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PEBBLES: A COMPUTER CODE FOR MODELING PACKING, FLOW AND RE-CIRCULATION OF PEBBLES IN A PEBBLE BED REACTOR

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ABSTRACT

A comprehensive, high fidelity model for pebble flow has been developed and embodied in the PEBBLES computer code. In this paper, a description of the physical artifacts included in the model is presented and some results from using the computer code for predicting the features of pebble flow and packing in a realistic pebble bed reactor design are shown. The sensitivity of models to various physical parameters is also discussed.

INTRODUCTION

The knowledge of the packing and flow patterns (and to a much lesser extent the position) of pebbles in the pebble bed reactor is an essential pre-requisite for many in-core fuel cycle design activities as well as for safety assessment studies.

Among the in-core fuel cycle related data and studies that require the knowledge of the packing distribution and of the fuel motion patterns (i.e., velocity field) are the space-dependent Dancoff factors, zone-specific macroscopic transport and diffusion data (cross sections, diffusion coefficient), and fuel depletion prediction, which is complicated by the motion of the fuel. The characterization of the in-core fuel management features of the reactor also require the knowledge of the pebbles flow patterns, as these amount to a continuous on-line reshuffling of the fuel.

Among the safety related studies that require a knowledge of the pebble packing and flow patterns are, for example, (i) the study of feedback effects, as these depend on the availability and extent of the flow path for the coolant, (ii) the study of earthquake effects, as the motion from earthquakes can cause pebble bed densification and subsequent reactivity insertions and (iii) safety of the pebble bed during approach to the asymptotic state. The latter item pertains to the study of the intermediate states of the reactor during and following initial fuel loading, as the core approaches the final asymptotic equilibrium loading and burnup distribution pattern. All of the intermediate states are dictated by the successive positions of the pebbles as they move through the core.

From the above it is clear that a computer code is needed that provides the knowledge of the packing pattern of the pebble bed and that of the evolution of that pattern as the pebbles flow downward, are removed at the bottom of the core and recirculated to the top for some, while some fresh ones are added. The outcome of the first stages of the development of such a computer code for the analysis of the physics pebble bed reactor is presented in this paper. The paper exploits the code to explore the behavior of the bed of pebbles as pebbles are loaded, allowed to flow, and extracted at the bottom of the reactor. In addition the paper reports on the sensitivity of the model to certain physical parameters.

The computer code developed in this work embodies a method akin to the "discrete element method" (DEM) in which individual granules (pebbles in this work) are modeled explicitly [1] and the forces acting upon each are taken into account, providing the acceleration to which the pebble is subjected at every time step. The DEM method has been around for a long time and has been applied extensively in several areas of engineering ranging from mills to photocopy toner. In the following no comprehensive review of the literature is presented. Rather, only recent applications directly relevant to the modeling of the pebble bed reactor are surveyed.

The early German work on the AVR and THTR pebble bed reactors relied primarily on experiments to determine the pebble packing and flow patterns. Only three reports on the topic could be found in the English language [2,3,4]. These reports summarize the German experimental work used to determine the flow patterns for their experimental pebble bed

reactors. Only brief references to theoretical work are made in one the articles, but no methods are described and not theoretical/computational results are given [2]. More recently, du Toit used a Discrete Element Method (DEM) code to determine the packing of pebbles in a pebble bed reactor [5] applied it to determining the porosity of the bed for use in reactor thermal-hydraulics studies. In 2004, Reitsma reported the use of the PFC3D commercial package [6] for the comprehensive computational characterization of the pebble flow characteristics for the PBMR reactor [7] and its application to reactor design and fuel management. In 2005, Ougouag et al. presented two methods for the determination of the packing distribution of pebbles in a pebble bed [8]. The first of the methods, a Monte Carlo-based approach, is purely static and relies solely on geometric considerations. The second method uses a full DEM treatment. Both methods were then applied to the determination of spatially-dependent Dancoff factors [9]. Another model, based on the Kinetic Monte Carlo approach was presented at PHYSOR-2004 [10]. The most recent addition to computational models for the flow of pebbles in a pebble bed reactor that came to the authors' attention is the yet unpublished work of Rycroft and co-authors [11] in which they study some of the features and statistics of pebble flow in a vat representative of a pebble bed reactor. However, they did not use their method for any specifically nuclear reactor analysis application, although they discuss in their conclusions the potential impact of their pebble flow findings on the coolant flow and the burnup of fuel pebbles.

The work presented in this paper extends that of Reference [8]. The "dynamic method" of that reference is refined and its physical modeling of the pebble bed dynamic is completed. In particular, the present work adds the ability to extract pebbles at the bottom of the reactor vat as well as recirculate some of them while adding fresh ones at the top. The code that is developed allows the conduct of reactor-specific studies. Among other features, the code includes the capability to model earthquakes and their impact on core configuration (e.g., densification). The code has been used to provide data to nuclear engineering applications such as the computation of Dancoff factors [9] or the modeling of the first criticality of the HTR-10 reactor [12].

Although DEM codes are widely available (see for example Reference [13] for an introduction to the physics and extensive references), it was preferred in this work to develop an in-house code because of the need for extensive customization for treating nuclear reactor-specific problems. The approach taken here is that of the development of a code capable of simulations with as high a level of fidelity as possible in order to fully reproduce experimental behavior and, even in the absence of a suitable scaling theory, to confidently predict the behavior of larger systems such as the PBMR-400. A high fidelity code can also be used to study the sensitivity of the method to the various model parameters. In subsequent work it is planned to optimize and accelerate the code.

