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Three-dimensional Numerical Simulation of Quasi-static Pebble Flow

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Abstract *To investigate the influence of the drainage rate and the particle contact model on the main features of the pebble flow, a quasi-static pebble flow of full scale German HTR-MODUL pebble bed is performed with up to 360,000 frictional graphite spheres. The treatment of the sphere-wall boundary condition is analyzed to avoid underestimating the friction of pebble near the wall. The streamlines, diffusion of pebbles and velocity profiles of pebble flow are drawn and analyzed. It shows that the streamlines and diffusion of pebbles inside the pebble bed are barely affected by the drainage rate and the particle contact model used. However, it reveals that the drainage rate and the contact model obviously influence the pattern of velocity profiles. It demonstrates that the quasi-static pebble flow and the Hertzian model are optimal choices of the neutronic physical design of the pebble bed reactor when the residue time of pebbles is particularly concerned.*

Key words: Pebble Flow; Granular Flow; Discrete Element Method; Sphere Packing; Pebble Bed

1. Introduction

As one of the main candidates for the next generation of nuclear power plants [1], the advantages of the pebble bed type high temperature reactor (HTR) include online refueling, passive safety features, and a high coolant outlet temperature. Besides more efficient electricity production, these features also have numerous applications for process heating and hydrogen production. The pebble bed reactor uses spherical graphite pebbles as fuel elements. In a pebble bed reactor, fuel pebbles form a randomly stacked bed inside a graphite reflector through which the helium coolant is pumped. The fuel pebbles circulate very slowly during the reactor operation.

The behavior of fuel pebble flow within a pebble bed reactor is an important issue. The streamline pattern of pebble flow and the diffusion of pebbles determine the design of refueling, and the velocity profile of pebble determines the residue time of pebble in the reactor, which are key factors of the reactor physical design. A vast amount of research has been carried out in order to accurately model pebble packing in a reactor core for the purpose of neutronic analysis, including the computation of the burnup distribution [2, 3], the effective thermal conductivity [4], the dust production [5], and the flow and thermal field coupling [6-8].

Over the past few decades, pebble circulation has been modeled as a dense quasi-static granular flow driven by the gravity. Although the kinematic model [9] and the microscopic model for random-packing dynamics has been proposed [10, 11], there is no reliable continuum model to predict the mean velocity in silos of different shapes [12]. Recently, much effort has been made to obtain realistic pebble flow features by the high fidelity Discrete Element Method (DEM) [13-17]. In recent years, small scale pebble bed simulations have been carried out with less than 30,000 pebbles [15-17].

However, the influences of boundary constrains for small scale problems are quite different from large scale ones.

Cogliati and Ougouag [18, 19] developed the PEBBLES code for modeling pebble flow for a large scale PBMR reactor. PEBBLES adopts a Hookean model as the particle contact model. However, the number of pebbles and the pebble drainage rate involved in computation are not quite clear.

The first known large scale pebble flow simulation by DEM code is shown by Rycroft [20, 21], with up to 440,000 frictional, viscoelastic 6cm-diameter spheres draining in a cylindrical vessel with a diameter of 3.5m and a height of 10m. In Rycroft's work, the streamline and velocity profiles are obtained, and the diffusion and mixing of pebbles are analyzed. For the reason of infeasible data collection, the Hookean model is adopted, the drainage of pebbles is not controlled on purpose, and the rate of removing pebbles is much faster than it is in the reactor core. In addition, the numerical simulation timestep of DEM has to scale according to $K_n^{-1/2}$ where K_n is the normal stiffness of the pebbles, otherwise the computation goes divergent and fails. Therefore, a realistic stiffness coefficient definitely leads to a much lower timestep. For computational feasibility, Rycroft uses a physically unrealistic value of normal stiffness which is significantly softer than that of typical fuel pebbles in pebble bed reactors. As a comparison, in this work, a physically realistic stiffness coefficient is used.

