MODELING STATIONARY AND DYNAMIC PEBBLES IN A PEBBLE BED REACTOR

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ABSTRACT

This paper presents a numerical study of the stationary and dynamic pebbles in a pebble bed reactor (PBR) by means of discrete element method (DEM). At first, the packing structure of stationary pebbles is simulated by filling process until the settling of pebbles into PBR. The packing structural properties are obtained and analyzed. Subsequently, when the outlet of PBR is open during the operational maintenance of PBR, the stationary pebbles start to flow downward and are removed at the bottom of PBR. The dynamic behavior of pebbles is predicted and discussed. Our results indicate the DEM can offer both macroscopic and microscopic information for PBR design calculations and safety assessment.

Keywords: Discrete Element Method (DEM), Pebble Bed Reactor (PBR), Packing Structure, Hopper Flow, Granular Flow

1. INTRODUCTION

To address the long-term challenge of global climate change, developing reliable, clean, safe and affordable energy resources has gained more attentions and renewal interests all over the world. As the only large-scale emission-free energy resources, nuclear power has been considered as a very promising option and becomes even more attractive as the re-introduction of Pebble Bed Reactor (PBR) to this field. PBR uses pyrolytic graphite pebbles as the neutron moderator, and an inert gas such as helium as the coolant. The helium gas is heated to a very high temperature and used to drive a turbine to generate electricity. Compared with the traditional light water reactor, PBR has lower risk and higher thermal efficiency. In PBR, the pebbles are randomly packed in a cylindrical vessel. The thorough knowledge of packing structures is essential to improve the thermal efficiency and assess the safety.

In general, PBR has a central core comprised entirely of reflector graphite pebbles surrounded by a larger annulus of entirely fuel pebbles. Pebbles are dropped into the top of the core and are allowed to freely fall onto the pebble pile. The graphite pebbles are dropped only in the center while the fuel pebbles are dropped on the periphery. The pebbles are drained out through the bottom and reinserted at the top. The positions of the pebbles are determined entirely by granular flow, and random dropping from the top of the core. In PBR, pebbles enter at the top of the reactor vessel and pass through the bed and out through the base of the vessel via an extractor. Of special importance is the information such as pebble pathway, and relative velocity through the bed. This information is crucial since excessive time spent in parts of the bed could result in severe irradiation and thermal damage to the pebble with possible escape of fission products. The extreme case would be the permanent fixation of a given pebble or group of pebbles in a region of the vessel. The feasibility of the recycling of pebbles in a pebble bed reactor depends on the maintenance of satisfactory pebble flow through the vessel, its outlet, and the pebble extractor. Therefore, accurate flow characterization and description of the dynamics of pebbles in

PBR is important with respect to the basic reactor design calculations, optimization of fuel cycle and burn-up calculations, and monitoring of fuel integrity over its lifetime.

Obviously, understanding the packing structures and flow patterns of pebbles in PBR is highly needed for design optimization and safety assessment. In the past, significant efforts have been made to mathematically determine the packing structure of particles and numerically describe the dynamics of flowing particles. Generally speaking, those methods can be classified into two types: macroscopic and microscopic length scales. As a consequence, for the packing of mono-sized spheres, structural properties such as packing density, radial distribution function, and coordination number distribution, etc have well established for general applications in term of macroscopic concept. Simulation algorithms with only geometrical consideration thus far suffer from a serious drawback, ie, poor accuracy, since they cannot explicitly take any force into account. This deficiency can be overcome by means of the so-called Discrete Element Method (DEM) proposed by Cundall and Strack in 1979. The method, sometimes referred as the granular dynamics simulation as compared with the molecular dynamics simulation, has been widely used in the study of solid-solid and/or gas-solid interaction in dynamic systems. On the other hand, the behavior of pebbles in PBR exactly falls into the category of granular materials widely recognized in both scientific and industrial communities.