NOMENCLATURE

$C_{||}$: normal dashpot constant
$C_{\perp}$: tangential dashpot constant
$\mathbf{F}_{ij}$: force from pebble j on pebble i
$\mathbf{F}_{ci}$: force of the container on pebble i
$\mathbf{F}_{g}$: force of gravity on the pebble
$\mathbf{F}_{||ij}$: normal force between pebbles i and j
$\mathbf{F}_{\perp ij}$: tangential force between pebbles i and j
$\mathbf{F}_{sij}$: static friction force
$\mathbf{g}$: acceleration of gravity
h: Hooke's law constant
h_s: coefficient for force from slip
I_i: moment of inertia of pebble i
l_{ij}: overlap depth of pebbles i and j
m_i: mass of pebble i
$\hat{\mathbf{n}}_{ij}$: unit vector pointing from the position of pebble i to that of pebble j
$\mathbf{p}_i$: position vector of pebble i
r_c: radius of the inner (fueled) zone of pebble
r_i: radius of pebble i
r_o: outer radius of entire pebble
$\mathbf{s}_{ij}$: slip distance perpendicular to the normal force between two pebbles
$\mathbf{v}_i$: velocity of pebble i
$\mathbf{v}_{ij}$: relative velocity between pebbles i and j
$v_{\max}$: maximum velocity below which static friction is assumed to exist in this model
$\mathbf{v}_{||ij}$: component of the relative velocity of pebbles i and j along the line joining their centers
$\mathbf{v}_{\perp ij}$: component of relative velocity of two pebbles normal to the line joining their centers
μ: kinetic friction constant
μ_s: static friction coefficient
$\boldsymbol{\omega}_i$: angular velocity of pebble i
ρ_c: density of the inner (fueled) zone of the pebble
ρ_o: density of pebble outer zone

METHODOLOGY

The high-fidelity pebble flow model developed in this work treats each pebble as a discrete element. A systematic identification of relevant forces that act on each pebble is carried. They are then incorporated into a dynamic model. Newton's law of motion is applied to the resultant of all forces acting on a pebble and the acceleration of that pebble is obtained. The motion of the pebble is then determined for a short time step and the position at the end of the time step determined. Since the number of pebbles under consideration is very large, and since all have to be explicitly modeled, the size of the computation effort can grow very quickly and result in impractical computer CPU times for realistic simulations. For these reasons, a number of refinements are added to the computational strategy. In this section the relevant forces are identified and the most salient CPU-time-conserving computational algorithm enhancement is described.

Each pebble is subjected to two types of forces: potential and contact. The natural potential force is the weight of the pebble. Two other forces are treated as potential forces for the sake of algorithm convergence. These are the normal contact (elastic) forces between pebble pairs and between a pebble and the container wall. Although in a macroscopic picture this treatment might appear to be unrealistic, from a strict consideration of the microscopic underlying mechanisms, it can easily be recognized that the treatment is valid, provided properly chosen Young moduli are used. The contribution from potential forces on pebble *i* is expressed as

$$\mathbf{F}_i = \mathbf{F}_{ci} + \mathbf{F}_g + \sum_{j \neq i} \mathbf{F}_{ij} \quad ,$$

where $\mathbf{F}_{ij}$ is the force from pebble *j* on pebble *i*, $\mathbf{F}_{ci}$ is the force of the container on pebble *i* and $\mathbf{F}_g$ is the force of gravity on the pebble. The $\mathbf{F}_{ij}$ force is normally expressed as the product of Young's modulus and the "overlap" distance over the two pebbles. As for all very rigid bodies, the overlap distance is of necessity a very small fraction of the dimension of the pebbles. The contact forces of interest in this model are friction forces. They are discussed later.

The external forces applied to the pebbles cause accelerations and torques. The accelerations and torques are then used to determine the linear and angular velocities that arise from them. The time derivatives that are used for these determinations are

$$\frac{d\mathbf{v}_i}{dt} = \frac{m_i \mathbf{g} + \mathbf{F}_{ci} + \sum_{i \neq j} \mathbf{F}_{ij}}{m_i} \quad ,$$

$$\frac{d\mathbf{p}_i}{dt} = \mathbf{v}_i \quad ,$$

and

$$\frac{d\boldsymbol{\omega}_i}{dt} = \frac{\sum_{i \neq j} \mathbf{F}_{\perp ij} \times r_i \hat{\mathbf{n}}_{ij}}{I_i} \quad ,$$

where $\mathbf{v}_i$ is the velocity of pebble *i*, $\mathbf{p}_i$ is the position of pebble *i*, and $\boldsymbol{\omega}_i$ its angular velocity. $\mathbf{F}_{ij}$ is the total force on pebble i from pebble j, $\mathbf{F}_{\perp ij}$ is the tangential force on pebble *i* exerted by pebble *j* and $\mathbf{F}_{ci}$ is the force of the container wall on pebble *i*. The remaining variables, referring to pebble *i*, are the mass m_i, the radius r_i, the moment of inertia I_i, the normalized vector $\hat{\mathbf{n}}_{ij}$ pointing from the position of pebble *i* to that of pebble *j*, and **g**, the gravitational acceleration. The principal vectors for two interacting pebbles are illustrated in Figure 1.

The velocities (linear and angular) of individual pebbles can translate into the existence of relative motion from which kinetic friction forces arise.

