

# **A Collective Dynamics-based Method for Initial Pebble Packing in Pebble Flow Simulations**

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## **Abstract**

In the simulation of pebble flow in Pebble-Bed High Temperature Reactors (PB-HTR's), high-fidelity methods, such as Discrete Element Method (DEM), are usually employed to simulate the dynamic process of the pebble circulation. Such simulation normally takes extraordinarily long time to reach the dynamic equilibrium state, in which the pebble distribution is statistically steady. However, if an initial dense packing of pebbles can be provided, which is close to the realistic packing at the equilibrium state and can be easily implemented without much computational effort, then the high-fidelity pebble flow simulation can take much less time to reach the dynamic equilibrium state. In this paper, a collective dynamics-based method is developed to generate an initial pebble packing for the subsequent high-fidelity pebble flow simulations. In the new method, pebbles are packed by two processes: a sequential generation process allowing overlaps and an overlap elimination process based on a simplified normal contact force model. The latter provides an adaptive and efficient mechanism to eliminate the overlaps accounting for different overlap size and pebble size, thus can pack tens of thousands of pebbles within several minutes. Applications of the new method to packing pebbles in both cylindrical and annular core geometries are studied for two types of PB-HTR designs: HTR-10 and PBMR-400. The resulting packings show similar radial and axial packing fraction distributions compared to the dynamic equilibrium packing state produced by the DEM pebble flow simulation. Comparisons with other existing random packing methods, such as the gravitational deposition method, have shown that the developed method not only exhibits excellent computation efficiency, but also presents desirable potential in other applications as a general packing algorithm for packing mono-sized or poly-sized spheres in a large container.

**Key words:** Pebble bed reactor, initial pebble packing, discrete element method, random sphere packing, gravitational deposition method, granular flow

## 1. Introduction

Recently, Pebble-Bed High-Temperature Reactors (PB-HTR's) have received much attention in the development and demonstration of advanced reactor systems for the next generation nuclear power plants (Bardet et al., 2008; Forsberg et al., 2008; Gougar and Davis, 2006). Several designs have been proposed and studied. In a typical PBMR-400 configuration (NEA, 2005), one of the conceptual PB-HTR designs, a total of about 450,000 graphite fuel pebbles are loaded into the reactor core and circulate slowly during the reactor operation. In each fuel pebble, a total of about 15,000 TRISO fuel particles are randomly distributed in the fuel zone. Such a design leads to many unique features and excellent performances, such as high fuel burnup, online refueling capability and inherent passive safety. To provide reliable evaluations of these features, and especially the neutronic, thermal-hydraulic and safety performances, one of essential efforts is the accurate modeling of fuel pebble circulation in a reactor core (Auwerda et al., 2010; Cogliati et al., 2011; Park et al., 2010; Terry et al., 2002). Recently, much effort has been made to obtain the realistic distribution of the pebbles in PB-HTR systems by high fidelity pebble flow simulations (Cogliati and Ougouag, 2006; Li and Ji, 2010, 2011; Rycroft et al., 2006a; Rycroft et al., 2006b) and apply the obtained distribution to perform reactor core analysis (Auwerda et al., 2010; Kloosterman and Ougouag, 2007; Kloosterman and Ougouag, 2005).

Normally, pebble circulation can be modeled as a dense quasi-static granular flow driven by the gravity. Discrete Element Method (DEM) has been widely used (Bagi, 2005; Cogliati and Ougouag, 2006; Landry et al., 2003; Li and Ji, 2010, 2011; Makse et al., 2000; Rycroft et al., 2006a; Rycroft et al., 2006b; Silbert et al., 2002; Silbert et al., 2001) to model the sphere contact mechanics and predict the long-term dynamic behavior of granular flow. In PB-HTR's, due to the complicated physical interactions of pebble-to-pebble, pebble-to-reflector wall, and pebble-to-fluid, and the high-fidelity mathematical models used for computing these solid-related normal/shear and fluid-related drag/buoyancy forces, the dynamic simulation of pebble flow using DEM or coupled DEM and Computational Fluid Dynamics (CFD) method is computationally intensive. Thus, it normally takes a considerably long time to reach the dynamic

equilibrium state, i.e. a state that the pebble distribution is statistically steady after several circulations. However, if a quasi-equilibrium state pebble configuration can be constructed as an initial packing for the subsequent full dynamic simulation, the equilibrium state can be obtained quickly, which will greatly relieve the heavy computational burden and increase the overall efficiency in pebble flow simulation. In practice, it is desirable that the initial quasi-equilibrium state packing: (1) should present similar packing fraction distribution to the equilibrium/realistic state produced by the subsequent high-fidelity simulation, whose typical average packing fraction ranges within 55% to 63% and belongs to random loose packing (Makse et al., 2000; Rycroft et al., 2006b; Scott and Kilgour, 1969; Silbert et al., 2002; Song et al., 2008; Zamponi, 2008); (2) can be generated in a very cheap way without too much computational effort when within the 55% to 63% packing fraction range; (3) can be applied to both cylindrical and annular packing regions with a computational efficiency that is nearly independent of geometry complexity. Based on these three requirements, a new, fast and efficient random packing method is needed to provide an initial packing of a large number of pebbles at high packing fractions in complex reactor core geometries, and the development of such method is the major effort in this paper.

