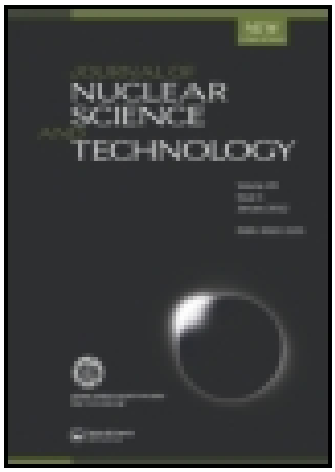


Journal of Nuclear Science and Technology
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/tnst20

# A review on numerical models for granular flow inside hoppers and its applications in PBR

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Published online: 10 Dec 2014.

To cite this article: Yushi Tang, Liguo Zhang & Qiuju Guo (2014): A review on numerical models for granular flow inside hoppers and its applications in PBR, Journal of Nuclear Science and Technology, DOI: 10.1080/00223131.2014.986553

To link to this article: http://dx.doi.org/10.1080/00223131.2014.986553

*Journal of Nuclear Science and Technology*, 2014
http://dx.doi.org/10.1080/00223131.2014.986553

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**REVIEW**

# A review on numerical models for granular flow inside hoppers and its applications in PBR

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(*Received 4 July 2014; accepted final version for publication 6 November 2014*)

Granular flow is the shearing motion of a collection of discrete solid particles which are commonly seen and widely utilized in various industrial applications. One of the essential applications of dense slow granular flow in engineering is the pebble flow in pebble-bed nuclear reactor (PBR). A number of numerical models have been established for researching the basic physical mechanisms and properties of granular flow. For the purpose of generating an appropriate model for high temperature reactor-pebblebed modules (HTR-PM) in the future, numerical models on granular flow in hoppers and some of their previous applications on PBRs are reviewed. In this paper, basic transport and contact mechanisms of granular flow are firstly introduced, then kinetic theory from gas molecules and plastic theory from metal mechanics approaches give descriptions of the macroscopic behavior of rapid flow and quasistatic flow regimes, respectively, subsequently kinematic continuum method and discrete element method (DEM) are presented to describe the bulk features of dense slow flow in hoppers. Since various kinematic models, DEM models and their modified versions for dense slow granular flow in hoppers have been experimentally verified and applied in prediction of pebble flow in PBRs, a promising model for HTR-PM is expected with further work to generate pebble flow profile in the future.

**Keywords: granular flow; discrete element method; kinematic model; PBR; burnup measurement/assay**



## 1. Introduction

Granular materials are commonly seen in nature and widely utilized in various industrial applications and daily life. Granular particles display a complex range of properties for their solid- or liquid-like state depending on the applied conditions, the fluid-like nature might be firstly recorded in quotation taken from Jacques [1] (ca. 98–55 B.C.). The storage and flow of granular materials in hoppers are of great importance in engineering applications. However the basic physical mechanisms and properties of liquid-like granular flow have been poorly understood [2]. Generally numerical simulations based on simplified theory have been utilized to study the physical mechanism of granular flow with a number of specific parameters provided while experiments are intuitional but limited information can be obtained.

Granular flow modeling began with the paper by Coulomb (1773) who firstly described the yielding of granular materials as a frictional process [3]. The flow was initially studied through some simple experiments and approximate analysis, providing empirical formulations for engineering problems. Bagnold [4] was the first to try and model a granular material from the point of individual particles, justifying his constitutive law of frictional stress tense with experiments performed on a suspension of particles in a shear cell. During the next several decades, a number of experiments on rapid shearing flow explained that energy was transmitted through interparticle collisions, but not continuous friction. After the 1970s, basic microscopic physical mechanism on interparticle collision was studied and developed [5]. Subsequently kinetic model was established for rapid granular flow with the concept of "granular temperature" initially proposed by Ogawa [3] out from molecular dynamics (MD), the simulation result was reproduced by Monte Carlo simulation. Decades later, Cundall and Strack developed a program for two-dimensional disks based on discrete element method (DEM) and were considered as pioneers of researching granular flow from the aspect of discrete individuals [6]. Meanwhile, the continuum models for dense slow granular flow have also been proposed, one is the plastic theory with the Mohr–Coulomb yield criterion, another is the kinematic model based on the continuous limit of

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random-walk/void model by Litwinszyn [7] which generated a diffusion equation from a constitutive law, followed by the spot model which was recently proposed as one of the statistical kinematic models for velocity profile. However the models for different flow regimes are incomplete as the flow state is rather difficult to nearly exact characterize.

