Granular flow in pebble-bed nuclear reactors: Scaling, Dust Generation, and Stress

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Abstract

In experimental prototypes of pebble-bed reactors, significant quantities of graphite dust have been observed due to rubbing between pebbles as they flow through the core. At the typical operating conditions in these reactors, which feature high temperatures, pressures, and a helium atmosphere, limited data is available on the frictional properties of the pebble surfaces, and as a result, a conceptual design of a scaled-down version of a pebble-bed reactor has been proposed to investigate this issue in detail. However, this raises general questions about how the granular flow in a scaled facility will emulate that in a full-size reactor. To address this, simulations of granular flow in pebble-bed reactors using the discrete-element method (DEM) have been carried out in a full-size geometry (using 440,000 pebbles) and compared to those in geometries scaled down by factors of 3:1 and 6:1. Differences in velocity profiles, pebble ordering, pebble wear, and stresses are examined, and the effect of friction is discussed. The results show complex behavior due to discrete pebble packing effects, although several simple scaling rules can be derived.

Keywords: granular flow, dust generation, numerical methods

1. Introduction

Pebble-bed nuclear reactors are a type of gas-cooled high temperature reactor (HTR) that are currently under study as part of the Generation IV initiative, and offer many potential advantages over current reactor technology, such as passive safety, continuous refueling, and proliferation resistance. However, early prototypes have identified a number of potential safety concerns, such as the generation of large amounts of graphite dust as the pebbles flow past each other and against the moderator. During the reactor operation, the dust may become activated, and may accumulate both in the reactor core and the heat exchange system. The characteristics and amount of the generated dust are not well-known, nor is its potential for release during a fast flow velocity increase.

Currently the most extensive data on dust generation is available from the German prototype Arbeitsgemeinschaft Versuchreaktor (AVR) (Gottaut and Krüger, 1990; Kissane, 2009). During
the reactor’s twenty-year operation span, it is estimated that 50 kg to 60 kg of dust was generated, and the median diameter of the dust particles was 1 µm. The concentration of the dust circulating the reactor was only a very small fraction ($10^{-7}$) of the total. It is expected that oil and air ingress incidents during the early operation may be responsible for the significant portion of the dust. Furthermore, several different types of fuels were employed over the reactor’s lifetime, with the earlier fuel designs being less durable than those used later. The relevance of this data to modern reactor designs and graphites is therefore limited.

Recently, a number of research groups have carried out studies that are relevant to the dust generation problem. One significant issue is that the frictional and wearing properties of graphite are not well-known at the typical helium atmosphere, temperatures, and pressures within the reactor, and several experimental studies have aimed to properly characterize these (Brendlé and Stempfle, 2003; Sheng et al., 2003; Luo et al., 2005). Two recent survey articles on frictional properties (Luo et al., 2010) and wear (Cogliati et al., 2011) summarize the available values in the literature. Building on this work, a finite-element analysis of individual pebble interactions has been constructed to more accurately characterize the dust produced during a pebble–pebble contact (Rostamian et al., 2012). In other work, computational fluid dynamics (CFD) simulations of gas flow around pebble assemblies have been conducted (Lee et al., 2007; Hassan, 2008; Wu et al., 2010), which may have important consequences for dust transport. Another recent study has examined the consequences of dust generation for the reactor system as a whole (Stempniewicz et al., 2012).

To complement this work a conceptual design of an experimental facility has been proposed (Lind et al., 2010) that would enable the generation of dust to be studied in a holistic manner. The facility would consist of a core simulator coupled to a heat exchanger. In tandem with analytical work, the project would characterize the aerodynamics of the core and heat exchanger, investigate the amount of dust generated and the locations most prone for deposition, and examine both normal operating conditions as well as fast depressurization events. Due to cost constraints, the experimental facility would be a scaled-down version of a full-size reactor. A suitable full-size reference design is the pebble-bed modular reactor (PBMR) (Kadak, 2007), which features a cylindrical reactor vessel of height 10 m and diameter 3.5 m, with approximately 440,000 pebbles of diameter 6 cm. Several designs in which the geometry is scaled down, but the pebble size is kept the same, have been considered, significantly reducing the number of pebbles required.

However, despite a large amount of study, there is still no complete theoretical description for how dense granular materials will flow, and hence no simple way to understand how pebble flow in a scaled facility will relate to that in the full-size geometry, or how this will affect pebble wear and dust generation. Granular flows have been of great interest in a number of different fields such as engineering (Levy and Kalman, 2001) and geology (Hutter et al., 1994; Hutter, 2005), and in the past two decades have attracted renewed interest from physicists (Jaeger et al., 1996; Kadanoff, 1999), particularly due to their relation to the glass transition (Liu and Nagel, 1998; Keys et al., 2007). Their rheology is complex, allowing for a solid-like behavior and the ability to support stress, but also exhibiting a transition to liquid-like flow (Aranson and Tsimring, 2001; Rycroft et al., 2009a). Granular materials exhibit many complexities at the level of a single particle, with forces being inhomogeneous (Mueth et al., 1998; Blair et al., 2001) and concentrated along extended force chains (Utter and Behringer, 2004; Majmudar and Behringer, 2005) making it difficult to define a
continuum theory. In the slow, dense, quasi-static limit that is appropriate for modeling the pebble bed, the packing geometry of the pebbles themselves strongly influences the flow, since in order to move, pebbles must have enough space available to rearrange with their neighbors (Rycroft et al., 2006a).