Random packing of spheres by computer simulation has experienced a long history. Literatures show that much effort has been made by many researchers for random packing of spheres at high packing fractions since last century (Bagi, 2005; Clarke and Wiley, 1987; Cooper, 1988; Finney, 1976; Jodrey and Tory, 1985; Makse et al., 2000; Mrafko, 1980; Mueller, 2005; Nolan and Kavanagh, 1992; Ougouag et al., 2005; Scott and Kilgour, 1969; Silbert et al., 2002; Song et al., 2008; Soppe, 1990; Visscher and Bolsterli, 1972; Zamponi, 2008). In general, packing algorithms can be classified into two models (Clarke and Wiley, 1987): sequential model and collective model. In the sequential model, spheres are generated one by one (or group by group) based on certain rules that ensure the randomness of packing and no overlaps between spheres. For most sequential packing approaches, the newly inserted spheres are either positioned randomly or following a constructive rule such as layer-by-layer method. Typical examples are Monte Carlo based rejection sampling trial methods (Cooper, 1988; Ougouag et al., 2005), gravitational deposition methods (Mueller, 2005; Visscher and Bolsterli, 1972), or the combination (Soppe, 1990), and domain triangulation methods (Bagi, 2005; Cui and O'Sullivan,

2003). Sequential models are easily implemented but fail to precisely attain the required total sphere quantity at high packing fractions, especially for the case of mono-sized sphere packing within a complex geometry, such as the PB-HTR core geometry. In the collective model, spheres (center points) are generated randomly permitting overlaps, and then the overlaps are eliminated by a collective rearrangement process: moving overlapped spheres apart while adjusting the sphere diameters at the same time (Clarke and Wiley, 1987; Finney, 1976; Jodrey and Tory, 1985; Mrafsko, 1980). Compared with sequential models, collective models are usually more time-consuming for random close packing (63%~64% packing fraction (Zamponi, 2008)) but more efficient for random loose packing and can attain the total sphere quantity or packing fraction exactly. From the perspective of physics, random packing algorithms can also be classified into geometry-based model and dynamics-based model (Bagi, 2005). A geometry-based model, for example, the sequential trial method mentioned above, does not account for any realistic forces. While dynamics-based models adopt realistic forces to perform the sphere rearrangement, which are closer to the actual configuration but more computationally intensive compared with the geometry-based models. Many engineers even use the DEM simulation itself for the sphere packing initialization (Bagi, 2005; Ougouag et al., 2005), by firstly generating loosely packed spheres and then densifying the packing through realistic forces. This approach is effective but extremely costly due to the intensive computation requirement for DEM. Another widely used dynamics-based approach is the Gravitational Deposition Method (GDM) (Mueller, 2005; Soppe, 1990; Visscher and Bolsterli, 1972), which also belongs to the sequential model. In this method, spheres are dropped into the container one by one and then find their equilibrium positions under gravity and normal contact forces. As pointed out above, being a sequential model, the gravitational deposition method cannot precisely control the total sphere quantity within a confined space.

In this paper, a new collective dynamics-based method, named as Quasi-Dynamics Method (QDM), is developed to obtain a quasi-equilibrium state packing of pebbles, as a static initial packing for the subsequent high-fidelity simulation of coupled pebble flow and coolant fluid flow in PB-HTR's. Both the initial packing and the dynamic pebble flow simulation have been implemented in a recently developed code PEBFD (Li and Ji, 2010, 2011). In the new method for the initial packing, pebble positions (center points) are firstly generated randomly within the

reactor core region allowing overlaps. Then a simplified normal contact force model is adopted to move overlapped pebbles apart using a nearest neighbor search technique (Ougouag et al., 2005). The dynamics-based nature of this method brings a pebble distribution closer to the equilibrium/realistic pebble arrangement produced by high fidelity simulation methods, such as the DEM, in PB-HTR's. Meanwhile, the simplified normal contact force model and the nearest neighbor search technique greatly improve the efficiency of the initial packing. The developed method is applied to the pebble packing for two typical PB-HTR designs: a full core size HTR-10 configuration and a scaled PBMR-400 core configuration. In both applications, radial and axial pebble distribution profiles are calculated and compared with those obtained by the high-fidelity DEM simulation. It demonstrates that the developed QDM can generate an assembly of pebbles that is close to the realistic configuration. The efficiency of the QDM is compared with the other conventional initial packing method, the gravitational deposition method, and shows excellent efficiency performance. Besides above PB-HTR applications in which the pebbles have uniform radii, poly-sized sphere packing is also studied using QDM to prove its potential as a general sphere packing approach.

## 2. Methodology Description

Assuming to pack  $N$  spheres with known radii  $r_i$  ( $i=1$  to  $N$ ) in a container, the developed method first generates  $N$  spatial points that are uniformly distributed within the container. Each point is a center of a sphere. Due to the finite size, some spheres may overlap with each other or overlap with the container wall. Next, a simplified normal contact force model is employed to calculate “normal contact forces” for each sphere based on the size of each overlap. A total “force” can then be calculated by summing up all the “normal contact forces” due to overlaps and this total “force” is used to move each sphere to a new position. The moving direction and distance are determined by the calculated total “force” and the sphere size. In this way, sphere overlaps are eliminated iteratively while all the spheres are constrained within the container boundary. The key idea in the developed method is assuming a “repulsive force” in all the overlaps and eliminating these overlaps by displacing each sphere based on the total net “repulsive force” at each step.