One of the essential applications of models on dense granular flow in engineering is in the pebble flow of pebble-bed nuclear reactor (PBR) which is currently being developed as a more economical, efficient and safer energy supplier around the world [8]. High temperature reactor-pebblebed modules (HTR-PM) being developed now by Tsinghua University is such a pebble-bed reactor which is in the shape of an upper cylindrical vessel and a bottom funnel. It is important to gain a more detailed understanding of pebble flow in the core, thus revealing some basic physics of granular flow and giving implications for the reactor design in PBR, whereas the pebble flow in dynamic core is not fully understood. So far most of the information on pebble flow in PBRs was generated through experiments which could only provide limited information, hence numerical models on granular flow in hoppers have been proposed and have succeeded in various applications of PBRs. For instance, the positions and velocities of tracked pebbles reproduced by kinematic model and DEM were used to study the basic granular physics in draining silos such as the mean streamlines, core diffusion and mixing, etc. Additionally other outstanding issues directly relevant to physical reactor design and testing, such as the geometry dependence of the mean streamlines and wall effects, have been well analyzed with numerical tools [8]. Consequently the simulations can contribute to the reliable prediction of reactor physics like power output, heat transfer efficiency, fuel burnup, etc., which rely on pebble flow profiles as an empirical input; furthermore the DEM simulation of coupled pebble flow and coolant flow with the computational fluid dynamics (CFD) approach has been introduced in the analysis of PBR thermal-hydraulics for accurate simulations of more core physics characteristics [9,10]. These simulation results can be reference data for the design factors in PBR. The ultimate purpose of this research on pebble flow is to generate the burnup distribution of fuel pebbles especially those being discharged out of the core, consequently investigating the probability for the actual burnup of fuel pebbles exceeding the safety burnup limit with the approach of burnup measurement [11], which is essentially related with the containing capability of radioactivity in reactor safety. Therefore some of models' previous applications on PBRs are reviewed for giving implications on generating an appropriate model for pebble flow in HTR-PM in the future.

This paper starts with an introduction of the basic transport and contact mechanism in granular flow. It continues with brief descriptions of two extreme granular flow regimes. It then gives introductions on two different models, the DEM model and the kinematic model, for dense slow/quasistatic flow. Later it introduces some of the proposed models' applications on PBRs. Last section is the summary.

## 2. Basic transport and contact mechanism

Granular flow is the shearing motion of a collection of discrete solid particles. It is commonly considered as a two-phase flow in which the spaces between particles are filled with gas or liquid. However, it is generally assumed in granular flow research that particles are large and heavy in the sense that they will not be affected by the interstitial fluid. Cohesion originated from surface forces or related phenomena such as liquid bridges can be neglected for large particles with small surface area to volume ratios [3]. Therefore in general the influence of the interstitial fluid is neglected and friction and collision between cohesionless particles are the concern.

In a dense gravity-driven granular flow, interacted solid particles can be line-linked and stably form a force chain which allows the force distribution within the material to be visualized (see Figure 1). These quasiliner structures support the bulk of external load and gravity of the particles within the material, giving rise to the frictional property and contact stress tense of granular flow. In a shearing material, these force chains are dynamic structures. It will quickly become unstable and collapse after the material is rotated slightly by the shear motion [6].

The derivation of contact force between two spherical particles in a cohesionless dense granular flow can be originally explained by Hertz and Mindlin–Deresiewicz solutions.

In a dense granular flow, forces are largely generated by interparticle contacts like collision and friction. When two spherical particles are pressed together, three analytical forms of normal interaction laws could be applied: Hertzian interaction, continuous interaction and Hooke's law spring interaction [2]. Concerning the nonlinearity of the contact response, Hertz (1882) derived the elastic solution of normal contact force between two spheres with the assumption that the square root of the contact area is small compared to the radius of curvature $R$ [3]. The interparticle normal force given by Hertz is as follows:

$$f_n = \frac{4}{3} R^{1/2} \frac{E}{1-\nu^2} \delta^{3/2} \tag{1}$$

where $E$ is the Young's modulus, $R$ is the radius of curvature, $\nu$ is Poisson's ratio and $\delta$ is the depth of the contact deformation (the distance the contact has been compressed). Then the normal stiffness of particle is given as the derivative of $f_n$: $k = \frac{df_n}{d\delta}$.

In addition to the normal force, there is also a frictional component of contact force, the expression of tangential force is much more complicated which will

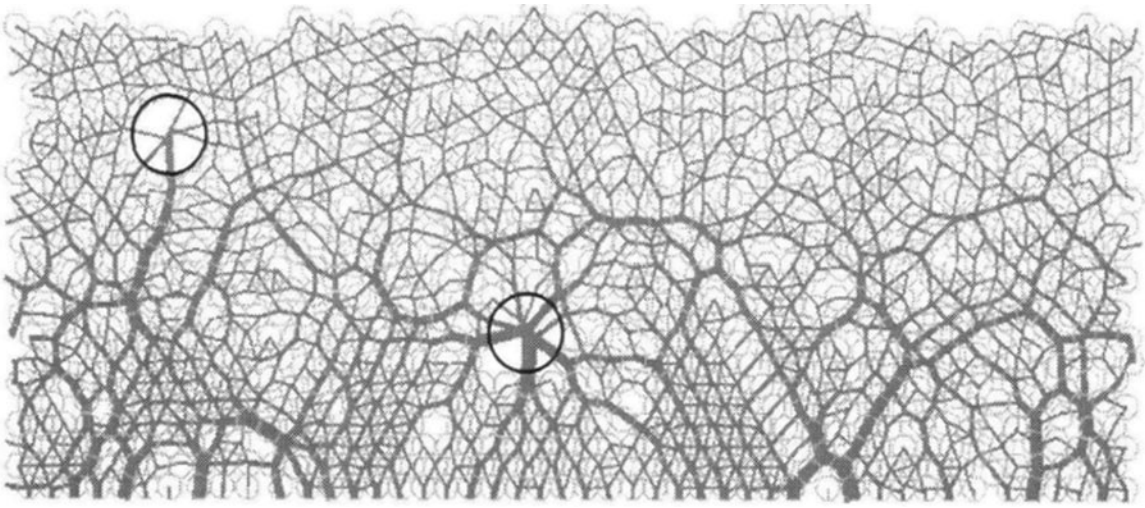

Figure 1. Force chains and constructions as particles are static (circles in light color are particles, lines in deep color are force chains with the thickness of lines being proportional to the interparticle contact force) [6].