In the absence of a theoretical description, the available data on granular flow in pebble-bed reactors consists of experimental studies in scaled-down geometries (Bedenig et al., 1968; Kadak and Bazant, 2004) or simulations carried out using the discrete-element method (DEM) whereby the position, velocity, and angular velocity of each pebble are individually tracked and updated according to Newton’s Laws, using a frictional contact model to evaluate the forces that each pebble experiences. Due to the stiff contact equations required to simulate hard particles, DEM simulations are computationally intensive but are feasible on a parallel computer; they have been employed to analyze granular flows in many situations such as on inclined planes (Silbert et al., 2001) and static granular packings (Landry et al., 2003), and have been shown to be in good quantitative agreement with laboratory granular flows (Rycroft et al., 2009b). In relation to pebble-bed reactors, several DEM studies have examined the structure of static packed beds (Ougouag et al., 2005; du Toit, 2008), whereas others have analyzed flowing packings using both commercial software (Venter and Mitchell, 2007; Moormann, 2008) as well as in-house codes (Cogliati and Ougouag, 2006) that offer more flexibility to examine issues relevant to reactor design, including dust production (Cogliati and Ougouag, 2008). Full-size reactor simulations (Rycroft et al., 2006b) have been carried out and also compared to experiment (Jiang et al., 2012). The simulations can be used to analyze bulk flow features such as velocity profiles, but are also useful in determining pebble-based statistics such as pebble residence times and pebble diffusion, which may be useful in determining the propensity for rare events, that could affect individual pebble peaking factors (Sobes et al., 2011).

In the current study, we aim to understand how flows in a scaled reactor will relate to the full-size geometry, and in particular investigate how pebble wear will differ. While the results are of direct relevance to the design of the proposed experimental facility, they also highlight the more general challenges in scaling of dense granular flows. We identify several areas where scaling presents some significant challenges, but also derive some general rules about how various quantities of interest will behave as a function of scale. Given the ambiguities in the frictional properties, we also systematically examine the role of friction. We place a particular emphasis on simulations with a Coulomb friction of $\mu = 0.35$. This value is consistent with the ranges reported by Luo et al. (2010) and we expect it to be a reasonable match to the conditions within the proposed facility. In a recent conference paper (Rycroft et al., 2012), we have also presented a variety of results for $\mu = 0.5$ for comparison.

2. Methods

2.1. Pebble contact model

The DEM simulations are carried out using the Large Atomic/Molecular Massively Parallel Simulator (LAMMPS) developed at Sandia National Laboratories (Plimpton, 1995; LAMMPS website). The code is widely used and provides a framework for carrying out particle simulations interacting under a diverse variety of forces. For a given simulation domain, the code decomposes the domain into a rectangular grid of regions, assigning each to a separate CPU thread. Each
which is small enough to be neglected. The model also makes use of a Coulomb friction coefficient $k$ values of correctly capturing the granular dynamics without creating prohibitively large elastic oscillations.

Physically realistic value, and the value of 2 typical hard materials like glass, where a value of $10^9 mg/d$ would be appropriate. However, since the simulation timestep must scale according to $k_n^{1/2}$, it is not computationally feasible to use a physically realistic value, and the value of $2 \times 10^5 mg/d$ was found to be a reasonable compromise, correctly capturing the granular dynamics without creating prohibitively large elastic oscillations.

The spherical pebbles interact according to a spring–dashpot contact model. If a pebble and its neighbor are separated by $r$, and they are in compression, so that $\delta = d - |r| > 0$, then they experience a force $F = F_n + F_t$, where the normal and tangential components are given by

\[
F_n = f(\delta/d) \left(-k_n \delta n - \frac{\gamma_n \nu_n}{2}\right) \tag{1}
\]

\[
F_t = f(\delta/d) \left(-k_t s_t - \frac{\gamma_t \nu_t}{2}\right). \tag{2}
\]

Here, $n = r/|r|$ is a normal vector at the point of contact between the pebbles. $k_{n,t}$ and $\gamma_{n,t}$ are the elastic and viscoelastic constants respectively, and $\nu_{n,t}$ and the normal and tangential components of the relative surface velocity. The function $f$ can be modified to consider different force models; here, Hookean contacts employing $f(\xi) = 1$ are primarily used, but an alternative model approximating Hertzian contacts using $f(\xi) = \sqrt{\xi}$ is also discussed. $s_t$ is the elastic tangential displacement between spheres, obtained by integrating tangential relative velocities during elastic deformation for the lifetime of the contact. It should be noted that this adds a significant computational complexity to the simulation, since it requires tracking the history of every pair of pebbles that are in contact. The model also makes use of a Coulomb friction coefficient $\mu$, so that if $|F_t| > \mu |F_n|$ and a local Coulomb yield criterion is exceeded, then $F_t$ is rescaled so that it has magnitude $\mu |F_n|$ and $s_t$ is modified to that Eq. 2 is upheld—this issue is discussed in more detail in Sec. 4 on pebble wear.