The simplified normal contact force model that is used to calculate the “repulsive force” is described as follows: according to contact mechanics (Johnson, 1985), for two spheres  $P_i$  and  $P_j$  with radii  $r_i$  and  $r_j$ , relative normal speed  $v_{n,ij}=(\mathbf{v}_i-\mathbf{v}_j)\cdot\mathbf{n}_{ij}$  and overlap size  $\delta_{ij}$ , the realistic normal contact forces  $\mathbf{F}_{n,ij}$  can be given as:

$$\mathbf{F}_{n,ij} = \sqrt{\frac{r_i r_j}{r_i + r_j}} (k_n \delta_{ij}^{1.5} - \gamma_n \delta_{ij}^{0.5} v_{n,ij}) \mathbf{n}_{ij}, \quad (1)$$

where  $k_n$  and  $\gamma_n$  are material elastic and viscoelastic constant separately, and  $\mathbf{n}_{ij}$  is the unit normal vector.

Different from the high-fidelity simulation of pebble flow, the initial packing procedure does not have to account for all the realistic physics. Therefore a simplified and linearized contact force model is adopted:

$$\mathbf{T}_{ij} = K_s \sqrt{r_{ij}} \delta_{ij} \mathbf{n}_{ij}, \quad (2)$$

where  $r_{ij}=r_i r_j / (r_i + r_j)$ ,  $K_s$  is a constant associated with the sphere elasticity and usually much less than the true value of  $k_n$ .

For a sphere with radius  $r_i$ , similar normal contact force  $\mathbf{W}_i$  can be formulated if the sphere overlaps with the container wall with an overlap size  $\delta_i$ :

$$\mathbf{W}_i = \sqrt{r_i} K_w \delta_i \mathbf{n}_i, \quad (3)$$

where  $K_w$  is a constant associated with the boundary elasticity and  $\mathbf{n}_i$  is the wall normal direction. The total contact force acting on the  $i^{\text{th}}$  pebble  $\mathbf{F}_i$  is calculated by the vector summation of  $\mathbf{T}_{ij}$  over all the overlapped spheres and  $\mathbf{W}_i$ :

$$\mathbf{F}_i = \sum_{j \neq i}^M \mathbf{T}_{ij} + \mathbf{W}_i. \quad (4)$$

And the displacement for  $i^{\text{th}}$  pebble is determined by:

$$\Delta \mathbf{X}_i = K_d \frac{\mathbf{F}_i}{r_i^3}, \quad (5)$$

where  $K_d$  is a constant. The moving direction is determined by the total contact force  $\mathbf{F}_i$ .

Eqs. (2) and (3) form the central scheme of the QDM. It linearizes the terms in the high-fidelity model for the normal contact force. This linearization is motivated by regarding the sphere-to-sphere or sphere-to-wall overlap as a compressed spring system. The overlap elimination process would be a step-by-step spring relaxation procedure. The step size is determined by a force that is linear to the overlap size in each step. This is the simplest and the fastest model to calculate the “repulsive” force between any two overlapped spheres, which is the basic calculation that has to be done for each sphere in the container. Considering that tens of thousands of contacting pairs may exist in a typical PB-HTR geometry (>20,000 contacting pairs for HTR-10), the simplified linear model can provide high efficiency in the overall QDM procedure.

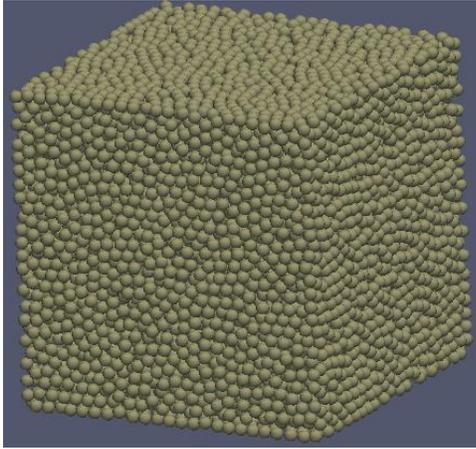
The constants  $K_s$ ,  $K_w$ , and  $K_d$ , are associated with sphere stiffness, wall stiffness and step size, which have significant impact on the algorithm convergence performance. In practice, for mono-

sized sphere packing,  $K_s$  can be chosen as  $K_s = \sqrt{\frac{2}{r}}$  such that  $K_s \sqrt{r_{ij}} = 1$  to simplify the expression of Eq. (2). The wall stiffness  $K_w$  can be set as  $K_w/K_s > 2$  (wall is much stiffer than sphere) to ensure that the average sphere-to-wall overlap is smaller than the average sphere-to-sphere overlap and consequently to well satisfy the boundary constraints. For the step size, generally a larger  $K_d$  leads to a faster convergence because two overlapped spheres can be easily separated by a large moving distance. However for a specified geometry, a critical step size  $K_d^c$  exists such that for  $K_d > K_d^c$ , the algorithm will be divergent. Numerical results indicate that  $\frac{K_d^c}{r^3} \rightarrow 1$  as the system geometry approaches infinity. This is demonstrated by packing mono-