not only depend on normal force but also evolve much dramatically with its loading history [3,6]. Mullier found that the analytic form of complex theory firstly proposed by Mindlin and Deresiewicz (1953) for micromechanical contacts could well describe the behavior before gross sliding [12] (when the surfaces of the two particles slip relative to another). Such a gross sliding critical condition could be initially explained by Mohr–Coulomb yielding criterion (1773) which is usually expressed in the form below for cohesionless particles:

$$\tau \leq \sigma \tan \phi \tag{2}$$

Here, $\tau$ is the shear stress, $\sigma$ is the normal stress, the constant $\phi$ is assumed to be material properties and $\tan \phi$ is generally what we call a "frictional coefficient" as $\mu$. When $\tau > \sigma \tan \phi$ (or as $F_t > \mu F_n$), the material yields and begins to gross slide, then frictional force is assumed as a constant value given by Amonton's law, $F_t = \mu F_n$ [2]. In general, $F_t$ is changed because surface friction coefficient is changed due to the removal of the asperities during gross sliding.

Differences will be present if the material yields plastically as the contact force is concerned. Walton [13] and Thornton [14] made analyses of Hertzian contacts with plastic yielding, it is shown that the normal force $f_n$ is nearly linearly related with $\delta$ during the loading period, indicating a nearly constant normal stiffness $k$. Nevertheless, the unloading gives another linear curve with a different steeper slope, indicating a constant but larger $k$. This can be explained physically that it is the flat indentation caused by plastic deformation in the particle surface which leads particles to lose contact early that makes the difference. This bilinear behavior has led to the "spring–dashpot" contact model which has been used in many computer simulations [3].

## 3. Models on extreme granular flow

Granular flow has been mostly studied from the aspects of experiment, basic theory and numerical simulation. Experiments are intuitional and can provide verification for proposed theories and models, but limited information of physical mechanism can be obtained. Numerical models based on simplified theory have been utilized to provide a number of specific parameters to study the microscopic physical mechanism of granular flow.

Generally, granular flow can be roughly divided into two categories, quasistatic flow and rapid flow, based on the flow velocity. Particles in a very slow shearing motion form the quasistatic flow regime, whereas particles with rapid shear velocity in rapid flow regime can move randomly in the intervals of collisions and the solid concentration is not that high. Campbell [3] has recently been able to unify the various flow theories and conclusively divided the field into two broad regimes, the elastic and the inertial, depending on whether the force chains are formed in the flow. The elastic flow regime in which the force is transmitted through the force chains is mainly observed in dense granular flow, and is divided into the elastic–quasistatic (or quasistatic flow) regime and the elastic–inertial regime based on whether there is an apparent dependence of stresses on the shear rate. The inertial regime encompasses flows with low solid concentration, no stable force chains and frequent interparticle collisions, and is divided into inertial–noncollisional regime and inertial–collisional (or rapid flow) regime depending on whether the dominant particle interaction is binary collision. Although the flow has been reclassified by Campbell, two extreme granular flow regimes are still discussed in this section. In general, the two extreme flow regimes, the quasistatic flow and rapid flow, can be numerically simulated by frictional plastic model and

kinetic model, respectively, in which the flow are both considered as continuity.

### 3.1. *Slow flow/quasistatic flow*

The flow of cohesionless quasistatic granular materials in conical hoppers was modeled by Nguyen et al. [15] using a perfect plastic continuum representation of the material. Hence the past plasticity theory was mostly adopted in the theoretical analysis for hopper flow in slow flow regime. Tüzün [16] made a overview on the work of plasticity theory.

In quasistatic flow, the particles keep touched and rubbed in a critical state in the sense that the flow behaves incompressibly with the density fixed at the critical concentration. The quasistatic models which relate stress and density to predict velocity field or mass flow rate [17] were derived from metal plasticity theory (or soil mechanics) applying a Mohr–Coulomb frictional yield condition. As a result, the material is treated as a continuous plastic solid, but not as individual particles. The basic principles and governing equations were generated by Sokolovski [18] and the theory was further simplified by the concept of "critical state". It is assumed in the metal plasticity theory that the flow begins to collapse once the tense situation satisfied a yield criterion, many yielding conditions for granular material have been established and various frictional plastic models have been proposed, i.e. the double shearing model, plastic potential model and double slip model for free rotation, etc. [5].

Whereas there are problems when they are used to predict qualitative features of hopper flow, especially the deviation problem attributed to boundary conditions [17]. Besides, the solutions available for hoppers possessed shock-like velocity discontinuities [8] and unphysical highly oscillatory behavior; some solutions also failed to describe the observed gravitational flow patterns of granular particles in a confined geometry [7], casting serious doubts on the validity of the continuum models.

### 3.2. *Rapid flow/collisional flow*

The rapid flow model is derived using models from the kinetic theory of gases. It is assumed particles in rapid flow interact by instantaneous collisions, and this is similar to the behavior of gas molecules although the interparticle collision with energy dissipating is more complex. Therefore the developed kinetic theory of gas has opened a door for rapid flow model and it was firstly applied to granular flow by Savage and Jeffery [19]. As intermolecular collisions will induce random velocities that are reminiscent of the thermal motion of molecules, a "granular temperature" was also superimposed on the velocity field representing the random, thermal-like, kinetic energy of the particles. Granular temperature generates relative interparticle motion in two primary modes of particle transport, which are collisional transport mode driving the particles to collide and streaming transport mode mixing the diffusive particles. Boltzmann function is the basis of the theory and a group of Navier–Stokes-like equations are generated through the kinetic theory [3].