In the above equations, the contact forces $\mathbf{F}_{ij}$ and $\mathbf{F}_{\perp ij}$ are calculated using Hooke's law assuming a force linearly proportional to the depth of overlap, and the kinetic friction is calculated using a dashpot model following Wait [14] and Rapaport [15]. Therefore, the contact forces are given by

$$\mathbf{F}_{\parallel ij} = h l_{ij} \hat{\mathbf{n}}_{ij} - C_{\parallel} \mathbf{v}_{\parallel ij}, \; l_{ij} > 0$$

and

$$\mathbf{F}_{\perp ij} = -\min\left(\mu \left|\mathbf{F}_{\parallel ij}\right| \; , \; C_{\perp} \left|\mathbf{v}_{\perp ij}\right|\right) \hat{\mathbf{v}}_{\perp ij}, \; l_{ij} > 0 \, ,$$

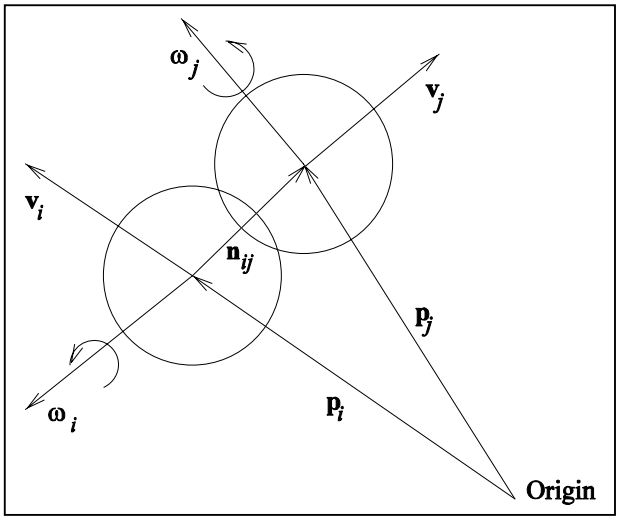


Figure 1. Principal Vectors in the Interaction of Two Pebbles.

where $\mathbf{F}_{\parallel ij}$ is the normal force between pebbles (parallel or along, the line between their respective centers) and $\mathbf{F}_{\perp ij}$ is the tangential force between them (perpendicular to the line between the centers). In the first equation, *h* is Hooke's law constant, l_{ij} is the overlap depth of the two pebbles, and $\mathbf{v}_{\parallel ij}$ is the component of the relative *surface* velocity of the pebbles along the line joining their centers. In the second equation, μ is the kinetic friction constant, and $C_{\parallel}$ is the normal dashpot constant, $C_{\perp}$ is the tangential dashpot constant, and $\mathbf{v}_{\perp ij}$ is the component of their relative velocity normal to the line joining their centers. The combined components of all forces acting on the pebble are used for calculating its acceleration, and the tangential forces are used for calculating the torque, as shown above. The components of the relative *surface* velocity between a pair of pebbles are calculated from the relative velocity, $\mathbf{v}_{ij}$, according to

$$\mathbf{v}_{\parallel ij} = (\mathbf{v}_{ij} \cdot \hat{\mathbf{n}}_{ij}) \hat{\mathbf{n}}_{ij}$$

and

$$\mathbf{v}_{\perp ij} = \mathbf{v}_{ij} - \mathbf{v}_{\parallel ij} \quad ,$$

whereas the relative *surface* velocity is calculated as the difference between the surface velocities at the center of the

region of contact. The surface velocity combines the translation velocity of the pebble, and the speed at which it is rotating. The equation for calculating the relative velocity is

$$\mathbf{v}_{ij} = (\mathbf{v}_i + \boldsymbol{\omega}_i \times r_i \hat{\mathbf{n}}_{ij}) - (\mathbf{v}_j + \boldsymbol{\omega}_j \times r_j \hat{\mathbf{n}}_{ji}) \quad .$$

The mass of the pebble is computed taking into account the variable density of its two constituent zones (the fueled zone and the outer graphite shell). With these considerations, the mass of the pebble is given by

$$m = \frac{4}{3}\pi[\rho_c r_c^3 + \rho_o (r_o^3 - r_c^3)]$$

where ρ_c is the density of the inner zone of the pebble, r_c is the radius of said inner zone, and ρ_o is the density of the outer zone, while r_o is the outer radius of the entire pebble. With the same notations, the moment of inertia is given by [16]

$$I = \frac{8}{15}\pi[\rho_c r_c^5 + \rho_o (r_o^5 - r_c^5)]$$

The forces exerted by the container wall on the pebbles that are in contact with it are computed as if the container wall were the surface of a pebble with zero linear and angular velocity and with normal direction between the wall "pebble" and the actual pebble taken as perpendicular to the container surface.

In addition to the forces already discussed, static friction is modeled since it is present, and a major contributor to the physical behavior of the pebble bed. Indeed, without static friction, the pebble bed model achieves packing densities that are significantly higher than those observed in experiments. Further, in the simplest early models we devised, ignoring friction and torque, the pebble bed tended to form ordered arrangements that are similar to crystalline structures of materials. The addition of static friction allows truly random packing to occur naturally in the simulations. In our method, static friction is accounted for by monitoring the distance that each pebble surface has moved relative to its immediate neighbors in a given time step. A force is then added that counteracts sliding motion when the magnitude of the relative velocity is below a preset threshold. This pseudo static friction is calculated (in a somewhat unphysical way) by assuming that it is proportional to the slip that has occurred between the two pebbles. The calculated force is limited to a maximum given by the product of the static friction coefficient by the normal force between the pebbles. It is further corrected by a factor that makes it more physical. The added factor assumes its maximum value of 1 when the slip component of the pebbles relative velocity is zero and allows a smooth decrease to zero when the maximum cutoff velocity is reached above which static friction is assumed not to occur. With this model, the pebbles are allowed to slide with respect to one another, but the sliding increases the slip, and thus the force counteracting the slip. This method is reasonable for small slips, but breaks down for large ones. A coding artifact (i.e., parameter) allows large slips to be zeroed or shortened to a specified size. However, the method remains valid in most cases, since the time steps used in the modeling and the relative velocity threshold of applicability are small. In order to save time, this method is used instead of the method based on the definition of static friction (i.e., the normal force times the static friction coefficient). The latter more correct approach would require time consuming calculations in order to determine the direction of the force and its magnitude. Such computations would use computer time faster than just proportional to the number of pebbles since they require solving for the friction for all the pebbles that are in static contact with each other. For 450,000 pebbles this is not computationally feasible. With the method used in this work, the static friction force, $\mathbf{F}_{sij}$, is given by