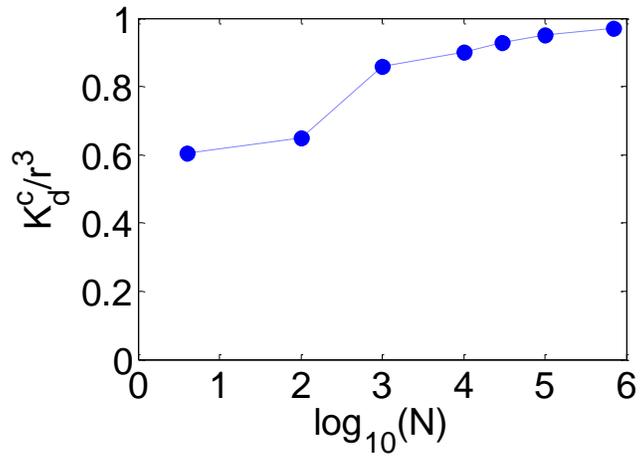
sized spheres in a cubic container as shown in Fig. 1a. To observe the behavior of  $\frac{K_d}{r^3}$  as the system size increases, we fix the size of the cubic container and decrease the radius of the spheres. At each different radius, the packing fraction is kept approximately constant at 60%. The system size (also the number of spheres in a container) impact on the critical step size  $K_d^c$  can be obtained as shown in Fig. 1b. It is required that  $K_d < r^3$  to ensure the algorithm convergence. For a smaller container, a larger margin, defined as  $r^3 - K_d$ , should be kept when choosing the value of  $K_d$ . For PB-HTR application, since the number of pebbles within the reactor core is the order of  $10^4$  for HTR-10 geometry and  $10^6$  for PBMR-400 geometry with packing fraction greater than

60%, it is suggested to choose  $\frac{K_d}{r^3} \sim 0.9$  to achieve both high efficiency and robust performance.

As for general poly-sized sphere packing,  $K_s$  can be chosen as  $K_s = \sqrt{\frac{2}{r_{\max}}}$  where  $r_{\max}$  is the maximum sphere radius. The wall stiffness  $K_w$ , can be chosen by following the same  $K_w/K_s > 2$  rule as in the mono-sized packing. For the  $K_d$ , it is suggested to follow a conservative  $K_d < \bar{r}^3$  rule ( $\bar{r}$  is the average radius) to ensure the convergence.



(a) Cubic packing geometry



(b) Impact of sphere number  $N$  on  $K_d^c$

**Fig. 1.** Investigation of impact from sphere number  $N$  on  $K_d$

By choosing appropriate values for parameters  $K_s$ ,  $K_w$ , and  $K_d$  based on the above guideline, the spheres are moved to a new configuration at each iteration, and these procedures will be repeated until the maximum overlap is less than a pre-determined threshold value. To illustrate the robust convergence performance of the algorithm qualitatively, the sphere configuration with overlaps can be deemed at an excited state with elastic potential energy stored. Then the simplified contact force will drive the pebbles to a new configuration without overlaps, corresponding to one of the possible lowest energy states. Since the sphere size is taken into account in the algorithm, it can handle both mono-sized and poly-sized sphere packing problems. It is worth to mention that there exists a packing fraction upper limit for the QDM, which is as high as around 64.3% and corresponds to the maximal randomly jammed state (or random close packing state) (Zamponi, 2008). In this extreme situation, most or all the pebbles are in jammed state, in which

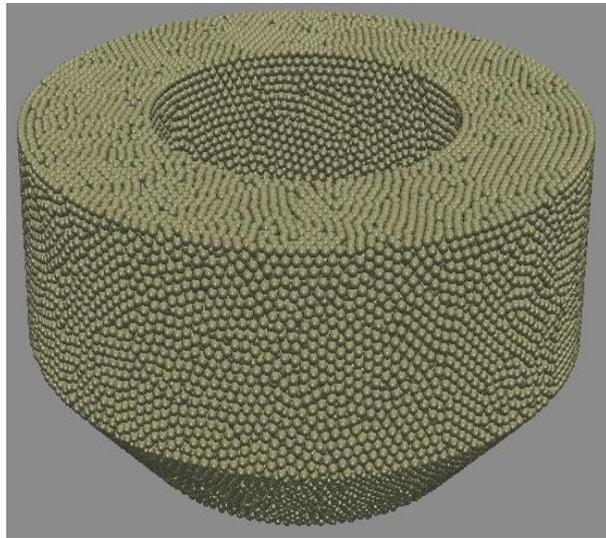
significant contact forces exist but the summed net force  $F_i$  for each jammed pebble equals to zero or is very small. Hence no further motion (separation) can be obtained according to Eq. (5).

### 3. Applications of the QDM to Initial Pebble Packing in PB-HTR's

The developed method is applied to providing initial pebble packings in two typical PB-HTR configurations. The first configuration is shown in Fig. 2a. A total of 29,600 pebbles are randomly generated within a full core HTR-10 geometry, which is a cylindrical core at the radius of 90cm and height of 180cm, with a 45 degree conic bottom. The second configuration is shown in Fig. 2b. The initialization of 66,300 pebbles is performed within a PBMR-400 annular core with reduced height, which has an outer radius of 185cm, an inner radius of 100cm and a height of 120cm. All the pebbles have a uniform radius of 3cm. In our simulations using the developed high-fidelity DEM code under realistic PB-HTR configurations (Li and Ji, 2010), the pebble volume packing fraction ranges from 61% to 63%, therefore the efficiency of the proposed method should be evaluated within this packing range. The comparison of pebble packing distributions with the high-fidelity DEM-based pebble flow simulation is made to demonstrate that the QDM can generate a packing configuration similar to the dynamic equilibrium state. The high efficiency of the QDM is also demonstrated by comparing with the traditional gravitational deposition packing method.