However there are several problems that should be figured out with this formulation. The most obvious one is that the limited capability of applications of rapid flow theory for the reason that rapid flow is rarely found naturally and can only be simulated in computer or found in high-speed laboratory shear cells. Thus systems such as hoppers cannot be modeled by rapid flow theory. Besides, there are no correlations in the velocities or positions of colliding particles with the assumption of Boltzmann's "Stosszahlansatz" or molecular chaos in the theory, however, it is likely that the velocities and positions will be strongly related as the particles will interact many times at large concentration [20,21].

Moreover, elastic parameters of particle like stiffness which is important for the description of granular flow are not included in frictional plastic and kinetic continuum models, leading to the neglection of the microscopic aspect of granular flow. With various disadvantages of the two models being presented, appropriate models for dense slow granular flow are required to simulate the unique features and gain a more detailed understanding of granular flow in hoppers.

## 4. Models on granular flow in hoppers

The dense slow or quasistatic high solid concentration granular flow found in hoppers is still poorly understood although the motion of particles has been researched from many different aspects of the flow with various theoretical techniques, for example, Beverloo's equation for predicting mass discharge rate, Janssen's differential slice force balance method for wall stress [2], Monte Carlo simulation with Langevin equation for granular flow trajectories [22] and Baxter's radiography method for observation of the density wave, etc. [17].

For a more detailed understanding of dense granular flow in hoppers as well as for implications from pebble flow for PBR design, the flow velocity of granular/pebble flow inside a (conical) hopper should be well numerically generated. On the whole, kinematic continuum method and DEM have been proposed and have succeeded in describing the bulk features of dense slow flow in hoppers.

### 4.1. *Kinematic model*

The flow profile of dense slow/quasistatic flow can be modeled by two approaches based on continuum theory. One is based on the plastic theory with the Mohr–Coulomb yield criterion which was introduced in the quasistatic models in the previous section, however, many simulations thus far have consequently led to the doubtful validity of the quasistatic models based

on plastic theory. The second approach which ignores the stress field and attempts a purely kinematic description, starting from an empirical constitutive law, is called kinematic model (diffusion equation). The kinematic model is possibly the only continuum theory available for flow velocity profile in a slowly draining hopper [8].

Litwinszyn firstly considered the possibility that the velocities can be determined by purely kinematic effects and introduced a stochastic model in which particles perform random walks into voids. Mullins proposed an equivalent stochastic model in terms of "voids" and developed the continuum limit [23,24]. Subsequently, Nedderman and Tüzün [16] have derived a continuum equation (diffusion equation with a third variable) on this approach from a constitutive law relating horizontal velocity $V_x$ and horizontal gradient of vertical velocity $V_z$ which is expressed as follows when a void is generated at locations $x$ and $z$:

$$V_x = -B\nabla_\perp V_z \tag{3}$$

where $\nabla$ is the horizontal gradient, $B$ is the "diffusion length", a parameter related with granule material and core geometry and is typically in the range of one to three times of the granule diameter. The assumption behind Equation (3) is that the upper particles tend to drift down to the region of a faster downward velocity, where there is more free volume to accommodate. Considering the small density fluctuation in dense granular flow, with the combination of incompressibility condition (Equation (4)), a diffusion equation for downward velocity is obtained as Equation (5),

$$\frac{\partial V_z}{\partial z} + \frac{\partial V_x}{\partial x} = 0 \tag{4}$$

$$\frac{\partial V_z}{\partial z} = B\nabla^2 V_z \tag{5}$$

where $\nabla^2$ is the horizontal Laplacian. Equation (5) is in the form of a diffusion equation, in which the vertical coordinate acts like "time". When an "initial condition" is given for downward velocity $V_z$ at the orifice, where $Z = 0$, the velocity diffuses upward. Boundary condition on Equation (5) assumed at the side walls of a hopper is that the velocity is parallel to the wall. Nedderman derived an analytic similarity solution (Equation (6)) for a two-dimensional flat-bottom silo with a point-like orifice at $z = 0$ acting as the source of velocity [25],

$$V_z = \frac{Q}{\sqrt{4\pi Bz}} \exp\left(-\frac{r^2}{4Bz}\right) \tag{6}$$

where $Q$ is the flow rate per unit thickness of the silo and $r$ is the radius of the silo. On solving the boundary-value problem above, the implicit Crank–Nicholson integration scheme [8,17] has been used to generate numerical solutions to the partial differential equation in Equation (5). A range of parameter $B$ values have been measured experimentally by various groups [17,25,26], and the experimental flow field qualitatively predicted by kinematic model with a single fitting parameter $B$ for steady flows of noncohesive materials in simple geometries were viewed as successes of the model.

