-sized pebble bed. There are no such obvious layers formed by the large particles, which is perhaps because only few large particles were present in our scaled model. However, it appears that the range of the wall effect is determined by the tiny particles.

Figure 4(b) shows the packing factor of mixed pebble beds as a function of the large-to-tiny particle diameter ratio $\varepsilon$ and the large-to-total particle volume ratio $v$. It can be seen that, for the same diameter ratio larger than 1, the maximum value is reached at the range of volume ratio between 0.6 and 0.7. While for larger diameter ratios, a higher packing factor can be obtained at the same volume ratio. The results agree well with those obtained by a packing algorithm in [12]. When $\varepsilon = 5$ and
\( v = 0.6 \), the packing factor is 0.75. As a result, it can be concluded that a possible packed bed which meets the neutronics requirements is obtained when the volume ratio is around 0.6–0.7 as well as the diameter ratio is not less than 5.

4. Conclusions

In this paper, the DEM was applied to produce prototypical pebble beds consisting of mono-sized \( \text{Li}_2\text{TiO}_3 \) particles for fusion blankets, as well as beds consisting of multi-sized \( \text{Li}_2\text{TiO}_3/\text{Be}_{12}\text{Ti} \) particles for a WCCB. After that, the packing structure of the pebble beds concerned was investigated. According to the current simulation, the packing factor of a mono-sized bed reaches the value of 0.62–0.64. A possible \( \text{Li}_2\text{TiO}_3/\text{Be}_{12}\text{Ti} \) mixed pebble bed which meets the neutronics requirements can be found where the large-to-tiny particle diameter ratio is not less than 5 and the large-to-total particle volume ratio is around 0.6–0.7.

However, the thermal and mechanical requirements of pebble beds and the recovery and sweep capability of tritium in the bed are not considered in the paper. As the next step, further studies need to be performed to determine how the pebble bed packing structure affects the thermo-mechanics of the bed and how the required packing structure impacts the purge gas sweep capability. In addition, it is also necessary to improve the calculation method and accuracy of the packing factor.

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Disclosure statement

No potential conflict of interest was reported by the authors.

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