Appropriate values of the contact model parameters have been considered in a number of previous studies. The initial calibration was carried out by Silbert et al. (2001), who found that values of $k_n = 2 \times 10^5 mg/d$ and $\gamma_n = 50 \tau^{-1}$ were appropriate for simulations of granular flows on inclined planes with 20,000 spheres of height 40d. This value of $k_n$ is significantly softer than for typical hard materials like glass, where a value of $10^9 mg/d$ would be appropriate. However, since the simulation timestep must scale according to $k_n^{1/2}$, it is not computationally feasible to use a physically realistic value, and the value of $2 \times 10^5 mg/d$ was found to be a reasonable compromise, correctly capturing the granular dynamics without creating prohibitively large elastic oscillations.
Simulation parameter                                | Typical value                          
---                                             | ---                                    
Normal elastic constant \( k_n \)              | \( 2 \times 10^6 \text{mg/d} \)         
Tangential elastic constant \( k_t \)          | \( \frac{2}{7} k_n \)                   
Normal viscoelastic constant \( \gamma_n \)     | \( 50\sqrt{10} \tau^{-1} \)            
Tangential viscoelastic constant \( \gamma_t \) | \( 25\sqrt{10} \tau^{-1} \)            
Friction coefficient \( \mu \)                 | 0.2, 0.35, 0.5, 0.65, 0.8               
Timestep                                       | \( 2.5 \times 10^{-5} \tau \)          

Table 1: Typical values of the pebble contact model parameters used for the simulations in the paper.

Silbert et al. (2001) make use of a ratio \( k_t / k_n = 2/7 \) for numerical convenience, since it makes the period of the normal and shear oscillations identical under the Hookean model. Although a value of \( k_t / k_n \) of approximately \( 2/3 \) would be more realistic based on the Poisson ratio of typical materials, changing the value of \( k_t / k_n \) did not have a strong effect on the particle dynamics.

In the previous full-size simulations of pebble-bed reactors (Rycroft et al., 2006b), the above values were adopted, and were sufficient to carry out a variety of analyses. However, subsequent work has shown that the above parameters can lead to spurious vertical oscillations in velocity that grow in significance at higher points in a drainage simulation (Rycroft et al., 2009b), which are not present in corresponding laboratory experiments. These oscillations occur rapidly, and it was found that they only had a weak effect on macroscopic flow features such as velocity profiles. However, beyond a height of around \( 60d \), they had a significant effect on microscopic quantities that were measured, such as autocorrelations in pebble velocity. Since one of the main aims of the current study is to investigate the microscopic quantity of wear, a value of \( k_n \) of ten times larger than previous work was considered, which was shown to mitigate the vertical oscillations. To accommodate this, the timestep was decreased by a factor of four, which remains feasible given progresses in computer technology.

In this study, it was chosen to focus on the Hookean contact model. While the Hertzian model provides a more realistic description of the contact force between two spheres, the additional factor in Eqs. 1 and 2 means that the effective spring constant is significantly lower for the small particle overlaps that are typical for slow, dense flows, and this can lead to particularly large spurious vertical oscillations (Rycroft et al., 2009b). We therefore decided to adopt the Hookean model, since it is widely used, and we considered that the additional realism of the Hertzian model did not outweigh the potential for numerical complications. Table 1 summarizes the typical parameters used throughout this study. For the typical pebble mass and diameter considered, the normal spring constant is \( k_n = 5.9 \times 10^7 \text{N/m} \) in physical units. The values of the viscoelastic constants are scaled up by a factor of \( \sqrt{10} \) for consistency, to preserve the same coefficient of restitution for two pebbles colliding in free space.

2.2. Geometry and initial packing generation

The reactor geometries are specified in a cylindrical \((r, \theta, z)\) coordinate system with gravity pointing in the negative \( z \) direction. The reactor is composed of several wall objects that are added to the simulation, with pebble–wall interactions being handled with the same contact model as pebble–pebble interactions. In the reactor, the moderator is a different type of graphite than the
pebble surfaces, and it could be expected that a pebble–wall friction coefficient could differ from the pebble–pebble friction coefficient. Simulations by Rycroft et al. (2006b) have shown that changing the pebble–wall friction parameter by itself can have significant effects on bulk flow properties. However, in the absence of friction coefficient data for the materials at the reactor conditions, the pebble–wall friction coefficient was chosen to match the pebble–pebble friction coefficient for all simulations.