(a) HTR-10: cylindrical core geometry



(b) PBMR-400: annular core geometry

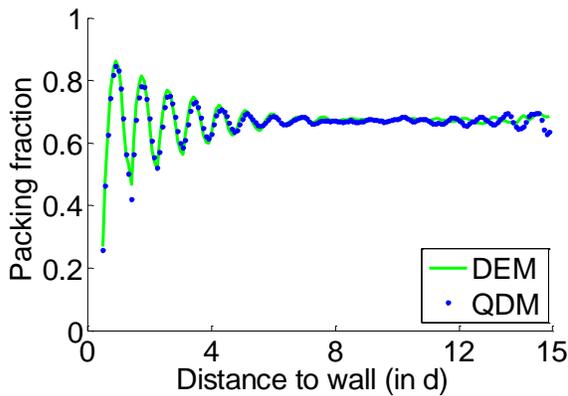
**Fig. 2.** Pebble packing initialization in cylindrical and annular PB-HTR's

### **3.1 HTR-10 initialization**

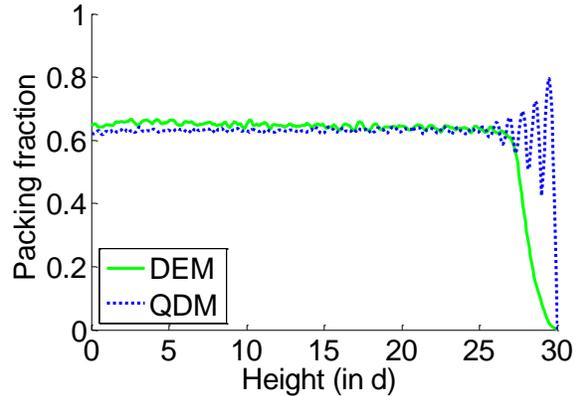
During the normal operation in HTR-10, pebbles are injected at the top of the reactor core region and removed from the conic bottom. The high fidelity pebble flow simulation based on the DEM follows the actual pebble loading and discharging processes in HTR-10. In the DEM simulation, it starts with an initial pebble configuration is generated either by the QDM or by other pebble initialization techniques such as the Gravitational Deposition Method (GDM), and there is no boundary constraint on the top of the newly loaded pebble. According to previous work (Li and Ji, 2010), the packing statistics can reach near-stable state in the cylindrical HTR-10 core within one fuel circulation cycle, attaining an average packing fraction as high as 63% for the pebble occupied region. A static packing at the same packing fraction and with the same amount of pebbles is generated by the QDM, where the values of constant parameters are chosen as  $K_s=0.8165 \text{ cm}^{-0.5}$ ,  $K_w=2.3 \text{ cm}^{-0.5}$ , and  $K_d=24.0 \text{ cm}^3$ . In order to achieve the specified packing fraction using the QDM, a top surface constraint is applied to preventing pebbles “floating” at the top of the pebble bed. This may introduce oscillatory packing fraction distribution near the top of the surface. However, as shown later, the bulky region still shows the similar packing statistics to the DEM simulation. In practice, once the pebble circulation starts with the initial packing generated by the QDM, the oscillatory change in the packing fraction near the top will vanish quickly.

The radial and axial packing fraction distributions are compared between the QDM and the high-fidelity DEM simulation, especially in the cylindrical core region. The radial packing fraction distribution is obtained by calculating the ratio between the area occupied by spheres and the total area on the cylindrical surface at each radial position (Toit, 2002). Similarly, the axial packing fraction distribution is calculated as the fraction of the area occupied by the spheres to the total area on the horizontal cross-sectional surface at different height of the reactor core region. The comparison of the pebble radial distributions is shown in Fig. 3a. It can be seen that the QDM resembles the realistic HTR-10 packing statistics under the operation condition (given by high-fidelity simulation) except for minor differences near the central zone. Because of uniform radial spacing, smaller amount of pebbles fall into the inner radial intervals, hence the

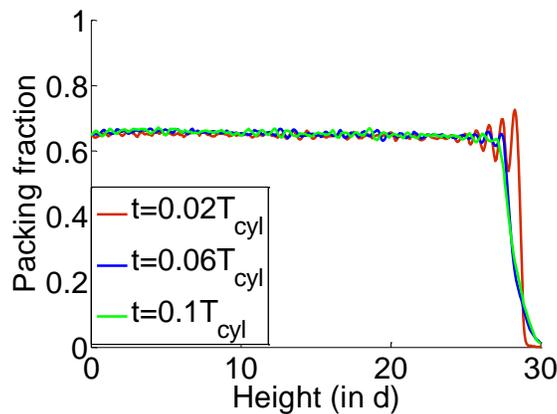
variation of the radial packing distribution in the central zones becomes larger as approaching the center. The axial pebble packing distribution comparison is shown in Fig. 3b. It can be observed that the average packing fraction is well maintained throughout the core region in both the QDM and the DEM, except for the top region of the pebble bed. This is because the QDM uses a constrained top surface while the DEM does not. As indicated above, this oscillation diminishes quickly after DEM simulation starts. If we denote  $T_{cyc}$  as the average time needed for a pebble to travel from the top of the reactor to the outlet bottom in the high fidelity DEM simulation (which takes around 1,200s of physical time and 1 week of single thread CPU time on a DELL T7500 3.6GHz workstation), it is observed that the oscillation becomes insignificant within  $0.1 T_{cyc}$ , as shown in Fig. 3c.