$$\mathbf{F}_{sij} = -\min\left(\mu_s \left|\mathbf{F}_{\|ij}\right| , h_s \left|\mathbf{s}_{ij}\right| \left[1 - \frac{\left|\mathbf{v}_{\perp ij}\right|}{v_{\max}}\right]\right) \hat{\mathbf{s}}_{ij} \quad , \quad \left|\mathbf{v}_{\perp ij}\right| < v_{\max}$$

where μ_s is the static friction coefficient, $\mathbf{F}_{\|ij}$ is the normal force, h_s is the coefficient for force from slip, $\mathbf{s}_{ij}$ is the slip distance perpendicular to the normal force between the two pebbles, $v_{\max}$ is the maximum velocity below which static friction is assumed to exist in this model, and $\hat{\mathbf{s}}$ is the unit direction vector of the slip. The bracketed factor allows the static friction to smoothly vanish as $\mathbf{v}_{\perp ij}$ approaches $v_{\max}$. The static friction given by the above equation is combined with the rest of the tangential force given above as $\mathbf{F}_{\perp ij}$ to give the total tangential force, $\mathbf{F}'_{\perp ij}$,

$$\mathbf{F}'_{\perp ij} = \mathbf{F}_{sij} + \mathbf{F}_{\perp ij} \quad .$$

Details on the computation of the slip magnitude will be given in a forthcoming Idaho National Laboratory (INL) external topical report.

The incorporation of a static friction model, albeit an approximate and simple one, into the model results in the capability of modeling such things as angles of repose and a sloping free surface. With sufficiently high static friction coefficients, the model inherently limits increases of the packing fraction (with gentle enough loading, packing fractions of 0.59 are possible), without analyst intervention. The primary disadvantages of the model that incorporates static friction are that the algorithm requires about twice as much time compared to the one without static friction and the algorithm requires more memory per pebble.

MODEL IMPLEMENTATION AND CODE FEATURES

The method described above has been implemented into the PEBBLES code written in FORTRAN95. The code is currently implemented and optimized to run on a single processor machine. However, it was also used on a cluster machine with, as expected, limited speedup (about a factor of 3-4 on 8 processors before overhead overwhelms any gains).

Restructuring the algorithm and mapping the code to a large number of processors is planned for the near future. Despite this, the algorithm used is not entirely naïve. In order to lower the computational burden of evaluating the forces between all pairs of pebbles, only neighboring pebbles are considered. This is done by tracking only neighbor interactions as in the Neighbor List (or Verlet List) approach [17] while limiting the tracking zone dimension through the use of Cell Lists [15]. This approach results in a number of evaluations that grows proportionally to the number of pebbles rather than proportionally to the square of that number. The implementation of this approach in the PEBBLES code is naturally limited to immediate neighbors, since no interaction occurs with non-neighboring pebbles. The cell list is also limited to the immediate neighbors as well. The approach is illustrated in Figure 2 and it proceeds by first partitioning the domain into cubic zones with one pebble long sides. Then, at the start of each time step the search for pebbles that interact with a given pebble is carried out only in the cells adjacent to the pebble's own cell.

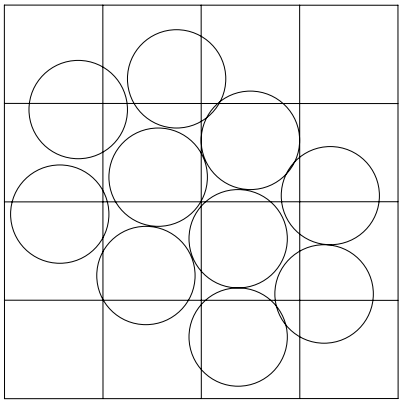


Figure 2. Example of Interaction Zones (Cells)

Since there are a bounded number of pebbles in each cell, and there are a bounded number of cells that a given pebble could interact with, the time spent processing interactions each time step increases linearly with the number of pebbles, which greatly speeds up the computation when large numbers of pebbles are being processed. The overall computation time is slightly higher than linear since an increase of the number of pebbles in the model results in a lower fraction of the computations being effectively treated within the cached portions of memory. In addition, an increase in the size of the problem results in fewer boundary cells being part of the computational model and therefore higher overall computational times (boundary cells involve fewer interactions as there are no pebbles on one of their sides).

The code allows the modeling of pebble recirculation by simulating the periodic (on-demand) removal of pebbles from the bottom of the reactor vat through one or more chutes while pebbles are added at the top of the vat. The initial time and subsequent frequency of chute openings are user supplied input parameters. Each time the chute is opened, the bottom most pebble is removed (and a pebble is added on top is recirculating is modeled). If the reactor model includes multiple chutes at the bottom, they will each in turn have a pebble removed from them.

The code allows the modeling of shaking of the vat according to a protocol (magnitude, duration, and shape of the shaking-induced walls and floor displacements) that is user specified. The shaking can be simulated by combinations of sine waves in any direction or using a user-specified table of displacements. The shaking feature can be used to model moderate shaking to allow enhanced packing in correction that correct for approximations made when running very large problems that would otherwise require excessively long computational times. More importantly, the feature can be used to model the effect of earthquakes on the packing and flow of the pebble bed.

The code can tally the velocity field on a rectangular or a cylindrical grid. The code can also tally the probability that a pebble changes from on grid location to another, as it moves down the vat. The total energy of the pebbles can be computed; however the potential energy from pebbles overlap is currently ignored.

Post-processing treatments include the computing, via deterministic methods, of the packing fraction distribution radially, axially, and both radially and axially. The packing fraction distribution can be calculated on an arbitrary grid using a stochastic method.

The code also produces a most important edit for application to neutronics, namely the pebble flow velocity field from which the flow paths of pebbles starting anywhere at the top of the reactor are determined. These last two applications are obtained from the velocity tallies that are generated and saved and are provided on a rectangular or a cylindrical grid at the user's option.