To carry out the scaling study, four different reactor geometries have been considered, and the parameters describing these are given in Tab. 2. Firstly, full-size simulations with 440,000 pebbles, matching the same geometry as previous studies (Rycroft et al., 2006b) and based on the MIT modular pebble-bed reactor design (Kadak, 2007) have been carried out. A 3:1 scaled geometry using 16,500 pebbles, and a 6:1 scaled geometry with 2,050 pebbles have been considered. Finally, a tall geometry with 13,900 pebbles has been considered, in which the reactor radius is scaled by 6 but the height is left the same—which is referred to as “tall 6:1” in this study. While this geometry has a different aspect ratio to the original design, it was of particular interest for its ability to simulate a depressurization event, and replicate the important aerodynamic parameters for dust removal by gas flow. For each of the four geometries, the reactor is composed of a cylindrical exit pipe of radius \( r_p \) that extends downward from \( z = z_p \). The top of the exit pipe is joined to a funnel with a slope of 30° with the horizontal, which then meets a cylinder of radius \( r_r \) that forms the main reactor vessel.

In constructing the scaled geometries, the fundamental quantity that is scaled is the reactor radius \( r_r \). The full-size value of 29\( d \) is based on a radius of 1.75 m from the MIT design, and the values of 10\( d \), 5\( d \), and 5\( d \) for the other geometries follow the scaling ratios, although rounded to the nearest whole \( d \) for numerical convenience. The other parameters follow the scaling ratios as closely as possible, although in certain cases some immediate challenges are faced. For the full-size geometry, an exit pipe of radius \( r_p = 5d \) is used. However, it is well-known that granular flows have a tendency to jam when the outflow pipe radius is less than 2.5\( d \) (Zuriguel et al., 2003), and thus the natural values of \( r_p \) in the scaled geometries would be too small. They were therefore chosen to be

<table>
<thead>
<tr>
<th>Simulation parameter</th>
<th>Full-size</th>
<th>3:1 scaled</th>
<th>6:1 scaled</th>
<th>Tall 6:1 scaled</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of pebbles</td>
<td>440,000</td>
<td>16,500</td>
<td>2,050</td>
<td>13,900</td>
</tr>
<tr>
<td>Exit pipe radius ( r_p )</td>
<td>5( d )</td>
<td>3.5( d )</td>
<td>2.5( d )</td>
<td>2.5( d )</td>
</tr>
<tr>
<td>Exit pipe height ( z_p )</td>
<td>10( d )</td>
<td>3( d )</td>
<td>2.5( d )</td>
<td>2.5( d )</td>
</tr>
<tr>
<td>Reactor radius ( r_r )</td>
<td>29( d )</td>
<td>10( d )</td>
<td>5( d )</td>
<td>5( d )</td>
</tr>
<tr>
<td>Pebble insertion height ( z_i )</td>
<td>180( d )</td>
<td>60( d )</td>
<td>30( d )</td>
<td>180( d )</td>
</tr>
<tr>
<td>Wear cutoff height ( z_w )</td>
<td>135( d )</td>
<td>45( d )</td>
<td>22.5( d )</td>
<td>135( d )</td>
</tr>
<tr>
<td>Pebble insertion rate ( R_i )</td>
<td>774( \tau^{-1} )</td>
<td>86.6( \tau^{-1} )</td>
<td>19.0( \tau^{-1} )</td>
<td>19.0( \tau^{-1} )</td>
</tr>
<tr>
<td>Pebble pouring time ( t_P )</td>
<td>750( \tau )</td>
<td>1000( \tau )</td>
<td>250( \tau )</td>
<td>1000( \tau )</td>
</tr>
<tr>
<td>Drainage time ( t_D )</td>
<td>2750( \tau )</td>
<td>4000( \tau )</td>
<td>4750( \tau )</td>
<td>4000( \tau )</td>
</tr>
<tr>
<td>Drainage snapshot interval ( t_s )</td>
<td>5( \tau )</td>
<td>2( \tau )</td>
<td>0.5( \tau )</td>
<td>( \tau )</td>
</tr>
<tr>
<td>Typical CPU threads</td>
<td>256</td>
<td>4</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>Computation time</td>
<td>130.6 s/( \tau )</td>
<td>130.3 s/( \tau )</td>
<td>16.9 s/( \tau )</td>
<td>85.3 s/( \tau )</td>
</tr>
</tbody>
</table>

Table 2: Parameters describing the geometry, insertion process, and computation time for the four families of simulations.
3.5d and 2.5d for the scaled runs to avoid this problem. Furthermore, granular materials tend to have lower packing densities near walls due to additional pebble ordering, and thus the number of pebbles in the 6:1 is slightly smaller than what would be expected based on volume scaling alone.

For each of the geometries, initial pebble packings are created by plugging the exit pipe with a horizontal wall at \( z = z_p \), and then randomly raining pebbles in from a fixed height of \( z_i \) at a given rate \( R_i \); details of this process can be found in previous work (Landry et al., 2003). For each of the four geometries, five initial pebble packings are created using the friction coefficients listed in Tab. 1. Friction has a relatively weak effect on the generated packings, with packing densities in the full-size geometry varying from 63.8\% for \( \mu = 0.2 \) to 63.2\% for \( \mu = 0.8 \). Each simulation is run for an interval \( t_P \) which is long enough for all pebbles to be inserted and come to rest. At the end of each simulation, a snapshot of the exact pebble configuration is stored, which includes information about all of the tangential displacements \( s_t \) at pebble contacts that are required in the history-dependent contact law.