However, the problem with simple kinematic "continuum" method is that, in the main, it ignores the effects of microstructure of the bulk and relies on an assumed (often over-simplistic) constitutive equation. Therefore this approach with its continuum formulation cannot predict particle-level diffusion and mixing as well as the formation of stagnant and cascading zones [7]. Meanwhile there are some statistical kinematic models proposed for velocity profile, the void model (earlier in 1972) and spot model (2002) [17], both of which postulate mechanisms for random-packing dynamics. Mullins (1979) developed the void model and suggested that the motion of granular particles in a confined geometry, for example, a hopper with a hole at the bottom, may be considered as the particles drift passively in response to the upward motion of voids generated after the discharge of particles through the hole. The kinematic model can be considered as a continuum limit of the void model. Therefore it can be understood that the parameter $B$ in kinematic model is originated from the void model as a diffusion length for free volume. Decades later Caram and Hong revisited the void model (random-walk/stochastic model) and implemented it in computer simulations on a triangular lattice [7], indicating that it correctly predicted the presence of stagnant and cascading zones, although the model was later claimed to face serious problem when predicting diffusion and mixing [17]. To address the contradiction, a more realistic mechanism, the spot model, originating from a cooperative diffusion mechanism in a dense random packing was proposed by Bazant et al. [27,28]. The void is replaced by extended "spots" of slightly enhanced interstitial volume and causes all affected particles to move in the opposite direction to the spot as an entity. The spot model was testified to capture many essential features of dense drainage and produce accurate flowing packings in wide silos [17] while problems like nonphysical interstitial site and spheres stacking have recently been found out [29].

Regardless of its ignorance to any specific microscopic mechanism, these kinematic models are simple to use and applicable in various geometries of dense slow granular flow. However it is noted that the kinematic models have other limitations as the velocity is generated with only one determined parameter which is too simple to capture all the aspects of velocity profiles in hoppers. It was found that $B$ increased with the local velocity as well as the conical angle, so a nonlinear constitutive law was proposed and modifications on boundary conditions and spot dynamics were suggested to better describe the general field [8,17]. In addition, some researchers [26] considered that the wall friction related

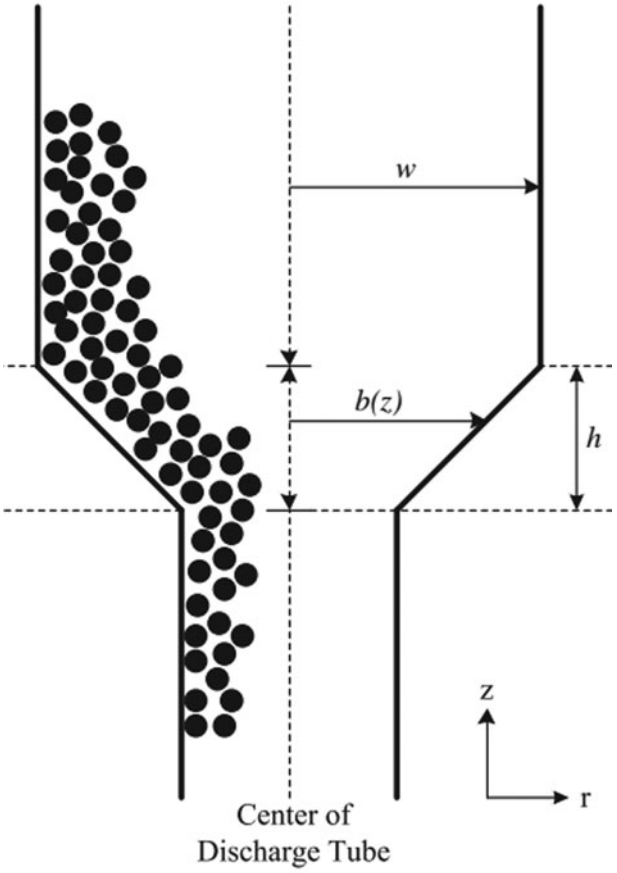


Figure 2. The horizontal view of the pebble reactor depicting the notations of Equation (7) [26].

with particle properties was not pertinently included in Equation (5) and it was difficult to analyze pebble velocity in conical hoppers and PBRs having annular core and defuel chutes with an application of this model, therefore in the study, with frictional terms added in Equation (5) and assumptions made upon the flow, a modified kinematic equation without changing $B$ is given as follows. The horizontal view of the pebble reactor with an upper cylindrical region, a conical funnel and a bottom discharge tube is given as Figure 2

$$\frac{\partial V_z}{\partial z} = B\nabla^2 V_z - f_b V_z H(r - b(z))H(h - z) - f_w V_z H(r - w)H(z - h) \quad (7)$$

where $\nabla^2$ is the horizontal Laplacian, $H$ is the Heaviside function, $f_b$ is the velocity reduction coefficient of the conical wall boundary, $b(z)$ is the distance from the reactor central axis to the wall in cone region, $h$ is the height of the cone region, $f_w$ is the velocity reduction coefficient of the cylindrical wall boundary, $w$ is the distance from the central axis to the wall in the upper cylindrical region (Figure 2). Therefore the right two terms are added for velocity reduction due to the conical wall and cylindrical wall boundary. The specific coefficients used in this modified model were acquired by cylindrical core experiments. The point Kernel method was adopted in this work for solving Equation (7) in models of complex pebble reactor with annular core, and the pebble velocity profile was verified by experiments with annular core model.

### 4.2. *Discrete element method*

The dynamics of the system are followed at the micro-contact level by this approach. Inspired by the MD method, Cundall and Strack [30] originally proposed DEM, upon which they developed programs for two-dimensional disks and three-dimensional spheres to further research the microscopic mechanism of granular flow. Subsequently it was viewed as a success of DEM and has been developed as a critical numerical tool to simulate granular dynamics. Generally, DEM starts from treating individual particles (and their physical characteristics) as separate entities in the model and afterwards attempts to give a description of time evolution of the assembly with Newton's equations of motion applied to predict particle trajectories in discrete time steps.