With all of these great works, there are still some uncertainties yet to be cleared. Such as, how do drainage rate and particle contact models influence the main features of the pebble flow, such as streamline pattern, diffusion of pebbles and velocity profile? In fact, the pebble flow in HTR is so slow that the original disturbance caused by the removal process of the pebbles is completely decayed before the next takes place [22]. Although the previous experimental work by Choi [12, 23] has shown that the main features of the flow are predominately governed by geometry and packing constraints, the influence of the drainage rate on the main features of the pebble flow is still not quite clear. Besides the issue of drainage rate, the Hookean model is often adopted by most DEM code for the sake of computational feasibility despite its unrealistic linear spring hypothesis. Thus there is a demand to do the comparison of the influences of the Hookean model and the Hertzian model on the main features of the pebble flow.

The main aim of this work is to investigate the influence of the drainage rate and the particle contact model on the main features of the pebble flow. For this purpose, the DEM code with both Hookean and Hertzian models is implemented in C/C++ language and optimized to run in parallel. The quasi-static pebble flow of a full scale German HTR-MODUL pebble bed is performed with up to 360,000 frictional graphite spheres draining in a cylindrical vessel of diameter 3m and height 9m.

2. Method

2.1 DEM method

DEM is based on the concept that individual material elements are considered to be separate and contacted only along their boundaries by appropriate physically based interaction laws. The interaction of forces between each contact pair are determined according to a constitutive relationship or interaction law. Based on Newton's 2nd law, the dynamic equation for pebble i is

$$\mathrm{m}\boldsymbol{a}_i = \sum_j \boldsymbol{F}_{ij}^c + m\boldsymbol{g} + \boldsymbol{F}_i^e \quad , \tag{1}$$

where m is the mass of the pebble; $\boldsymbol{a}_i$ is the translational acceleration; $\boldsymbol{F}_{ij}^c$ is the contact force between pebbles i and j; $\boldsymbol{F}_i^e$ is the resultant of all externally applied forces that could also include forces from the pebble interaction with other phases not explicitly modeled, such as fluid flows, electric/magnetic fields etc. In the current work being conducted, no such external forces, except for gravity, are considered. Also note that, during the static packing generation and even the subsequent recycling of the fuel spheres, the motion of the spheres is quasi-static at the most, the rotational motion is negligible, and therefore the rotational motion is ignored to reduce computational costs and improve simulation performance.

The contact force between a pebble i and another pebble is represented by $\boldsymbol{F}_i$,

$$\boldsymbol{F}_i = F_n\boldsymbol{n}_i + F_t\boldsymbol{t}_i \quad , \tag{2}$$

where $F_n\boldsymbol{n}_i$ is the normal contact force with $\boldsymbol{n}_i$ being the unit normal direction vector and F_n being the magnitude; while $F_t\boldsymbol{t}_i$ is the tangential force with $\boldsymbol{t}_i$ being the tangential direction unit vector and F_t being the magnitude. As shown in [20],

$$\boldsymbol{F_n} = \boldsymbol{f}\left(\frac{\boldsymbol{\delta}}{\boldsymbol{d}}\right)\left(-\boldsymbol{k_n\delta} - \frac{\boldsymbol{\gamma_n v_n}}{\mathbf{2}}\right) \ , \tag{3}$$

$$\boldsymbol{F_t} = \boldsymbol{f}\left(\frac{\boldsymbol{\delta}}{\boldsymbol{d}}\right)\left(-\boldsymbol{k_t s_t} - \frac{\boldsymbol{\gamma_t v_t}}{\mathbf{2}}\right) \ , \tag{4}$$

where δ is the normal overlap, *d* is the diameter of pebble, γ_n and γ_t are the elastic and viscoelastic constants, v_n and v_t are the normal and tangential componentsof the relative surface velocity. s_t is the elastic tangential displacement between spheres. The function f is customized for different contact model. The Hookean model employs $f(\xi) = 1$, while the Hertzian model uses $f(\xi) = \sqrt{g(\xi)}$ [24, 25].