Table 2 also provides details of the computations, listing the typical number of CPU threads used for each run, as well as the wall clock time required to compute one unit of simulation time. The full-size simulations are by far the most computationally expensive, and were carried out at the Swiss National Supercomputing Centre on ROSA, a Cray XE6 system with 47,872 cores. All other simulation runs were carried out on a variety of Linux machines and Mac Pros, with the typical computation times in the table corresponding to a particular Linux machine with two quad-core 2.6 GHz AMD Opteron processors. In general, due to the short-range force model where pebbles only interact when they are in contact, the code exhibits very good parallel efficiency and doubling of CPU threads will reduce the simulation time by almost half. Memory and disk usage are relatively small, with processor power being the limiting factor.

### 2.3. Pebble drainage

For each of the initial pebble packings, a drainage simulation is carried out by removing the horizontal wall plugging the exit pipe, and letting the pebbles fall out under gravity. The flow rates under gravity are typically much faster than would be expected in real reactors, where a mechanism may be employed to remove pebbles individually, and a flow rate of one pebble per minute would be more reasonable. However, previous work has shown that for dense granular flows in the quasi-static regime, the overall flow rate has a weak effect on the features of flow, allowing for time to be scaled out. This is because at slow flow rates, kinetic effects play a weak role, and the flow is largely determined by geometrical features of how pebbles flow past one another. Choi et al. (2004) have shown that the amount of particle diffusion in slow, dense granular drainage experiments is invariant over a large range of flow rates. In granular drainage simulations, Rycroft et al. (2009b) have shown that artificially inhibiting the flow rate at the exit pipe results in a scaling of the bulk velocity profiles to a high degree of accuracy. It is therefore reasonable to expect that the results of our simulations can be connected to a real reactor by scaling the time variable.

A custom routine was added to the simulation that recycles pebbles that fall out of the exit pipe and reinserts them at the top of the packing. After every one hundred timesteps, any pebbles that have fallen into the region \( z < 0 \) are removed and randomly reinserted into the disk \( z = z_i \) and \( r < r_p \). The recycling routine requires cooperation between many CPU threads in the simulation, since pebbles have to be gathered across several threads, and the operation must ensure that the reinserted
Table 3: Average pebble drainage rates for each simulation geometry and each value of friction, given in units of $\tau^{-1}$.

<table>
<thead>
<tr>
<th>$\mu$</th>
<th>Full-size</th>
<th>3:1</th>
<th>6:1</th>
<th>Tall 6:1</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>152.4</td>
<td>52.3</td>
<td>18.4</td>
<td>19.4</td>
</tr>
<tr>
<td>0.35</td>
<td>133.3</td>
<td>45.0</td>
<td>15.5</td>
<td>16.1</td>
</tr>
<tr>
<td>0.5</td>
<td>124.4</td>
<td>41.6</td>
<td>14.2</td>
<td>14.7</td>
</tr>
<tr>
<td>0.65</td>
<td>120.1</td>
<td>39.9</td>
<td>13.6</td>
<td>13.8</td>
</tr>
<tr>
<td>0.8</td>
<td>117.5</td>
<td>38.9</td>
<td>13.4</td>
<td>13.4</td>
</tr>
</tbody>
</table>


pebbles do not overlap with existing ones, and hence it is more efficient to carry out every hundred timesteps rather than continuously. To avoid a buildup of pebbles within the disk, which would prohibit further insertions, the recycled pebbles are given an initial downward velocity of $6d/\tau$ in the full-size simulations and $3d/\tau$ in the scaled simulations. Typical flow rates for each simulation geometry and each value of friction are shown in Tab. 3. Snapshots of the pebble positions are saved at intervals of $t_s$, which can be post-processed to carry out a variety of analyses. In addition, diagnostic routines to analyze pebble wear and stress are carried out within the simulation, and these are discussed in more detail in the following sections.

We carried out some preliminary drainage simulations to check that the choice of contact model did not have large effect on the results. Using the approximate Hertzian contact model in the 3:1 geometry with $\mu = 0.35$ and identical model parameters as given in Tab. 1, we found that for a variety of statistics (flow rate, velocity profile, wear generation, and stress) the simulation matched the corresponding Hookean simulation to within 5%. Simulations were also carried out using the Hookean model with $\mu = 0.35$ where the ratio of $k_t/k_n$ was changed to $1/2$ or $2/3$ and all other parameters were kept identical; differences of no more than 2% in wear and flow rate were observed. These differences are small compared to many of the other factors that are considered.