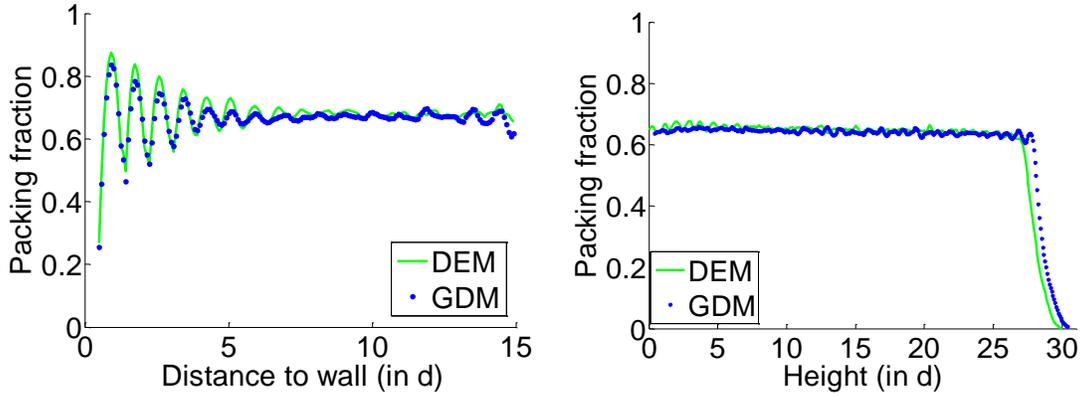
(a) radial distribution profiles of QDM



(b) axial distribution profiles of QDM



(c) quick diminish of the oscillation in axial packing fraction generated by QDM



(d) radial distribution profiles of GDM

(e) axial distribution profiles of GDM

**Fig. 3.** Comparison of radial and axial pebble packing fraction distributions produced by the DEM, QDM and GDM for the initial pebble packing in HTR-10

As a contrast, the radial and axial packing fraction distributions are also compared between the GDM and the DEM simulation. The results are shown in Fig. 3d and Fig. 3e. Since no constrained top surface is needed when the GDM is used to pack spheres, the resultant axial packing fraction distribution does not show the oscillatory behavior at the top region as appears in the QDM results. The average axial packing fraction in the bulk region is close to the steady state DEM result, similar to the QDM result. For the radial packing fraction distribution, the GDM does not show a close agreement with the steady state pebble flow result generated by the DEM, especially at the region near the wall.

The similarity of the radial and axial packing distribution between the initial packing generated by the QDM and the equilibrium packing generated by the DEM indicates that the computational time would be decreased significantly if the high-fidelity simulation starts with the pebble distribution generated by the developed initialization method, compared with other initialization technique such as starting from an ordered packing or a very loose random packing. Numerical results show that the DEM simulation starting with the initial configuration from the QDM can reach the steady state within less than  $0.5 T_{\text{cyc}}$  for HTR-10 geometry, while for GDM it is around  $0.6 T_{\text{cyc}}$  and for pouring method (or random sequential addition method) it takes slightly more than  $1.0 T_{\text{cyc}}$ . It takes even longer for ordered initialization, for example, the initialization with simple cubic (SC) structure takes between  $1.7 T_{\text{cyc}}$  to  $2.5 T_{\text{cyc}}$  (depending on the material friction coefficient and Young's modulus) to reach the steady state. For body-centered cubic (BCC)

initialization, local jamming near the bottom is likely to occur hence it may even terminate the pebble recirculation process at the non-steady state.

Figure 3 demonstrates that the QDM can generate an initial packing that is close to the dynamic equilibrium state, which can save computation time for the pebble flow simulation to reach the stable pebble flow status. In order to have a further idea about the relative efficiency of the QDM compared with other commonly used initialization method, the initialization time at various high packing fractions using the QDM and the GDM are recorded in Table 1.

**Table 1**

CPU time comparison between the Quasi-Dynamics Method and the Gravitational Deposition Method for the initial pebble packing in HTR-10 (29,600 pebbles).

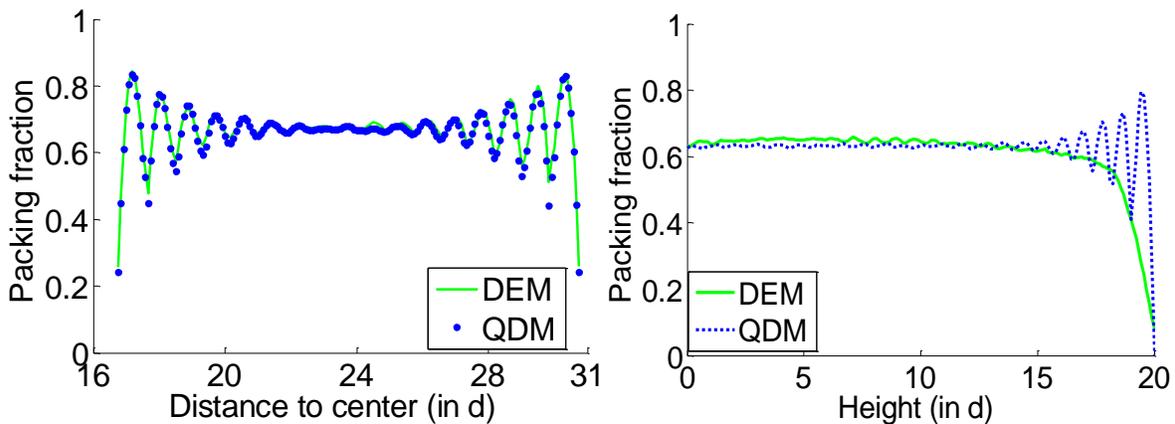
Packing fraction	61.5%	62%	62.5%	63%	63.5%
Quasi-Dynamics Method	~45s	~65s	~90s	~145s	~380s
Gravitational Deposition Method	~160s	~175s	~200s	N/A	N/A