The selection of a set of contact laws to be used for a particular application should be mainly based on the physical phenomena involved. In this work, the classic Hertzian contact model that governs elastic contact of two equal sized spheres in small strain deformation is adopted as the normal contact model. The tangential, or frictional, force between two contacting spheres is described by a tangential contact model in DEM. There are a few different models available to be considered. The Hertz-Mindlin-Deresiewicz model [26-29], which takes into account the interactions between the normal and tangential (frictional) forces and is regarded as the most accurate model, has been adopted as the tangential contact model.

In this work a physically realistic stiffness coefficient is used which is much higher than it is in Rycroft's work [20, 21]. Since the simulation timestep of DEM must scale according to $K_n^{-1/2}$ where K_n is the normal stiffness, the simulation timestep is much smaller in this work and it takes much more CPU time to perform the simulation. The computations are carried out on 8 Dell servers with 16-core 3.5GHz Intel processors, and it takes more than half a year to obtain the results.

2.2 Wall boundary

With regard to the sphere-wall boundary treatment, there is a prevalent method called the GHOST PEBBLE which seemingly comes from Computational Fluid Dynamics (CFD). As shown in Fig.1, to compute the contact force between a sphere and the wall, a GHOST PEBBLE is in a mirrored place along the wall. In this way, the formula of sphere-sphere can be applied at first glance. However, the following analysis reveals the drawback of the GHOST PEBBLE method.

For a given normal overlap δ_n, the magnitude of the normal contact force between spheres, F_n, is given by

$$F_n = \frac{4E^*}{3}\sqrt{R^*}\delta_n^{3/2} = K_n\delta_n \quad , \tag{5}$$

with the "secant" normal stiffness K_n defined as

$$K_n = \frac{4E^*}{3}\sqrt{R^*\delta_n} \quad , \tag{6}$$

where E^* and R^* are, respectively, the equivalent Young modulus and radius of the two spheres. In the current case, all the spheres have the same radius and material properties, and thus

$$E^* = \frac{E}{2(1-\nu^2)} \;\; ; \;\; R^* = \frac{d}{4} \quad , \tag{7}$$

in which E and ν are respectively, the Young's modulus and Poisson's ratio of the spheres. Energy dissipation due to plastic deformation, heat loss and material damping etc. during impact/contact is normally taken into account by adding a viscous damping term to the local contact force,

$$F_{nd} = F_n + 2m^*\omega_n\xi_n v_{nr} \quad , \tag{8}$$

where $m^* = m/2$ is the equivalent mass; ω_n is the instantaneous natural frequency; v_{nr} is the normal relative velocity of the contact pair; and ξ_n is the normal viscous damping coefficient. The instantaneous natural frequency ω_n, may be defined as

$$\omega_n = \sqrt{k_n^*/m^*} \quad , \tag{9}$$

where k_n^* is termed the (instantaneous) normal stiffness, which is well defined for a linear spring contact model, but is not so for a nonlinear contact model, such as the current Hertzian model. The normal damping ratio ξ_n is related to the normal coefficient of restitution, $0 \le e_n \le 1$, by

$$\xi_n = -\frac{\ln e_n}{\sqrt{\pi^2 + \ln^2 e_n}} \quad , \tag{10}$$

For the Hertzian model, the exact damped contact force can be obtained if the (instantaneous) normal stiffness k_n^* is taken as

$$k_n^* = \sqrt{1.25}K_n \quad . \tag{11}$$

For a sphere-wall contact case, however, the Hertzian formulas needs to be modified. According to the theory, the equivalent radius should take into considerations the radius of the cylinder. As the diameter ratio D/d between the main cylinder and the fuel sphere is very large, the wall can be considered as an elastic half-space. Also the wall of the reactor core is made of graphite bricks, so the same material properties as the fuel particles are used for the wall. Then the Hertzian model is still valid for a sphere-wall contact if we set

$$E^* = \frac{E}{2(1-\nu^2)} \;\; ; \;\; R^* = \frac{d}{2}; \;\; m^* = m \quad . \tag{12}$$

As is shown in formula (7) of sphere-sphere treatment, $R^* = \frac{d}{4}$, only a half of it's in this sphere-wall treatment by formula (12). Furthermore, formula (6) indicates that the sphere-sphere treatment results in a smaller stiffness. Since the normal contact force F_n is proportional to the stiffness by formula (5), and the tangential force F_t has magnitude μF_n where μ is the frictional coefficient, it means the effect of the GHOST PEBBLE method underestimates the friction of pebble near the wall.