3. Pebble ordering and velocity profiles

Figure 1 shows snapshots of the full-size, 3:1, 6:1, and tall 6:1 simulations for the case when $\mu = 0.35$. A central slice through each simulation is shown, by only plotting those pebbles whose centers are in the region $y > 0$. The snapshots are shown at $672.5\tau$, $80\tau$, $30\tau$, and $30\tau$ after the onset of drainage respectively; for the first three, this corresponds to approximately 20% of pebbles draining out of the container and being reinserted. Figure 1(d) is shown after approximately the same amount of drainage as Fig. 1(c).

The pebbles are initially colored in horizontal bands of width $24d$, $8d$, $4d$ and $4d$ respectively, and the deformation of the bands highlights the pebble flow. In the full-size geometry, the bands in the center of container remain horizontal, suggesting a uniform flow profile, although close to the wall the bands are curved, indicating a boundary layer of slower moving pebbles (Nedderman and Laohakul, 1980). In the lower part of the container, the colored bands undergo significant deformation as the pebbles flow out of the orifice, pointing to higher velocity in the region directly above the exit pipe. In the snapshots, pebbles retain their color as they are recycled, which leads to a band of mixed color at the top of the container.

The 3:1 and 6:1 simulations share many of the same qualitative features. The colored bands are
Figure 1: Snapshots of the (a) full-size geometry, (b) 3:1 geometry, (c) 6:1 geometry and (d) tall 6:1 geometry, all making use of a friction coefficient of $\mu = 0.35$. A central slice through each geometry is shown, by only plotting those pebbles with $y > 0$. The snapshots are shown after the $672.5\tau$, $80\tau$, $30\tau$, and $30\tau$ respectively from the initiation of drainage. For the first three, this corresponds to approximately 20% of the pebbles having been drained through the container. For the tall 6:1 geometry this corresponds to roughly the same amount of flow as the 6:1 geometry. Before drainage is initiated, the pebbles are colored in vertical bands of width $24d$, $8d$, $4d$ and $4d$ respectively, and the deformation of the bands highlights the pattern of flow; the two colors of pebbles are mixed together at the top of each simulation, when they mix together during reinsertion.

roughly horizontal in the middle of the container, but with evidence of a slower-moving boundary layer at the walls. At the exit pipe, the shapes of the deformed bands are qualitatively similar across the different scales. In the tall 6:1 simulation, the pebble flow near the exit pipe is very similar to the 6:1 simulation, since as discussed in more detail in Sec. 5 the height of the simulation does not have a large effect on the stress profiles.

To investigate the flow in more detail, time-averaged velocity profiles were computed by making use of the pebble snapshot information. Here, and in all subsequent analyses that employ time-averaging, each computation is started after 20% of the pebbles have drained, in order for the pebbles to reach a steadily flowing state. Pebble velocities are binned in horizontal strips of width $1d$, and as a function of the radial coordinate. If a pebble is at $x^n$ at one timestep and $x^{n+1}$ on the next timestep, then it is treated as having velocity $(x^{n+1} - x^n)/\Delta t$ at location $(x^{n+1} + x^n)/2$. Figure 2(a)
shows the velocity profiles in the full-size simulation with $\mu = 0.35$ at several heights that are not far above the exit pipe. As expected, the velocity is highest for small values of $r$ in the region above the exit pipe. At larger heights, the velocity profile becomes less pronounced and wider. The Gaussian shapes of the profiles are typical of dense granular drainage experiments (Samadani et al., 1999; Choi et al., 2005), and are approximately captured by the kinematic flow model (Nedderman and Tüzün, 1979).

The velocity profiles in the central region of the container are shown in Fig. 2(b). Over the range $0 < r < 25d$, the velocities are almost perfectly uniform, and the pebbles move downward with almost no rearrangement. For $r > 25d$, a boundary layer of slower flow is visible, in agreement with the snapshot of Fig. 1(a). Figure 2(c) shows the boundary layer in more detail, and also in comparison to the full-size simulations with different values of friction. Since the profiles are based upon pebble centers, these curves are plotted up to $r = 28.5d$, which is the closest a pebble
center can come to the wall. The simulations with higher values of friction have lower speed, and a noticeably wider boundary layer.

Some small oscillations in velocity due to the pebble packing structure are visible in Fig. 2(c), and to investigate this in more detail, profiles of number density are computed. The number density is a dimensionless quantity defined as the number of pebble centers per $d^3$, and can be computed by binning the pebble positions using the same procedure as for the velocity. Figure 2(d) shows the number density profile for the boundary layer for the different values of friction. It can be seen that the pebbles are ordered into layers that are very well-defined next to the wall and then become progressively more blurred in the bulk. In the center of the packing, the number density tends to a value of approximately 1.2. Since the volume of a pebble is $V_p = \frac{4}{3} \pi (0.5d)^3$, it follows that the pebble volume fraction is approximately $1.2V_p/d^3 = 63\%$, which closely matches the initial density of the pebble packing. The ordered layers of pebbles occupy roughly the same width as the boundary layer of slower velocity, suggesting the boundary layer's origin may be connected with the pebble size itself.