Setting to simulate the granular flow with DEM, a previous work is required that the interparticle forces shall be numerically described since most particles in a granular assembly will form contacts with several other particles. There are usually three models that are different in their description of interparticle contact [6].

The first one gives description on near-exact contact mechanism. The force–displacement theory on normal and tangential contact force by Hertz and Mindlin–Deresiewicz which was introduced in Section 2 has been adopted in this model for cohesionless dense particles. For the complexness when dealing with mutual-interactive, history-dependent contact forces, the incremental method was used in numerical simulation [6]. Group of Thornton [31] of Birmingham University has developed DEM simulation program for three-dimensional spheres based on this near-exact contact mechanics and has been recognized as a successful contributor in further promotion of DEM simulation in granular flow. The latter two models are simplified versions of the first model.

The second one is hard sphere model which treats particles as inelastic and collisions are all taken as instantaneous. It totally ignores physical mechanism of particle deformation and it is an over-simplification, consequently this model can only be applied in low solid concentration rapid granular flow and will not be discussed more here.

The last model, soft sphere model, was initially proposed by Cundall and Strack. Theories given by Hertz and Mindlin on contact force present a purely elastic contact, however, the material in dense granular flow actually behaves plastically during collisions as stated in Section 2. This can be simple-demonstrated by soft sphere model. Figure 3 is the schematic drawing of soft sphere model by Walton which is in the spring–dashpot

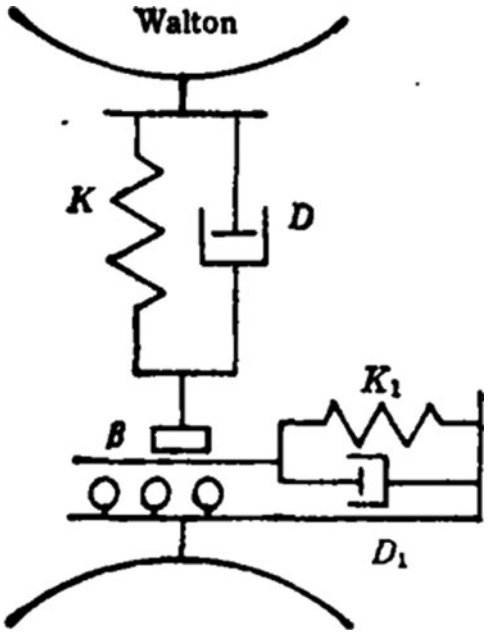


Figure 3. Soft sphere model for contact force in particle collision [31].

frame [32]. The spring designed for elastic part of interaction and the dashpot designed for dissipating energy co-state the main idea of soft sphere model that contact interaction is composed of elastic, kinetic energy damping and frictional components. Therefore the total contact force (both tangential and normal) at any time can be generally given as $F = k\delta - DM$, where $k$ is stiffness, $\delta$ is the depth of deformation, $D$ is damping coefficient and $M$ is the reduced mass [6].

Among all the contact models above, the model based on near-exact contact mechanism has no simplification in the description of contact force and can be applied to simulation of any flow regime which ranges from quasistatic flow to rapid flow, making it the best model to study microscopic mechanism of granular flow [6]. The soft sphere model is intuitive, making it easier to describe the system, it has been applied in many engineering problems and is the spirit of the TRUBAL program developed by group of Cundall.

The model is generally stated by a pebble motion which includes the transitional motion of the center of mass and the rotational motion about the center of mass. The basic functions of DEM are as follows [33]: Equations (6)–(8) give descriptions of normal and tangential forces $F_n$ and $F_t$ together with the Coulomb yielding criterion of frictional force. Equations (9)–(10) are functions giving the resultant force $F_c$ and its torch which are based on the Newton's equations of motion.

$$\begin{aligned} F_{cn} &= -k_n \cdot \delta_n + \beta_n \cdot V_n \\ F_{ct} &= -k_t \cdot \delta_t + \beta_t \cdot V_t \\ |F_{ct}|_{\max} &\le \mu\,|F_{cn}| \end{aligned} \qquad (6)\text{–}(8)$$

$$\begin{aligned} m\frac{dv}{dt} &= F_c + F_g \\ I\frac{d\omega}{dt} &= r \times F_c \end{aligned} \qquad (9)\text{–}(10)$$

where $F_{cn,ct}$ are the normal and tangential contact force, $k_{n,t}$ and $\beta_{n,t}$ are the elastic and damping coefficient, respectively, $V$ is the relative surface velocity components, $\delta$ is the deformation, $\mu$ is the frictional coefficient, $m$ is mass of element, $I$ is moment of inertia, $v$ is velocity of element, $\omega$ is angular velocity of element, $F_c$ is the resultant contact force, $F_g$ is the gravity of element, $r$ is the distance between the interacted two elements. Most of the DEM simulations on cohesionless granular flow are based on a modified version of the soft sphere model given the basic equations mentioned above. The position, velocity, and angular velocity of each pebble are individually tracked and updated according to the contact models and motion equations; the massive amount of precise data given by DEM are then used to reconstruct the flow profiles such as the mean flow, the mean flow velocity, streamlines, etc.