The sequence of operation for simulating pebbles recirculation was discussed above. For the initial vat filling the code offers two options. In the first (and oldest option), the simulation starts by determining initial locations and velocities for each of the pebbles. This information can be loaded from a file if one is available for the reactor under consideration. Alternately, the code can generate the needed initial loading. The simplest and quickest way to do so is to fill the reactor with an initial low density packing. A packing fraction of 0.15 can be generated by randomly filling the vessel with pebbles and displacing any overlapping ones. The angular and linear velocities are initialized to zero. Then, gravity is allowed to pack the pebbles. This method tends to generate low packing fractions compared to the second method. It also generates an initial pebble distribution with a level top surface. The second, and more realistic method, fills a chute above the reactor and then pours the pebbles into the reactor. This method generates a cone on the surface of the bed and results in higher packing fractions.

TEST MODELS DESCRIPTION

The PEBBLES code was tested using models of the HTR-10 [18] and the PBMR-400 [7] reactors.

The HTR-10 core region is a cylinder without an inner reflector. The radius of the core is 0.9m (inner radius of the radial reflector). The reactor contains 16,890 pebbles. The core height is about 2.171m from the top of the exit chute to the top of the fuel cone that forms at the top of the core as a consequence of refueling. For most analyses the results are presented for averages over the axially uniform portion of the core (i.e., for a portion of the core below the top fuel cone and above the vessel conus at the bottom of the reactor). This is done in particular for reporting the average packing density. However, it must be born in mind that all the details of the core height of this reactor are modeled. The choice of a zone of height approximately 60 cm in cylindrical portion of the core for reporting average packing avoids artifacts that may introduced by the bottom conus and by the significantly more random structure of the packing near the top cone.

The PBMR-400 reactor model assumes there are 451,197 pebbles in a cylindrical annular reactor core zone between two reflectors. The fuel zone is located between two radii at 1.0m and 1.85m. The model assumes 3 loading chutes and 3 exit chutes.

RESULTS: PHENOMENA PREDICTION AND CONFIRMATION

The PEBBLES code was used to model a variety of situations and to uncover or verify the occurrence of a number of phenomena that are known or suspected to occur in bed of granular media subject to recirculation or shaking. The various types of phenomena and the corresponding results are presented in turn.

Average packing density

Preliminary modeling of the average packing density for the PBMR-400 reactor has been carried out using an approximate method and without accounting for the effects of recirculation. The approximation stems from the approach used for simulating the loading of the reactor. In order to save computational time, it was assumed that the reactor is loaded with 90% of its fuel pebbles content using the initial low pack filling method described above, then the remaining 10% using the chute filling method, also described above. Since no shaking is imposed, the model is expected to produce unrealistically low packing fractions for the first 90% of pebbles loaded, whereas the remaining ones should correspond to more reasonable packing. There could therefore result a discontinuity of the packing fraction at the transition from the first 90% to the other 10%. This can be seen in Figure 3.

The expected discontinuity can be observed as a small increase in packing density at the 10 m location. The figure shows the radially average packing distribution versus the axial position. The averaging is carried out using for radial extent the maximum radial extent of the vat (i.e., the largest cylindrical radius of the vat) even in the discharge conus region and at the top of the core where the charge cone is present. This results in the tapering in the apparent density shown in the figure between 2 m down to 0 m and at the top of the reactor.

Pebble flow field determination

The PEBBLES code can be used for determining resting locations of pebbles as well as for simulating various motion effects (earthquake as mentioned above and flow as discussed here). The program can calculate a variety of parameters related to flow. The simplest is the path that each pebble takes through the reactor.

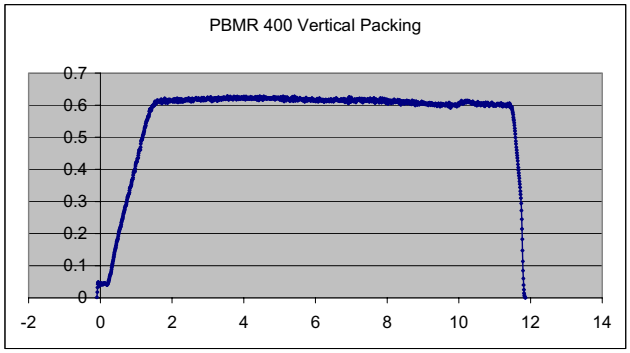


Figure 3. Approximate Radially Averaged Axial Packing Fraction in PBMR-400

Figures 4 and 5 show two perspective views of the paths four pebbles take as they are circulated through a reactor. The simulation results shown are for a 1000 pebbles vat over the course of time through which each pebble is recycled on average once.

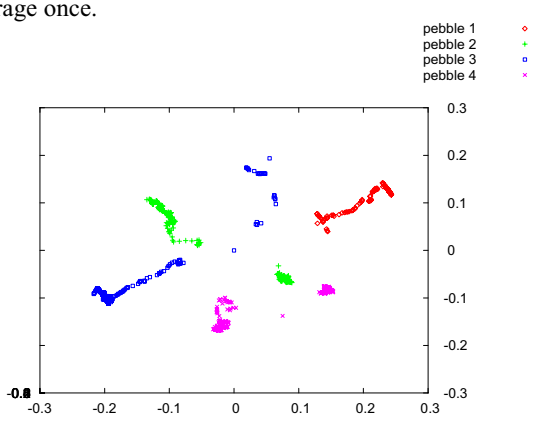


Figure 4. Pebble paths from top view of vessel.

The gate at the bottom of the chute was opened every quarter second to release one pebble that was then recycled to the top of the container. The chute is 6 pebble diameters wide and the entire vessel is 10 pebble diameters wide.

Figure 6 shows the velocity field of the pebbles in the model reactor vat. The flow field is also tabulated or

parameterized for use in a neutronics and burnup code such as PEBBED.