To compare the simulations at different scales, normalized velocity profiles were computed by rescaling the velocity by the total flux, and rescaling the radius by the reactor radius. Velocity profiles for the four simulation geometries with $\mu = 0.35$ are shown in Fig. 3(a), and it can be observed that in the scaled geometries, the boundary layer of slower flow takes up proportionally more of the flow profile. This is particularly apparent in the 6:1 geometries, where gradients in vertical velocity are visible across the entire profile, and no region of constant velocity is present. A plot of rescaled number density (Fig. 3(b)) shows a similar picture, with well-defined layers of pebbles in the 6:1 simulations being present across the entire profile. To examine the absolute widths of the ordered layers, the same curves are plotted in Fig. 3(c) as a function of distance from the wall. It can be seen that the layers are almost identical in structure in the full-size and 3:1 simulations, while they are more pronounced in the 6:1 simulation. In the full-size and 3:1 simulations, the presence of a homogenized central region may serve to dampen the ordering. Figure 3(c) also shows that the layers are highly pronounced in the tall 6:1 geometry. To investigate this further, the number density was plotted at several different heights (Fig. 3(d)), showing that the layers become more well-defined at lower levels, suggesting that over time, the pebbles move into a more ordered state.

The generation of highly ordered pebble arrangements is particularly significant in the 6:1 geometries. To examine this issue further, simulation times are referred to in cycles, with one cycle corresponding to when each pebble has been reinserted once on average. Figure 4(a) shows a snapshot of the 6:1 geometry with $\mu = 0.35$ after one cycle. Unlike Fig. 1, all pebbles are plotted, so that the pebble packing arrangements against the wall can be seen. For this snapshot, some pebbles appear ordered into regular hexagonal arrangements, but there is also a large amount of pebble disorder. Figure 4(b) shows the same simulation after twenty-five cycles, at which point the pebbles next to the wall have become highly ordered into a regular hexagonal arrangement—similar patterns have been observed in experiments (von der Decken, 1972) and simulations (Cogliati and Ougouag, 2006). The pebbles in this layer are still flowing, with pebbles falling out at the bottom, but as new pebbles are introduced they extend the ordered arrangement at the top; once established, this ordered structure can persist for a long duration.

To quantitatively study this phenomenon, a measure of boundary ordering for a given snapshot
Figure 3: Comparison of simulations at different scales with $\mu = 0.35$: (a) vertical velocity normalized by the total flux, as a function of normalized radius, for the four different simulation geometries (b) number density as a function of normalized radius for the four different simulation geometries, (c) number density as a function of distance to the cylindrical wall. In (a)–(c), the profiles are plotted at $z = 90d, 30d, 15d, 15d$ for the full size, 3:1, 6:1, and tall 6:1 simulations respectively. In (d), number density in the tall 6:1 simulation at different heights is plotted.

was introduced, by first finding the set of all pebble centers $\mathbf{x}_i$ that are within a distance $d$ of the cylindrical wall, and in the region $z_c < z < z_w + 1.1d$, where $z_c$ is the height at which the exit funnel meets the cylindrical wall. For each pebble position $\mathbf{x}_j$ in the range $z_c + 1.1d < z < z_w$, the number of neighbors can be computed as the number of pebbles with $i \neq j$ such that $|\mathbf{x}_i - \mathbf{x}_j| < 1.1d$, which corresponds when pebbles are touching or in very close proximity to each other. Boundary ordering is then computed as the average number of neighbors for pebbles in this set. Figure 4(c) shows the evolution of boundary ordering in the 6:1 simulations. Some of the simulations show evidence of random fluctuations in boundary ordering, but in all cases the amount of boundary ordering generally increases over time. For the runs with $\mu = 0.2$, $\mu = 0.5$, and $\mu = 0.8$, the boundary ordering reaches a value close to six (corresponding to the hexagonal arrangement) after several cycles and then barely deviates over the next thirty cycles. For $\mu = 0.35$ and $\mu = 0.65$ the runs exhibit some variations in boundary ordering, which could be attributed to random differences.
Figure 4: Boundary ordering effects in the scaled geometries. The figures are measured in terms of cycles, with one cycle corresponding to when each pebble has on average been recycled once. Simulation snapshots with \( \mu = 0.35 \) in the 6:1 geometry after (a) one cycle and (b) twenty-five cycles are shown. Boundary ordering, computed as described in the text, is shown as a function of cycles in (c) the 6:1 geometry, and (d) the 3:1 and tall 6:1 geometries. Since the typical simulation lengths reported in Tab. 2 for the tall 6:1 simulations cover approximately ten cycles, the curves in (d) are based on extended simulation runs.

between runs, but by thirty cycles these have also reached a highly ordered state.

Figure 4(d) shows the evolution of boundary ordering in the 3:1 and tall 6:1 geometries for selected values of the friction coefficient. The ordering in the tall 6:1 simulations appears to increase over time, and while some random variations are present, the boundary ordering sometimes reaches values close to six, suggesting that the entire layer of boundary pebbles can become highly ordered. This is in marked contrast to the 3:1 simulations, where boundary ordering never reaches values above 5.05 even after many complete cycles; similar behavior is seen in the full-size simulations.