From Table 1, it can be seen that the developed method is much faster than the gravitational deposition method over the range of packing fractions from 61.5% to 62.5%. As the increase of the packing fraction, the simulation time increases significantly due to the increase of average contacting neighbors for each pebble, while the gravitational deposition method only has a slight increase in CPU time. It is verified in our simulations that an upper packing fraction limit exists for the QDM, which is around 64.3% for HTR-10 geometry, corresponding to the maximal randomly jammed state (or random close packing). However, there is no lower packing fraction limit for the QDM. It is also verified that the gravitational deposition method can generate packings only with a more restricted range of the volume fraction, mostly between 60% and 62.5%. For the packings that are greater than 62.5% or lower than 60%, it becomes ineffective. For the realistic PB-HTR configuration, due to the large friction coefficient of graphite pebbles ( $\mu \sim 0.7$ ), the actual packing fraction is usually less than 63% (Makse et al., 2000; Rycroft et al.,

2006b; Silbert et al., 2002; Song et al., 2008) , within the range that the developed dynamic-based method has the best performance.

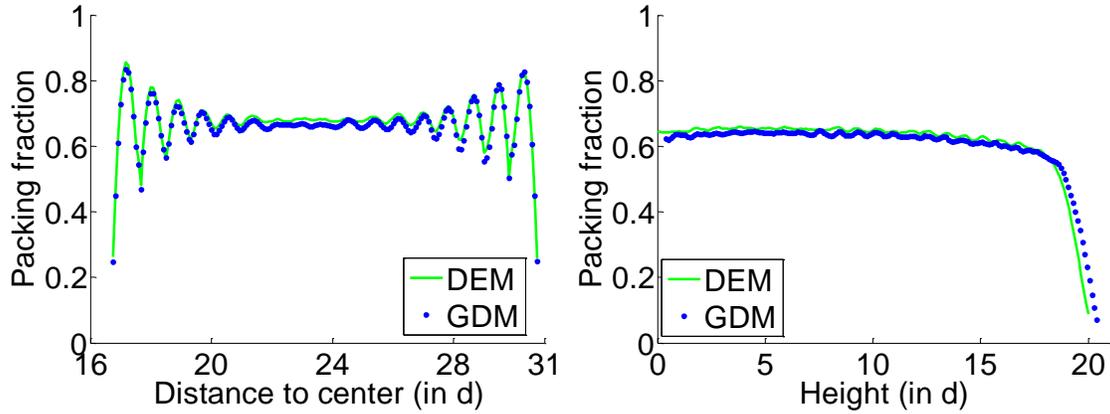
### 3.2 Scaled PBMR-400 initialization

PBMR-400 is another PB-HTR design with annular core geometry configuration. Section 3.1 has demonstrated the efficiency of the QDM in packing pebbles in the cylindrical core geometry of HTR-10, it is necessary to verify whether QDM can retain the same efficiency in a different geometry, such as the annular core geometry with greater height-to-radius ratio. Since the core measures 11m in height in the realistic PBMR-400 design, more than 450,000 pebbles are in the active core. Such a large geometry requires significant amount of computation time for high-fidelity DEM simulations ( $T_{cyl}=34$  days CPU time) on a DELL T7500 3.6GHz workstation without parallelization. Although parallelization can reduce  $T_{cyl}$ , it is beyond the scope of this paper. As it does not change the initial packing statistics generated by the QDM and the GDM, hence does not change their relative efficiency in reaching the steady-state pebble flow. In order to speed up the comparison, a core with the same radial geometry but has a reduced height of 1.2m is simulated with 66,300 pebbles inside. A DEM simulation for one fuel cycle is performed in which pebbles are injected from the top and removed from the conic bottom. Same amount of pebbles are packed using the QDM within the same geometry with the same parameter values as used in the HTR-10 geometry. The packing statistics for QDM are obtained and compared with the DEM simulation, as shown in Fig. 4a and Fig. 4b. As a contrast, the comparisons between the packings from GDM and DEM are also made, shown in Fig. 4c and Fig. 4d.



(a) radial distribution profiles of QDM

(b) axial distribution profiles of QDM



(c) radial distribution profiles of GDM

(d) axial distribution profiles of GDM

**Fig. 4.** Comparison of radial and axial pebble packing fraction distributions produced by the DEM, QDM and GDM for the initial pebble packing in PMBR-400

From Fig. 4, it can be observed that the QDM can still maintain its similarity to the DEM simulation in packing statistics, which is comparable with the GDM results. Although the results are obtained from a scaled PMBR-400 geometry, the QDM can handle the full core PMBR-400 geometry initialization within 3 hours on a on a DELL T7500 3.6GHz workstation. Due to the similarity in packing statistics between the QDM and DEM simulations, it is expected that the proposed method can significantly expedite the overall simulation time needed to reach the dynamic equilibrium state if the DEM simulation starts with the initial packing provided by the QDM, as proved in the HTR-10 geometry.

**Table 2**

CPU time comparison between the Quasi-Dynamics Method and the Gravitational Deposition Method for the initial pebble packing in PMBR-400 (66,300 pebbles).