Granular material can be described by a continuum approach stemmed from spatial local average theorem. In the continuum description, the macroscopic behavior of granular flow is described by the conserved equations facilitated with constitutive relations and boundary conditions. In the past, two continuum models developed within the framework of plasticity theory and kinetic theory of molecular dynamics have extensively been used to study the dynamic behavior of granular materials. They have been shown to be applicable to quasi-static and rapid flow regimes, respectively. However, they do not satisfactorily apply to a system in which different flow regimes coexist such as the granular flow in a

PBR/hopper. An alternative approach is DEM, which takes into account the distinct nature of granular materials without any global assumption, thus allowing a better understanding of the fundamental mechanisms of granular flow. To date, the pebble flows in PBRs are poorly understood and not easily accessible through experiments, and yet it has a major impact on reactor physics. Very recently, Zhao et al. (2009) performed a study on the pebble flow in a rectangular model PBR by using DEM. In this work, in view of real PBR geometry, DEM was employed to numerically simulate pebble dynamics in a cylindrical PBR.

2. HOPPER FLOWS

Hoppers are widely employed in engineering practice mainly due to their capacity to enhance flow conditions for granular materials. They must be properly designed for reliable control. Therefore, a comprehensive understanding of the dynamic behavior of the granular flow in a hopper, so called hopper flow, is essential. In addition, theoretical treatment of granular flow in hoppers provides a class of benchmark boundary value problems for analyzing and predicting the behavior of granular materials under external mechanical excitations. The relatively simple geometry, well-defined flow patterns but complicated flow characteristics have made the hopper flow an attractive case to study new research techniques for granular flows. For these reasons, the granular flows in hoppers has been an important topic of research worldwide for several decades. Especially, in recent years, the dynamics of the flow has been studied extensively by means of both experimental techniques and numerical simulations at a microscopic or particle scale. Such studies take into account the discrete nature of granular materials without requiring any global assumption needed in the previous macroscopic approaches and thus allows a better understanding of the underlying mechanism. DEM is again the most important simulation approach for this connection.

Granular flows in hoppers with various geometries have been studied. These studies are mainly focused on three aspects: wall stress/pressure, discharge rate and internal properties. The study of the bulk material pressure on the walls of a hopper is very important for the hopper design. It has extensively been investigated by means of analytical, experimental and numerical approaches. However, the fundamentals about the pressure are not comprehensively understood due to its dependence on many parameters such as the geometry of hopper, material properties of hopper and particles, and flow conditions. DEM studies can enhance the understanding. The wall pressures along the silo height obtained by discrete element simulations agree well with the results from finite element simulations,

analytical approaches or experiments (Langston et al., 1995a; Negi et al., 1997; Holst et al., 1999a, b; Rotter et al., 1998; Masson and Martinez, 2000a, b; Goda and Ebert, 2005). Furthermore, it has also been reported that the wall pressure is affected by particle shape (Cleary and Sawley, 2002) and air-assisted flow which leads to increased wall stresses (Langston et al., 1996). The wall pressure is also affected by inserts whose presence influences the force transmission patterns within a hopper, producing strong and localized loads on the walls and the inserts (Parisi et al., 2004).

The prediction of the particle discharge rate from the hopper is of importance for the effective operation and control of a transport system, and is difficult due to the complexity associated with granular flow such as inhomogeneous particle distribution, irregular velocity profile and diverse particle size and shape (Seville et al., 1997). Although various empirical formulations have been proposed, a complete description of discharge rate is still lacking due to its complexity. DEM simulations have been conducted to address this problem. It has been reported that the hopper discharge rate obtained by DEM is qualitatively in good agreement with the results obtained from experiments (Favier et al., 2001) and the empirical predictions (Langston et al., 1994, 1995a; Kano et al., 1998). The discharge rate is affected by particle characteristics and material properties. DEM simulations can quantify these effects. It has been shown that compared with spherical particles, the disc flow is about 20–30% faster (Li et al., 2004); the discs with aspect ratio 5 are discharged 40% faster than the spheres (Langston et al., 2004); and elongated particles produce flow rates up to 30% lower than for circular particles (Cleary and Sawley, 2002). DEM simulations also show that the discharge rate is not so sensitive to the stiffness of particles, wall roughness and damping coefficient, but is affected by particle friction (Langston et al., 1994, 1995a; Kano et al., 1998). Other properties such as hopper geometry and operation also affect the discharge rate. For example, the discharge rate largely depends on the hopper orifice and half-angle (Langston et al., 1994, 1995a; Kano et al., 1998). The ratio of the discharge rates from a vibrating

hopper to a non-vibrating hopper decreases with vibration except at the highest frequencies (Wassgren et al., 2002).