3. Static packing

The geometric parameters and structure of the HTR-MODUL core are shown in Fig. 2 and Table 1. Both the pebbles and the wall are assumed to be graphite with its relevant material properties listed in Table 2, and the same coefficient of restitution of e=0.6 is assumed for both pebble-pebble and pebble-wall impact. The friction coefficients between the pebbles and between the pebbles and the wall are assumed to be the same. A typical value of $\mu = 0.3$ is chosen if not stated otherwise.

In order to model the behavior of a static packing pebble bed and the subsequent flow pattern during the pebbles removing process, an initial pebble packing needs to be generated. Initial packing in DEM in general is a practical issue but numerically challenging. In the current case, the initial filling of pebbles could be modeled by DEM by continuously injecting pebbles from the top of the bed until the required number of pebbles is generated and the whole system reaches a static equilibrium. The extremely high computational time cost involved, however, prohibits the adoption of such a procedure.

Instead, a two-stage approach is employed in the project. In the first stage, around 360,000 pebbles with a diameter of d=6cm are randomly generated in the pebble bed zone using the progressive packing algorithm [30] which results in a packing fraction of around 50%. Then the compaction under gravity is simulated in the 2nd stage using DEM until a (quasi-)static equilibrium is reached. The convergence criterion is set such that the total reaction force acting on both the wall and the bottom surface should be the same as the total weight of the pebbles within a relative error of 10^{-5}. When the convergence criterion is satisfied, a global packing fraction of around 61% is achieved, which indicates a global static equilibrium. It is possible for global packing fraction of a pebble bed to reach 63% under vibration of some amplitudes and frequencies [31], and our DEM code can achieve such effects. However, according to the normal operating conditions of HTR-MODUL, the case of static packing with around 61% global packing fraction is adopted as the initial status of pebble flow simulation.

Fig. 3 displays the average radial fraction distributions at two heights Z=2m and Z=8m. Note that the unit of the x-axis is in *d*, the diameter of the pebble. It shows that the pebbles in the lower half (Z=2m) are more compact than are in the upper half (Z=8m), which seems reasonable. Yet, the fraction distributions at different heights follow the same pattern in the radial direction: a layered pattern can be identified in the vicinity of the wall along with severe oscillations, which confirms the observation of experiments [4]. **Note the packing fraction near the wall is higher than 0.74. It's based on the elastic deformation caused by the particle contact model which leads to the numerical overlap of the spheres.** Fig. 4 shows the packing fraction distribution in the axial direction of the main cylindrical section, which appears obviously nonlinear. The packing fraction for the most part of the cylindrical section falls between 0.605~0.625. The sharp decrease of packing fraction at the bottom is due to the influence of the bottom funnel.

4. Quasi-static pebble flow

As illustrated in Fig. 5, the pebble flow is simulated with periodically removing and recycling spheres. In the ANABEK experiments [32], the drainage process takes place extremely slowly, at a rate of about one pebble per second. According to the average velocity of pebbles in the ANABEK experiment, we drain the spheres at a rate of about 50 pebbles per second (50peb/s). Considering that there are 360,000 pebbles in total, the velocity of pebble in most region of the pebble-bed is about

0.001m/s, which is a quasi-static flow. In the following analysis, the results of a drainage rate of 200peb/s and the much faster drainage in Rycroft's work [20, 21] are used for comparisons.