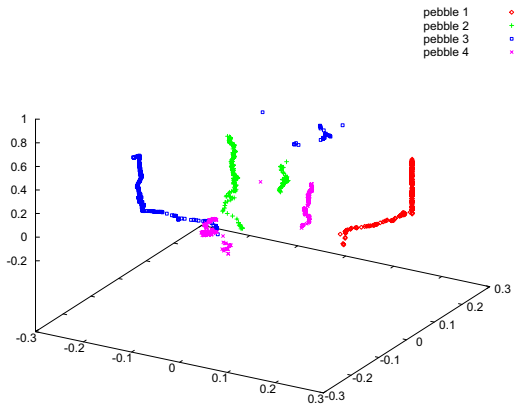


Figure 5. Pebble paths from side view of vessel.

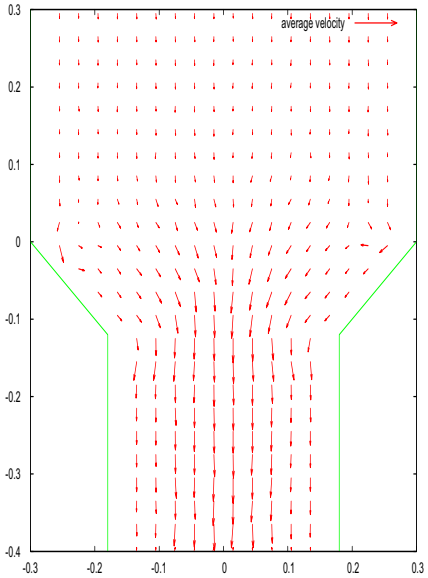


Figure 6. Flow field representation (arrow lengths are proportional to local average pebbles velocity)

Packing density spatial variation

Some of the obvious applications of the PEBBLES code are the determination of pebble locations within the pebble bed, the evaluation of the packing fraction of the pebble bed (i.e., the relative density of the bed), the determination of the packing spatial fluctuations, and the determination of pebbles flow patterns. The latter was discussed above. In this section the packing and it fluctuations are discussed. The packing patternss were modeled for various reactors, including the the HTR-10 and the PBMR-400.

A sample result of modeling the initial packing in a pebble bed using the PEBBLES code is shown in Figure 7. The figure shows that the packing is for the most part random, as no regular geometric features could be discerned.

In Figure 8 the output from PEBBLES is compared to experimental data obtained by Benenati and Brasilow [19]. The code was run multiple times with different initial conditions with data corresponding to lead spheres to conform to the conditions of the experiment.

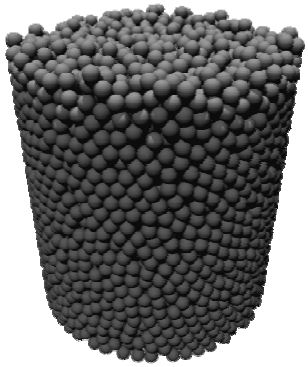


Figure 7. Sample pebble bed packing from PEBBLES code

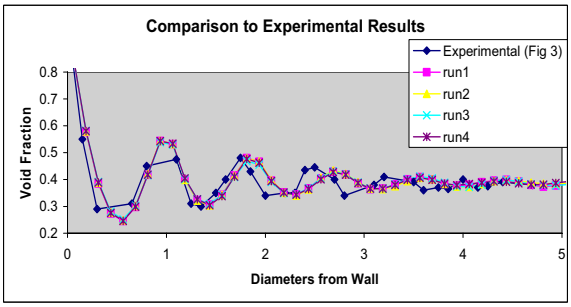


Figure 8. Wall effect density oscillations.

The model reproduces accurately the wall-effect oscillatory behavior and the average packing density. It must be noted that the packing density that is achieved depends on the friction factors and other physical characteristics of the material being simulated. It is possible that for materials with lower static friction coefficients, higher packing fractions may result. Therefore, accurate data for the parameters applicable to graphite coated pebbles are important to obtain and qualify.

Figure 9 shows the wall-effect spatial density fluctuations in the radial direction for the PBMR-400 reactor between about 4 meters and 8 meters above the bottom of the discharge chutes. The figure presents an axial average between those two heights.

Experience with modeling the bed density has put in evidence the dependence of the bed packing density on some physical parameters. For example, it was shown that larger values of the kinetic and static friction factors result in lower bed density predictions. It was also shown that larger dashpot force values also result in lower packing densities.

Modeling artifacts can also affect the final resting packing density: for example, a low initial packing (i.e.,

higher initial potential energy) results in higher final packing density. Because of this, care must be taken to ensure that the simulations actually reflect the correct initial state of the physical system.

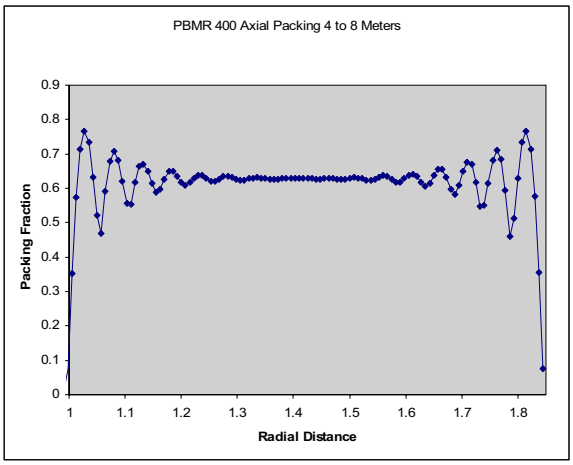


Figure 9. Wall-effect density fluctuation in the PBMR-400.

The wall-effect packing density fluctuations were demonstrated to have little if any neutronic impact [20]. However, they may be important for the thermal-hydraulic behavior of the bed [5].