It is important to understand the microscopic structure and its relations to the mechanisms governing the hopper flow. The DEM simulation takes into account the discrete nature of granular materials, and therefore is very effective for this purpose. In the past, particle velocity or kinetic energy, flow structure and force structure of granular materials in hoppers have been investigated. These studies are mainly focused on two aspects of these properties:

1. Spatial distributions: DEM simulations confirm that there are several different flow zones in a hopper flow (Langston et al., 1994, 1995b, 1996; Rong et al., 1995a, b; Rotter et al., 1998; Parisi et al., 2004). For example, there are generally four flow zones for the granular flow in a cylindrical hopper with flat bottom: stagnant, plug flow, converging flow, and transitional zones (Zhu and Yu, 2004). In different zones, the flow pattern, flow structure (Langston et al., 1997) and force structures (Langston et al., 1995b; Gutfraind and Savage, 1998; Parisi et al., 2004) are different. These studies indicate that the hopper flow can be qualitatively described in terms of these special distributions.
2. Statistical distributions: DEM simulation results show that the statistical distributions of the properties such as velocity, porosity and force can be used to describe the hopper flow quantitatively. It is suggested that variables such as porosity and force vary in a large range, and force distributions decay approximately in an exponential manner. Further comparison between the force distributions for unsteady and steady state flows in a hopper indicates that the steady state flows have less particles with large interaction forces, which can be attributed to macroscopically smaller resistance when particles transforming from plug flow to converging

flow for a steady state flow. In addition, the effect of hopper geometry and particle properties on the flow has also been quantified by these statistical distributions.

By a proper averaging method, macroscopic quantities such as density, velocity, stress and couple stress can be obtained based on DEM results. For hopper flow, the velocity, density, stress and couple stress distributions have been extensively investigated. These distributions are shown largely related to the corresponding microscopic structures. In particular, the results about velocity and mass density are qualitatively in agreement with the experimental results and the microdynamic analysis (Potapov and Campbell, 1996). The consistency between the micro-and macroscopic variables confirms the applicability of the average method to the hopper flows. Moreover, the results indicate that the distributions of the stresses are related to the force structures, controlled by the magnitude and direction of the interaction forces and the contact direction between particles (Langston et al., 1995b; Potapov and Campbell, 1996; Gutfraind and Savage, 1998; Masson and Martinez, 2000a, b). Only near the walls of the hopper, the couple stress is significant; when far from the walls, it can be ignored. The results also suggest that the treatments that employ plasticity models under the assumption that the material is always yielding are not valid, and hopper flows cannot be modeled as rapid granular materials (Potapov and Campbell, 1996). These studies also indicate that the combined approach of the discrete approach and the averaging method offers a convenient way to link fundamental understanding generated from DEM-based simulations to engineering applications often achieved by the continuum modeling.

3. SIMULATION METHODS

DEM simulations involve solving the equations of motion for the trajectory, spin and orientation of every particle in the flow. The collisions between particles and between particles and the surrounding boundary objects are also modeled. When it is necessary, moving boundary objects that the particles interact with are also considered.

The DEM variant (Cundall and Strack 1979, Feng et al. 2004, Zhang et al. 2002, 2003) used in this work is sometimes referred to as the soft sphere method. The particles are allowed to overlap when they collide with each other. A conventional linear spring dashpot model as shown in Fig. 1 will be used for estimating the inter-particle forces.

Assume the particle i interacts with a number of adjacent particles. The translational and rotational motions of particle i at any time t in a granular flow are determined by Newton's second law of motion, which can be written as

$$m_i \frac{dv_i}{dt} = \mathbf{f}_{f,i} + m_i \mathbf{g} + \sum_{j=1}^{k_i} \mathbf{f}_{ij} \quad (1)$$

and

$$I_i \frac{d\omega_i}{dt} = \sum_{j=1}^{k_i} \mathbf{T}_{ij} \quad (2)$$

where m_i , I_i , k_i , $\mathbf{v}_i$ and $\boldsymbol{\omega}_i$ are, respectively the mass, moment of inertia, number of contacting particles, translational and rotational velocities of the particle i ; $\mathbf{f}_{f,i}$, $m_i \mathbf{g}$, $\mathbf{f}_{ij}$ and $\mathbf{T}_{ij}$ are respectively the fluid drag force, gravitational force, and inter-particle force and torque from particle j , acting on particle i . Here j is one of the particles contacting i . The DEM algorithm is comprised of three essential parts:

1. A particle near-neighbor interaction list is constructed with the aid of an overlaying Cartesian grid. The mesoscopic size of the grid cells is chosen such that there is at most one particle in each cell. The surrounding cells are searched for neighboring particles. This grid search technique reduces the nearest neighbor search procedure to an $O(N)$ operation, where N is the total number of particles. This is essential for DEM simulations involving a large number of particles.
2. The collisional forces on each of the particles and the boundary objects are evaluated using the near-neighbor list and the spring-dashpot interaction model, and then transformed into the simulation frame of reference.
3. All the forces on the particles and surrounding boundary objects are summed and the resulting equations of motion are integrated to advance the positions in time. A second-order predictor-corrector scheme is used, with between 10 and 50 time steps required to integrate accurately each collision. This gives very small time steps, typically 10^{-3} to 10^{-6} s, depending on the length and time scales of each application.

Due to the relative motion among particles, it is necessary to update the near-neighbor list as often as necessary.

4. SIMULATION CONDITIONS

The PBR in our simulation is a cylindrical vessel and has a converging section with a 45 degree hopper half angle at the bottom as shown in Fig. 2. Its characteristic dimensions are assumed to be related to the diameter d of the particle: the overall height of the hopper is $87d$, and the diameter of the vertical wall part of the hopper is $20d$, while the outlet of the hopper is a circular orifice at the center of wedge-shaped bottom with $6d$.

The granular material is composed of 20,000 mono-sized particles. The physical data for the assumed visco-elastic material are given in Table 1. Inter-particle and particle-wall friction is specified by the same friction coefficient μ . For convenience, non-dimensional units mainly based on particle diameter, d , were employed, so that the force was normalized by mg , elastic modulus by mg/d^2 , and time by $(d/g)^{1/2}$. All results through the paper are illustrated in non-dimensional units for relevant parameters.

The packing in PBR is simulated by sedimentation of particles, which is more realistic and named as group method. Based on the group method, the granular materials are introduced into the top of the hopper by a group consisting of a few particles at a time and allowed to fall under gravity. The group method is quite different from the traditional method in that the traditional method enables a block of material to fall under gravity *en masse* until it collides with the hopper base. This is closer to the manner in which granular material is delivered into real hoppers and the magnitude and directions of the initial particle velocities are also artificially imposed with Gaussian random distributions, in which the mean value is 2.56 m/s and the pebbles are confined in a cone region with the head angle of 30 degree for dropping down. The growing bed in the hopper therefore has a longer time to relax and become better consolidated. During the particles settling on the bottom in the dynamic packing process, the orifice is kept closed until a quasi-static state occurs. The discharge process begins after an instant opening of the orifice. The discharge without material feedback from above is considered in the present simulations.

The behavior of a granular material during filling was controlled by the evolution of the total kinetic energy of granular material, expressed as the sum of all particle energies due to translational and rotational motion. The evolution of the kinetic energy to zero value is assumed to be a stabilization indicator of the filling process of granular material, so called quasi-static stage.

Consequently, all dynamic parameters of particles obtained at the end of the filling process are assumed to be the initial conditions for simulation of the discharge process, while a new time scale referred to initial discharge time $t = 0$ is employed for the sake of similarity. All simulations in this work were carried out on a PC computer with 64bit, 16GB RAM, CPU 2.4GHz (dual Quad Core). At the present of time, the DEM solver is not implemented by parallelization, it was run in serial to simulate various particle processes that are from filling, settling, discharge and leaving the vessel. The entire computations were proceeded to 382,000 time steps for non-dimensional time of 382, which has run 2 hours and 7 minutes on the PC computer. The discharge process starts from non-dimensional time = 80, in which the transition occurs at the 80,001st time step in the computation. Fig. 3 shows snapshots at different non-dimensional times to illustrate the formation of the pebble packing.