Packing fraction	61.5%	62%	62.5%	63%	63.5%
Quasi-Dynamics Method	~115s	~165s	~235s	~410s	~1,120s
Gravitational Deposition Method	~405s	~420s	~450s	N/A	N/A

The CPU time comparison between the QDM and the gravitational deposition method for the PBMR-400 application is given in Table 2. By comparing Table 1 and Table 2, it can be seen that, for both methods, the CPU time increases nearly proportionally to the increased pebble quantity, indicating that geometry complexity does not have much impact on the CPU time compared with the impact of total pebble amount. The geometry complexity has almost no impact on the upper limit of packing fraction that each method can achieve. Therefore it can be concluded that the QDM still exhibits higher efficiency and better applicability in the PBMR-400 core geometry. Similar as the HTR-10 case, for high-fidelity PBMR-400 DEM simulation starting with the QDM result, the system can reach the steady-state flow within  $0.45T_{\text{cyl}}$ , while the time is still  $0.6T_{\text{cyl}}$  with the GDM initialization. This is approximately 5 days of CPU time difference. As mentioned above, parallelization can reduce  $T_{\text{cyl}}$ , but will not change the packing statistics generated from either QDM or GDM, hence there will be no impact on the relative efficiency of QDM in quickly reaching steady-state flow.

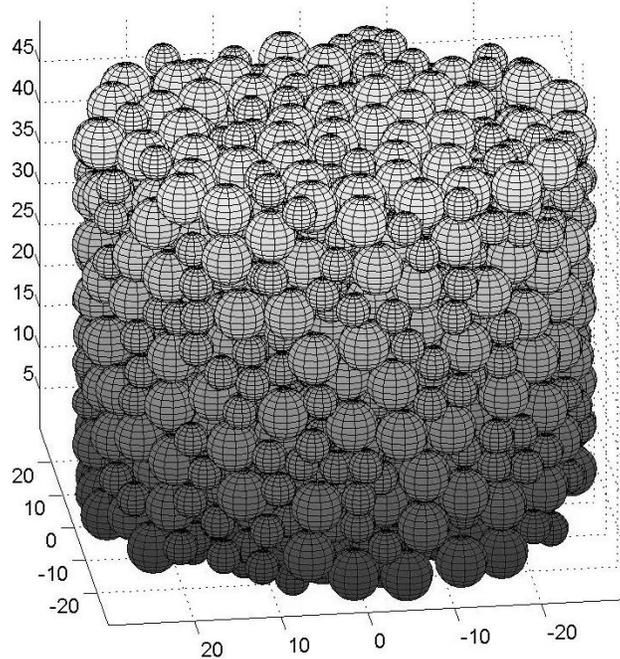
### 3.3 Poly-sized sphere packing

Since the radius impact is taken into account, the developed method can generate both mono-sized and poly-sized sphere packings. Previous sections have shown the applications of the QDM to the mono-sized sphere systems, such as HTR-10 and PBMR-400. To illustrate its capability to deal with the packing of poly-sized spheres, an example of packing 1,400 spheres within a 30cm radius and 60cm height cylinder is shown in Fig. 5. The spheres have two sizes,  $r_1=3\text{cm}$  and  $r_2=2\text{cm}$  which are sampled with equal probability. The CPU time of the QDM is around 3.8 seconds, while the packing of 1,400 spheres with uniform radius of  $r=3\text{cm}$  at the same packing fraction takes 3.4 seconds to converge. Therefore the size variation does not have much impact on the efficiency of QDM, and only some adjustment on the algorithm parameters is needed in

order to achieve best convergence rate, such as  $K_s = \sqrt{\frac{2}{r_{\text{max}}}}$  and  $K_d < \bar{r}^3$  as discussed in Section

2. The ratio of the maximum pebble radius  $r_{\text{max}}$  to the minimum radius  $r_{\text{min}}$  can be as high as  $r_{\text{max}}/r_{\text{min}}=10$  without affecting the computation efficiency too much. For higher  $r_{\text{max}}$ -to- $r_{\text{min}}$  ratio which is greater than 10, the cell-based nearest neighbor search approach in the QDM will

deteriorate significantly in efficiency due to the fact that there will be too many small spheres within a mesh cell.



**Fig. 5.** Poly-sized sphere packing: a total of 1,400 spheres are randomly packed in the cylindrical region with 30cm radius and 60cm height. Half amount of spheres have radius of 3cm and the other half have radius of 2cm.

#### 4. Conclusions

A collective dynamic-based sphere packing method is developed and applied to providing an initial packing of pebbles for the high-fidelity simulation of pebble flow in PB-HTR's. In the new method, pebble positions are first uniformly sampled to produce random dense packing at a designated packing fraction, allowing overlaps. And then enlightened by the normal contact force calculation used in high-fidelity DEM simulation, a simplified virtual contact force is adopted to eliminate the overlaps. Due to the dynamics-based nature, the radial and axial packing fraction distributions of the pebbles packed by the developed method are similar to the ones obtained by the high-fidelity simulation for an operating PB-HTR. Thus, the developed initial packing method can effectively speed up subsequent high-fidelity simulation in approaching equilibrium state.

The application of the QDM to two common PB-HTR designs, a full scale HTR-10 and a PBMR-400 design with reduced height are studied. The developed method demonstrates its capability in both designs. The efficiency of the QDM is demonstrated by comparisons with an existing packing method, the gravitational deposition method. It shows that the developed method is more efficient in providing an initial packing of pebbles within the range of packing fractions in PB-HTR's. Moreover, as a collective packing approach, the QDM can control the final packing fraction precisely compared with the gravitational deposition method. Since the developed method accounts for the pebble radius so it can pack both mono-sized and poly-sized spheres, giving it the potential as a general sphere packing approach for applications in granular material/flow study. Finally the dynamics-based nature enables the developed method to deal with complex constraints and boundary conditions, which is very useful for complicated PB-HTR core geometry.

### **Acknowledgements**

This work was performed under the auspices of the U.S. Nuclear Regulatory Commission Faculty Development Program under contract NRC-38-08-950.

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