Arching

An interesting feature of the PEBBLES code is that it reproduces experimentally observed phenomena without analyst intervention. For example, in the course of modeling the flow of pebbles through a reactor core and out the bottom chute, the code predicted the formation of arches of pebbles. That is, pebbles formed bridges above the chute and interrupted the flow down the chute. The "problem" was resolved by gradually increasing the diameter of the chute until the arching no longer occurred. The chute diameter to pebble diameter ratio at which this occurs in the model is essentially the same as the one observed in real experiments [21].

A systematic search for the non-bridge-forming chute diameter was carried out. For this purpose a model containing 2000 pebbles was devised. The pebbles were recirculated repeatedly. After 3991 pebbles have passed down the chute or when bridging occurs, whichever comes first, the simulation was stopped. For each chute diameter, the simulation carried out twice, each time with different starting conditions. The chute tube diameter was varied from 1 pebble diameter to 7 pebble diameters in ½ pebble diameter increments. The bounding cases are given by the largest friction factors that can apply to the real reactor. In order to make the simulations reflect the physics of the PBMR-400, a static friction factor of 0.65 and a kinetic friction factor of 0.4 were used. These were used for both pebble-to-pebble and wall-to-pebble friction. These data correspond to the properties of hot "graph-i-tite" graphite [22] in a helium atmosphere and at a temperature of 2450ºC, which is substantially higher than that of the PBMR In a second set of simulations the static and kinetic factors were taken as 0.35 and 0.25, respectively. These data correspond to cold (20ºC) graphite in an air atmosphere [22]. It was observed from the model results that for chute openings with diameters larger that are 5 pebble diameters bridging does not occur in the large friction cases, whereas in the low friction cases bridging does not occur for openings 4.5 pebble diameters and larger. This result appears to be practically insensitive to discharge conus slope. In practical applications, for conservatism, the discharge opening is designed with a larger diameter than the theoretical one found in these simulations, notwithstanding the conservatism in the model parameter used. Indeed, the values used for both the static and kinetic friction factors (in the high friction case) are substantially larger than those expected to prevail under the conditions of an operating PBMR-400 reactor. In such a reactor [21] the static friction factor would takes values between slightly less than 0.3 (at 1000ºC) and slightly under 0.64 (at 400ºC), whereas the kinetic friction factor would take values between slightly under 0.2 (at 1000ºC) and about 0.4 (at 600ºC). With larger friction factors, the propensity for bridging (or arching) is greater, so the chute dimensions that preclude arching with these data would a-fortiori preclude it for lower, more realistic, friction factors. The actual designs of pebble bed reactors use a slightly higher ratio than the computationally determined one. An experimentally determined chute-diameter-to-pebble-diameter ratio of 50/6 seems to have been adequate to reliably prevent arching in the AVR reactor [2].

Preliminary modeling of angle of repose

When a large number of pebbles is loaded gradually into a vat, they form a pile similar to that obtained when pouring sand on a table. The pile is wide at its base and narrow, seemingly to a "point," at the top. However, unless made of an extremely large number, the pile of pebbles would appear to be macroscopically less smooth than the pile of sand. The shape, nonetheless, stems from similar physical principles. The conical or nearly conical shape is the result of the various forces that are applied to the pebbles. The angle defined by the surface of the cone surface and the horizontal plane is termed the *embankment angle*. In a real pile, the periphery of the cone base is not shaped exactly as a circle and the embankment angle is not constant around the periphery. When the pile is being formed, a pebble added *softly* at the very top may remain there. Pebbles added carrying substantial kinetic energy have little chance of remaining at the top. Also, when pebbles are added, the cone that forms gradually increases in steepness until the slope of the pile surface reaches a critical value. At that critical point a minavalanche takes place and the pebbles flow down the slope to a position of equilibrium. At the critical slope, the angle between the pile surface and the horizontal plane is termed the *angle of movement*. The angle to which the pebble pile relaxes to is termed the *angle of repose*. It is obvious that the angle between the surface of the pile and the

horizontal plane any time lies between these two extreme values. A more detailed discussion of the phenomena just mentioned can be found in the book by Duran [23]. During a numerical simulation of the loading of a pebble bed (as during the actual loading of the bed), the embankment angles around the cone at the top of the pile, in any direction around the pile, may undergo the increase and decrease mechanisms described above. It follows that the actual embankment angle would always remain undetermined to the extent defined by angle of movement and the angle of repose. Another consequence is that in a simulation it is not ordinarily possible to define a unique angle for the entire cone. Theoretically an average angle or an angle distribution could be defined. In this preliminary work, the range of angles observed in the simulation is reported for one example related to the HTR-10 reactor. An illustration of the formation of an embankment angle (sometimes also termed angle of repose by abuse of language) is shown in Figure 10.

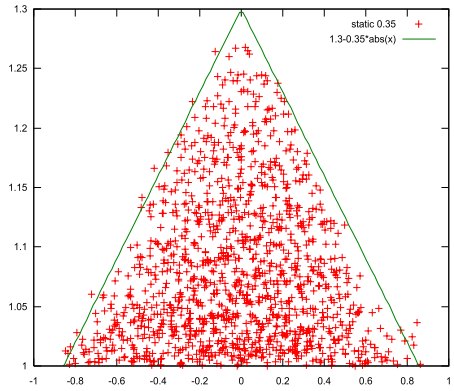


Figure 10: 2-D projection of pebble cone on HTR-10 (crosses represent centers of pebbles)

The PEBBLES code was used to model the pouring of individual pebbles (using the chute method) in the final stages of the filling of a vat with dimensions and shape those of the HTR-10 reactor. The initial stages of the filling process (which do not affect the presence, absence, or shape of the cone) were modeled as an initial dump of 14,000 pebbles into the vat. The positions of the individual pebbles are tallied after the total kinetic energy of the pebbles drops below a pre-set threshold. As the final stages of filling were modeled, a cone was indeed observed to form in the model results. The case presented here used a static friction factor of 0.35 for the pebbles. This is the friction factor of cold (20ºC) graphite pebbles in air [22], which corresponds to the conditions of the HTR-10 initial loading.