5. RESULTS AND DISCUSSION

In general, the packing of pebbles in PBR was analyzed mainly in terms of packing density, radial distribution function (RDF) and coordination number. Although packing density can also be defined either a local or global property, only global or overall packing density was employed, obtained by considering the section of a packing at least 3 particle diameter away from its bottom, wall and surface. The radial distribution function is the probability of finding one particle centre at a given distance from the centre of a given particle. Coordination number is the number of particles in contact with a considered particle. It varies with the definition of contact, ie. the critical distance of separation less than which two particles are defined to be in contact. Obviously, the larger the critical distance of separation, the larger the mean coordination number. In this work, the critical distance was set to $1.01d$. The mean coordination number was obtained from counting the contacts for all particles in the packing section used for the calculations of packing density, except for those about 1 particle diameter close to the wall to avoid the wall effect. In the past, the packing of mono-sized spheres has been comprehensively studied by mean of DEM method (Zhang et al., 2001) with special reference to variables affecting the packing dynamics, with the results analyzed in terms of packing density, RDF and coordination number. In their work (Zhang et al., 2001), it was found that packing density increases with dropping height and restitution coefficient, and decreases with deposition intensity and friction coefficient, which is consistent with previous experimental findings. In general, deposition intensity in the continuum sense is the average numbers of particles arriving per unit volume. In this work, deposition intensity is the average numbers of particles dropping into the PBR per unit time. Both RDF and coordination number distribution vary with these variables, in line with packing density. For a packing of high density, it has a clear split second peak in its RDF, like that observed for the dense random packing. However, as

packing density decreases, the first component of the split second peak will gradually vanish, giving an RDF more comparable to those observed in a sequential addition simulation. Mean coordination number can be correlated with packing density; it increases with dropping height and restitution coefficient, and decreases with deposition intensity and friction coefficient.

Fig. 4 gives the pebble velocity vectors during filling process, which is showing the pebble kinetic energy to zero value at the settled down stage. Fig. 5 shows the portion of packing structure extracted from the present simulation. Fig. 6 illustrates the overall mean density and mean contact number variations during compaction. The mean density of the compact is increasing with the time evolution until a final stable stage is achieved. Finally, the packing yields a packing of mean density up to 0.645, which suggests that a random dense packing (RDP) is obtained. This result is slightly higher than Finney's experimental value 0.636, but agrees with other theoretical values, for example, Berryman's (0.640). Simulation also shows that the mean coordination number increases with the compacting, the final mean co-ordination number is found to be 6.12, a widely accepted value.

The characteristics of discharge, indicating the transitional and final stages of the flow in hoppers, are illustrated in Fig. 7. The particles are colored by the initial height. Let us consider the discharge flow kinematics. The distribution of velocity fields has been extensively studied by the macroscopic experiments and simulations (Nedderman, 1992). However, the detailed motion of individual particles in the discharge flow is difficult to measure experimentally, particularly in 3D cases. Thus, following the classical macroscopic description of the discharge flow, there are five zones of flow inside the hopper with flat bottom: stagnant zones located at the bottom corners, a plug flow zone in the upper part, a converging flow zone in the lower part, a transition zone from plug flow to converging flow (where particles move toward the orifice), and a free particle fall zone. From the initial transient stage up to the

quasi-static ($t = 0.4$ s) flow, such flow patterns can be observed by the obtained velocity vectors of individual particles plotted in Fig. 8.

6. CONCLUSIONS

DEM method has been employed to simulate the stationary and dynamic behavior of pebbles in a PBR. The packing structure of stationary pebbles is obtained by a realistic filling process until the settling of pebbles into PBR. The structural properties, such as packing density, radial distribution function, coordination number distribution and homogeneity, are analyzed. The pebble pathway and relative velocity through the bed are predicted. Quantitatively, the dynamic behavior is in good agreement with the data available in literature.

The results presented in this paper demonstrate the DEM modeling is a very promising and feasible approach to analyze the granular flows in hoppers and show enormous potentials to study the pebble behavior in PBRs. Next, the present DEM model is to be extended to real geometry pebble beds. To investigate the effects of the gas flow on the pebble dynamics and heat transfer in the reactors, the coupling of DEM and computational fluid dynamics (CFD) would be employed to describe the discrete flow of pebbles and the continuum flow of gas, as well as the heat and mass transfer between them.