DEM has been developed as a critical numerical tool to simulate granular dynamics which can construct the complicated microscopic granular mechanism; it is more realistic-descriptive and has the advantage that no global assumptions are required on the material such as steady-state behavior or uniform constituency as in the continuum theory, besides the difficulties in describing the boundary conditions and particle properties in continuum model do not exist. However, the improper values of the contact parameters can lead to subsequent unexpected simulation problems [34], especially the stiffness $k_n$ in soft sphere model which can not be measured directly was considered to be relevant to $k_t$ and it is now usually given with an empirical value with no agreed applied rules [6]. Additionally a number of assumptions and constants determined from experimental data will be difficult given the large parameter space [26]. Besides the soft sphere model is somehow simplified which induces deviation from the real contact force, which may lead to some theoretical and conceptual problems [10], so further study and applications of the classical near-exact contact mechanism are required. Conclusively the selection of proper parameters and a more comprehensive theory to study and quantify the interaction forces between particles are of great importance in generating accurate results. These issues should be considered in the further development of force models.

## 5. Applications of models in PBR

So far studies on pebble flow in PBRs have focused on experiments with approaches including traditional phenomenological method, pebble marker

method and radiography method [35] while experiments can only provide limited, although important, information on pebble flow. Therefore the previous introduced kinematic models, DEM models and their modified advanced versions for dense slow granular flow in hoppers have been experimentally verified and applied in the predictions of pebble flow profiles in PBRs, thus revealing some basic physics of granular flow and providing implications for reactor design and in PBR.

With the massive amount of precise data about the position and velocity of each pebble, simulations have been carried out and compared to experiments to study the basic granular physics in PBR, e.g. bulk flow features such as the velocity field, pebble-based statistics such as the porosity distribution, and core diffusion and mixing which would be helpful in determining the propensity for rare events that could affect individual pebble peaking factors [36]. For instance, Rycroft et al. analyzed comprehensive basic flow features such as the mean velocity, diffusion and mixing, local ordering and porosity, etc. with kinematic and DEM methods [8]. Kim et al. proposed a modified kinematic model with experimentally determined coefficients to simulate the pebble velocity for reactors with annular core [26]. Li et al. investigated the trajectories and velocities as well as the particle diffusion at the interface of the "double zones" in PBR during monosized glass beads discharging using the DEM simulation code Granule developed by Thornton's group [37]. Wang et al. also analyzed the pebble dynamics in two-dimensional double-zone PBR using phenomenological method with DEM simulation [33].

Additionally many other aspects of granular flow in PBR cores of direct relevance for design and testing have been analyzed with kinematic models and DEM, i.e. numerical simulations have been studied on outstanding issues such as the sharpness of the interface between fuel and moderator pebbles (in both monodisperse and bidisperse cores), the geometry dependence of the mean streamlines, wall effects, etc. [8]. Scaling properties and graphite dust generation problem were analyzed with DEM simulations performed by using the code LAMMPS on both full-size and scaled-down geometries [36].

Consequently the simulations can contribute to the reliable prediction of reactor physics like power output, heat transfer efficiency, fuel burnup, etc., which rely on pebble flow profiles as an empirical input. However it is still difficult to accurately predict the realistic core physics with only DEM directly adopted in the simulation for the unique fuel design in PBR: hundreds of thousands of complex-structured fuel pebbles are constantly recycling in the core region and gas coolants are flowing under high pressure through the interstitial space of pebbles. The stochastic motion of pebbles, complicated pebble–coolant interactions and the coupling between the pebble and coolant flow make the predictions of flow properties quite difficult. Hence a more realistic particle–fluid modeling method for PBR considering the strong interactions among pebbles, coolants and reactor walls was proposed. The most widely used one is the coupled DEM-CFD approach [10] in which the particle flow is simulated with DEM model and the fluid quantities are computed with the CFD model. Whereas due to its high price and long computational time in large fluid–particle system, Li et al. proposed accelerated strategies to simulate the pebble–coolant system in PBR without loss of accuracy [9]. It is expected that with further work for the existed DEM-based approaches, more core physics characteristics can be more accurately simulated and provide implications for the design factors in PBR.

The ultimate purpose of this research on pebble flow is to generate the burnup distribution of fuel pebbles especially those discharged out of the core while the pebble burnup is thought to be only closely related to the pebble velocity profile (or pebble residence time: the time it takes to pass through a certain height) which can be obtained numerically by previous methods and the nonuniform distribution of neutron flux. The fresh fuel is supplied from the top of the core and the burned fuel is extracted from the bottom of the discharge tube; fuel pebbles with measured burnup exceeding the determined burnup safety level are discharged out of the reactor while pebbles with lower burnup are refueled to the reactor. The time-dependent analysis of burnup starts with the velocity profile using batch-tracking method [38,39]. The core region is firstly divided into several axial flow channels, and the distribution of residence times in different channels due to variations of velocity profile along different streamlines can then be generated. Different fluxes and residence times in different channels result in the distribution of fuel pebble burnup. With velocity profile and neutron flux profile obtained, the MCNPX modeling based on Monte Carlo code for the particle transport and the burnup calculation is performed to track the fuel pebble burnup during the circulation and the burnup distribution of pebbles discharged out can then be constructed as well. Meanwhile a model of the detecting system is set up to produce the measured burnup of discharged pebbles with a certain accuracy. Consequently the burnup distribution of discharged pebbles and the measuring accuracy of the detecting system can generate the probability for actual pebble burnup exceeding the burnup safety limit, thus revealing its impacts on the safety operation of PBR.