In the figure the red crosses represent centers of pebbles. The green line has a slope of 0.35 (i.e., makes an angle of 19° 17" from horizontal). This value is exactly the theoretical expected value for the angle of repose, α_r, as this angle and the friction factor, μ, are related by

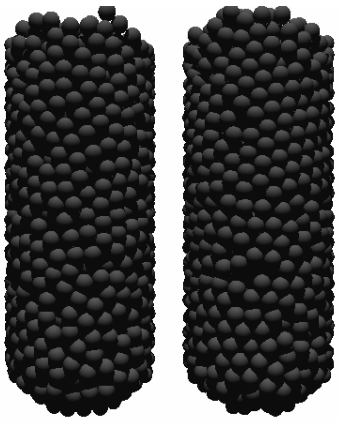
$$\mu = \tan(\alpha_r) \ .$$

The results presented above define limiting behavior of the pebble bed in a deterministic sense. In reality, although the methods used in this work are deterministic, the modeling of a very large number of pebbles that interact then fall in place may result in different configurations for each instance that the process is repeated. That is, the model behaves like a stochastic one in the same sense as an analog Monte Carlo model. Therefore, it should be expected that the results produced by running the PEBBLES code should be regarded as individual instances of a stochastic system, and the results (i.e., embankment angles and the angles of repose) as members of an ensemble. The spread in the embankment angle discussed above and the fact that the number of pebbles that constitute the cone is small further compounds this randomness. This "randomness" effect is observed in the numerical simulation where it is seen that the angle of embankment at various azimuthal positions around the cone base perimeter varies between 17° and 22°. The angle of repose is also affected by the kinetic energy of falling pebbles, as discussed above. For a drop from high chutes, the cone could either not form at all or form but remain shallower than the theoretical slope.

Results for angle of repose from the PEBBLES code have been used in the analysis of the HTR-10 first criticality [24]. Future work should consider the sensitivity of the effective multiplication factor to the embankment angle and to variations between the angle of movement and angle of repose in avalanches.

Circulation-induced short range ordering

The initial loading of the pebble bed vat appears to result in random packing as seen in Figure 7, above. Subsequently, as the pebbles are recirculated, some local order is observed to form, particularly near the vat walls. This is shown qualitatively in Figure 11.



Before After

Figure 11. Disorder before and local order after recirculation

A careful observation of the pictures before and after recirculation show that the total disorder that prevails before recirculation is simulated is no longer as prevalent after. Indeed, whereas the "before" picture shows a totally

disordered pebbles distribution, the "after" picture shows a crystalline-like structure over several areas of the bed lateral surface where the pebbles touch the vat wall. A similar behavior was observed experimentally [2].

Densification in earthquake

The PEBBLES code was used to model the effect of an earthquake on the pebble bed density. The results of that study are presented in a companion paper to be presented elsewhere.

Sensitivity of models to parameters

The sensitivity of models to various parameters has been systematically investigated with the PEBBLES code. As already mentioned above, it was shown that larger values of the kinetic and static friction factors result in lower bed density predictions. For example, a model using 0.1 for its static friction factor and 0.05 for kinetic friction factor gave packing fractions of 0.633 and 0.635. A lighter packing fraction of 0.61 was reached by the same model for 0.7 kinetic friction and 0.9 static friction. However, there is a wide range of both kinetic and static friction values for which little difference arises in the packing fraction. It was also shown that larger dashpot force values also result in lower packing densities. Another parameter that affects the packing fraction of the pebble bed is the Hooke's law constant between pebbles. Qualitatively, though somewhat counter-intuitively, it is obvious that a larger constant will result in a higher packing density if one considers that a larger constant will imply more bounce in pebble collisions and hence more motion and a better chance for pebbles to keep moving until a lower potential energy position (i.e., denser configuration) is reached. For the same example problem discussed above, using a kinetic friction factor of 0.40 and a static one of 0.65, for a Hooke's law constant of 1,000 kg/s^2 an average packing fraction of 0.611 is achieved. For a Hooke's law constant half that value, i.e. 500 kg/s^2, the packing fraction is 0.598.

Finally, as previously stated, modeling artifacts (such as height of pebble fall onto the bed) can also affect the final rest packing density and therefore modeling artifacts should be made to reflect the actual physical features of the actual system with high fidelity in order for the model predictions to be reliable.

DISCUSSION AND CONCLUSION

A method for modeling pebbles packing and flow in a pebble bed reactor has been developed and implemented into the PEBBLES code. The adopted approach is akin to the discrete element method. The code has been provided with the means to model behaviors and produce results that are relevant to the analysis of pebble bed reactors. Among the applications that have already been made possible by the new code is the computation of pebble locations in a pebble bed. The code was tested on several sample problems that are representative of the HTR-10 and PBMR-400 reactors. It was shown that the code reproduces experimentally demonstrated behaviors of a pebble bed. These behaviors include the wall-effect density oscillations, the short range ordering of the bed upon recirculation, the formation of a cone at the top of the pebble bed, and the bridging of pebbles at unloading chutes and an identification of chute diameters that prevent the bridging.

The new code has been used in reactor physics related applications presented elsewhere and those applications were referenced. Those applications included the modeling of pebbles locations within a pebble bed in support of the computation of spatially-dependent Dancoff factors, the estimation of the loading cone shape in the HTR-10 in support of a benchmarking project, and the prediction of pebble bed densification during the course of earthquakes. This latter application is presented in a companion paper to be presented elsewhere. The application of the results to the transient that results from such densification is currently being carried out.

On-going work either on the PEBBLES code or using the code include modifications (primarily code parallelization) to speedup its performance and replacement of the static friction model a by a physically fully justified formulation.

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