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NOMENCLATURE

d	particle diameter
$\mathbf{f}_{f,i}$	fluid drag force
$\mathbf{f}_{ij}$	inter-particle force
$\mathbf{g}$	gravity
I_i	moment of inertia
k_i	number of contacting particles
m_i	mass
t	time
$\mathbf{T}_{ij}$	torque from particle
$\mathbf{v}_i$	translational velocity

Greek letters

$\boldsymbol{\omega}_i$	rotational velocity
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Subscripts

i	particle index
j	contacting particle index

FIGURES TITLES

Fig. 1 Illustration of inter-particle forces including contact force and damping force

Fig. 2 The geometry of a cylindrical PBR with steep 45 degree wedge-shaped bottom

Fig. 3 Snapshots showing the formation of a packing of pebbles at different non-dimensional times: (a) 0.; (b) 10.; (c) 20.; (d) 30.; (e) 40.; (f) 50.; (g) 60.; and (h) 70.

Fig. 4 The velocity vectors of individual particles during filling at different non-dimensional times: (a) 0.; (b) 10.; (c) 20.; (d) 30.; (e) 40.; (f) 50.; (g) 60.; and (h) 70.

Fig. 5 The portion of packing structure extracted from the core of the cylindrical PBR

Fig. 6 Density and coordination number variation during filling process

Fig. 7 Flow patterns at different non-dimensional discharge times: (a) 0.; (b) 30.; (c) 60.; (d) 90.; (e) 120.; (f) 150.; (g) 180.; (h) 210.; (i) 240.; (j) 270.; (k) 300.; and (l) 302.

Fig. 8 The velocity vectors of individual particles at different non-dimensional discharge times: (a) 0.; (b) 30.; (c) 60.; (d) 90.; (e) 120.; (f) 150.; (g) 180.; (h) 210.; (i) 240.; (j) 270.; (k) 300.; and (l) 302.

TABLES

Table 1. Materials properties in the simulation

Variable	Value
Particle	Spherical
Number of particles	20,000
Particle diameter	0.06 m
Particle density	$2500 \text{ kg} \cdot \text{m}^{-3}$
Sliding friction coefficient (p-p or p-w)	0.3
Young's modulus	$1.54 \cdot 10^7 \text{ kg} \cdot \text{m}^{-1} \cdot \text{s}^{-1}$
Possion's ratio (p or w)	0.3
Damping ratio (p or w)	0.3
Time step	$7.8 \cdot 10^{-5} \text{ s}$
Simulation time	29.87 s

FIGURES

Fig. 1 Illustration of inter-particle forces including contact force and damping force

(a) 2d side view

(b) 3d view

Fig. 2 The geometry of a cylindrical PBR with steep 45 degree wedge-shaped bottom

(a)

(b)

(c)

(d)

(e)

(f)

(g)

(h)

Fig. 3 Snapshots showing the formation of a packing of pebbles at different non-dimensional times: (a) 0.; (b) 10.; (c) 20.; (d) 30.; (e) 40.; (f) 50.; (g) 60.; and (h) 70.

(a)

(b)

(c)

(d)

(e)

(f)

(g)

(h)

Fig. 4 The velocity vectors of individual particles during filling at different non-dimensional times: (a) 0.; (b) 10.; (c) 20.; (d) 30.; (e) 40.; (f) 50.; (g) 60.; and (h) 70.

Fig. 5 The portion of packing structure extracted from the core of the cylindrical PBR

(a)

Fig. 6 Density and contact number variation during filling process

(a)

(b)

(c)

(d)

(e)

(f)

(g)

(h)

(i)

(j)

(k)

(l)

Fig. 7 Flow patterns at different non-dimensional discharge times: (a) 0.; (b) 30.; (c) 60.; (d) 90.; (e) 120.; (f) 150.; (g) 180.; (h) 210.; (i) 240.; (j) 2708.; (k) 300.; and (l) 302.

(a)

(b)

(c)

(d)

(e)

(f)

(g)

(h)

(i)

(j)

(k)

(l)

Fig. 8 The velocity vectors of individual particles at different non-dimensional discharge times: (a) 0.; (b) 30.; (c) 60.; (d) 90.; (e) 120.; (f) 150.; (g) 180.; (h) 210.; (i) 240.; (j) 270.; (k) 300.; and (l) 302.