Then comes the technique of drawing streamline of pebble flow. There are two ways of implementation. One way is the Lagrange method of tracing individual pebbles through time adopted by Rycroft [21], which is simple to implement, but only applicable to fast drainage cases. The other way is the Euler method of interpolating the vector filed at the same instant, which is realized by this work for its time-efficiency. It takes two steps to figure out streamlines. First, the pebble bed is cut into 30mm thick slices. The velocity vectors of the pebbles touched by a slice are drawn in Fig. 6. Since the pebbles are randomly packed, the method of scattered data interpolation is used to figure out streamlines. In Fig. 7a, the centers of pebbles touched by a slice are represented by small circles, and some streamlines are drawn.

Fig. 7a reveals that the streamlines are almost vertical for most of the height and no lateral motion can be observed until at the height of around 2m. As the flow pattern plays such an important role in the pebble bed reactor, some experimental results regarding the pebble flow pattern are available [33, 34]. Fig. 7b displays the flow model of HTR-MODUL which is based on the German ANABEK experiments. A direct comparison is made in Fig. 7c by overlaying the average numerical result over the experimental result. It is evident that the numerical result matches the flow model of HTR-MODUL very well in the most part of the domain.

Considering a Pèclet number which is defined as

$$Pe_{\mathrm{x}} = \lim_{\Delta t \to \infty} \frac{2Vd\Delta t}{\langle \Delta x^2 \rangle} \ , \tag{10}$$

where V is the velocity of pebble and Δx is the horizontal displacement. It is interpreted as the distances (in units of d) for a pebble to fall before it diffuses by a diameter in the X direction. In this simulation of quasi-static full scale pebble flow, a Pèclet number of around 350 was observed, meaning that a pebble would have to fall twice the height of the core before diffusing by a single pebble diameter. It confirms the conclusion of Rycroft's work [21]. Through the comparison with faster drainage rate cases, it is found that the streamlines of pebble flow are almost the same pattern and the Pèclet number is on the order of 300 at different drainage rates and choices of either the Hertzian or the Hookean model.

Fig.8 shows the normalized velocity profiles at different drainage rates and different heights. Again note that the unit is in *d*. We can see the drainage rate affects the velocity profiles. The influence is more significant at the height closer to the outlet.

The comparisons of the normalized velocity profiles of the two different contact models at different heights are shown in Fig.9. It is obvious that the velocity profiles of the Hookean model are flatter, and the slope of velocity profiles is sharper near the wall. Rycroft adopts the Hookean model and shows similar features of the velocity profile. Through the comparison with the velocity profiles in Fig.11 of Kadak and Bazant's experiment [35], it demonstrates that the Hertzian model provides a more realistic description of the contact force between spheres than the Hookean model does. Since velocity profiles of pebble flow determine the distribution of the residue time of pebbles in the reactor which is important for pebble bed reactor design, the Hertzian model is worth numerical complications and the computation cost.

5. Conclusion

In this work, to investigate the influence of the drainage rate and the particle contact model on the main features of the pebble flow, using DEM method, a quasi-static pebble flow of full scale German HTR-MODUL pebble bed is performed with up to 360,000 frictional graphite spheres. The treatment of the sphere-wall boundary condition is analyzed to avoid underestimating the friction of pebble near the wall. The streamline is obtained by a Euler method, and compared with the flow model of HTR-MODUL based on the German ANABEK experiments. A Pèclet number around 350 is observed. Velocity profiles are drawn and compared with previous work in the literature. Through the numerical simulation and analysis, it demonstrates that, the streamlines and diffusion of pebbles inside the pebble bed are barely affected by drainage rates and particle contact models. However, we show that the drainage rate and the choice of a contact model obviously influence the pattern of velocity profiles. Since velocity profiles of pebble flow determine the distribution of residue time of pebbles in the reactor, it therefore shows that a quasi-static pebble flow and the Hertzian model are optimal choices of the neutronic physics design of pebble bed reactor when the residue time of pebbles is particularly concerned.

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