In consideration of our purpose on velocity profile of granular flow, the mean-velocity profiles predicted with DEM and kinematic model by Rycroft et al. are presented here for reference [8]. Simulation results of DEM have shown well-agreed velocity distribution with experiments in the upper cylindrical region and exhibit a smooth transition from a nearly uniform plug flow in the cylindrical region to a nonuniform, converging flow in the lower funnel region, which is consistent with the standard engineering picture of silo drainage. Compared to DEM, the simple kinematic model was found to give

a reasonable qualitative prediction of flow profiles, but failed to picture the rapid transition from converging flow to plug flow in the upper region with vertical walls seen in the DEM data and did not precisely predict the dependence of the flow profile on geometry.

## 6. Summary

Flow of granular materials in hoppers is important in wide variety of applications, one of which is in the pebble flow of PBR. Models of granular flow in hoppers and some of their applications in PBRs have been studied and reviewed here to provide implications for an appropriate flow model for pebble flow in HTR-PM in the future in that the pebble flow is quite related with reactor core physics especially the burnup distribution of fuel pebble which is our further purpose on this research.

The basic transport and contact mechanisms of granular flow are firstly introduced. The force chains within granular flow can be visualized as dynamic quasiliner structures that support the external load as well as the source of friction and contact stress tense of the flow. The derivation of contact force between two spherical particles in the cohesionless dense granular flow can be originally explained by Hertz and Mindlin–Deresiewicz solutions.

Generally numerical models based on simplified theory have been utilized to study the physical mechanisms of granular flow. In the low solid concentration high shear rate and compact quasistatic high solid concentration extremes, kinetic theory from gas molecules and plastic theory from metal mechanics approaches, respectively, give descriptions of the macroscopic behavior of the granular state. Whereas some simulation results obtained casted serious doubts on the continuum model based on metal plasticity, and applications of rapid flow theory are limited concerning that rapid flow is rarely seen naturally and industrially except for simulations and experiments in shear cells. Thus dense slow flow systems such as hoppers cannot be well modeled by these two extreme flow regimes.

Kinematic continuum method and DEM have been proposed to describe the bulk features of dense slow flow in hoppers. The kinematic model ignores the stress field and attempts a purely kinematic description, starting from an empirical constitutive law, and consequently generates a diffusion equation relating the downward and horizontal velocity components. It is simple to use and there are analytic and numerical results for steady flows of noncohesive materials in simple geometries which were viewed as successes of the simple kinematic model. However, problems with the kinematic continuum method are that, in the main, it ignores the effects of microstructure of the bulk and relies on an assumed (often over-simplistic) constitutive equation. Second, only one free parameter $B$ is used in the model without considering wall friction and geometry. Therefore statistical kinematic models like the void model and the spot model concerning microstructure have been proposed, a nonlinear constitutive law and modifications on boundary conditions and spot dynamics in kinematic models were also suggested, and a modified kinematic equation with two velocity reduction terms added for conical and cylindrical walls friction were put forward in conical hoppers.

Whereas the DEM focuses on the dynamics of the system at the micro-contact level. Generally, DEM starts from treating individual particles (and their physical characteristics) as separate entities in the model and afterwards attempts to give a description of time evolution of the assembly with Newton's equations of motion applied to predict particle trajectories in discrete time steps. Three contact models which are different in their description of interparticle contact force are introduced. Most of the DEM simulations on cohesionless dense granular flow are based on a modified version of the soft sphere model. DEM has been developed as a critical numerical tool to simulate granular dynamics which can construct the complicated microscopic granular mechanism, although soft sphere contact force model has unsettled problems on parameters and it is simplified, deviated from the real contact force. Hence selection of proper parameters and a more comprehensive theory to describe the interaction forces between particles are important in generating accurate results and should be considered in the further development of contact models.

Various kinematic models, DEM models and their modified advanced versions for dense slow granular flow in hoppers have been experimentally verified and applied in the prediction of pebble flow in PBRs. Some applications of models on PBR are introduced for revealing some basic granular physics and the important implications for reactor design in PBR. Consequently the reactor physics like power output, heat transfer efficiency and fuel burnup, which rely on pebble flow profiles as an empirical input, can be reliably predicted although further effort is required to accurately predict the realistic core physics with DEM-based approaches. As our purpose is on the distribution of pebble burnup which is closely related to velocity profile of granular flow, the mean-velocity profiles predicted previously with DEM and kinematic model are presented here for reference.

Yet some aspects of granular flow system is still something of a black art, the existed models of dense slow granular flow are required to satisfy unique engineering environment. In further research, a reliable prediction of burnup distribution of fuel pebble is expected with the simulated flow velocity profile, which will finally lead to investigating the probability of actual pebble burnup exceeding the safety burnup limit with the approach of burnup measurement concerning the containing capability of radioactivity in reactor safety. Hence a promising next step of our work would be to generate an appropriate model for pebble flow in HTR-PM with more further work and the collected information of

reviewed models, and combine the existing computational approaches to analyze reactor core physics which rely on pebble flow profile as an empirical input.

**Acknowledgements**

This work is supported by the National Science and Technology Major Project [grant number ZX06901] and the Key Laboratory of Advanced Reactor Engineering and Safety and Tsinghua University jointly.

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