The presence of boundary ordering is interesting from a scaling viewpoint since it is an example where the 6:1 scaled simulation exhibits fundamentally different behavior than at larger scales. In general, boundary ordering is likely to be detrimental to reactor performance, creating the possibility of pebbles remaining stuck in the ordered layer for a long duration, leading non-uniform pebble burn-up (von der Decken, 1972). Furthermore, ordering may lead to significant alteration in the distribution of interstitial volume within the reactor core, which has been shown to be associated with alterations in neutron scattering that may affect reactor performance (Lieberoth and Stojadinović, 1980; Larsen and Vasques, 2011).
4. Wear and residence times

As the pebbles flow through the reactor, they will slide against each other and against the reactor walls, causing wear and generating graphite dust. This section aims to quantify the dust generation and understand how it is spatially localized. Quantifying the amount of wear between two surfaces is a complex field, and a very large number of models are discussed in the literature. Many of these models are summarized by Meng and Ludema (1995), who note that the general picture of wear is poorly understood, citing how wear has been proposed to be a function of a great number of physical variables. For the current study, the situation is particularly unclear, since the properties of graphite at high temperature are not well-known. A recent survey article (Cogliati et al., 2011) noted that wear rates differing by several orders of magnitude have been reported, depending on the experimental conditions; little data is available for conditions similar to the reactor and the influences of factors such as pebble sliding velocity or contact force have not been researched in detail. Since we are unable to propose a model that may take into account the particular properties of graphite, we therefore make use of the classical model of Archard (1953), which is one of the simplest available. In this model, the volume of worn material is given by

\[ W = ks \frac{P}{p_m} \]  

(3)

where \( s \) is the sliding distance, \( P \) is the applied load, and \( k \) is the dimensionless parameter. The quantity \( p_m \) is referred to as the “flow pressure,” has units of pressure, and is roughly equivalent to a material hardness. For the purposes of this study, since \( k \) and \( p_m \) are not known, the amount of wear is measured in terms of \( sP \) with units of energy, \( md^2/\tau^2 \).

The wear model of Archard was also made use of in previous pebble simulations of dust production (Cogliati and Ougouag, 2008), where slip was computed in terms of the relative tangential velocities between pebbles. In the contact model employed in these simulations, presented in Eqs. 1 and 2, the amount of slip can be naturally quantified by making use of the tangential displacement \( s_t \). Consider two pebbles that are in a horizontal plane and are constrained so that they cannot rotate. Suppose the pebbles are brought into contact, and then one pebble is slowly displaced vertically by small amount. This will create an elastic tangential restoring force \( F_t \) given by Eq. 2. If the restoring force is below the Coulomb friction criterion, so that \( |F_t| < \mu |F_n| \), then if the pebble is allowed to freely move in the vertical plane, the combination of the elastic and viscoelastic tangential forces will cause the pebble to move back to its original position of contact, where \( s_t = 0 \). Thus this type of contact can be thought of as elastic and reversible, with no slip occurring.

Now suppose that as the pebble is displaced vertically, there is one instant when the elastic tangential restoring force exceeds the Coulomb friction criterion. In that case, the tangential displacement will be modified, so that \( s_t \) is replaced by \( s_t + c \) for some vector \( c \). If the pebble is allowed to move freely in the vertical plane, then in a similar manner to described previously, it will move back to where \( s_t = 0 \). However, this will be displaced by a vector \( c \) from its original point of contact. Hence, a modification of \( s_t \) due to the friction law corresponds exactly to the case when irreversible slip occurs between pebbles. This provides a succinct way to evaluate wear within the simulation: every time a pebble contact is evaluated, an additional step can be carried out to compute an amount of wear as the product of \( |F_n| \) and the magnitude of the modification to \( s_t \). Wear can also be computed at a pebble–wall contact using the same procedure.
It should be noted that our model neglects other potential mechanisms for wear, such as from pebble collisions, although due to the large contact forces and slow flow rates, it is reasonable to assume that wear from rubbing surfaces is the dominant effect. Other effects, such as alterations in pebble sphericity due to abrasion, which could affect pebble rolling dynamics against the walls, are also not considered, although the available data suggests that the wear will not be large enough to substantially affect the shapes of the pebbles. For the AVR, a wear generation rate of 5 kg/yr has been estimated (Cogliati et al., 2011), which is much smaller than the total pebble mass of approximately $2 \times 10^4$ kg.

4.1. Wear per pebble

For each pebble within the simulation, the amount of wear that it experiences as it flows through the reactor can be calculated by summing up all its individual wear contributions at each timestep. However, before proceeding, one difficulty has to be addressed: the simulation records a large amount of wear occurring at the top of the packing, as pebbles are reintroduced, fall under gravity, and undergo many collisions and contacts as they settle into a densely packed arrangement. Unlike in the bulk of the reactor, where the flow is quasi-static and previous studies suggest that the results can be scaled to match a real reactor flow rate, it is less clear how to scale the simulation results in the top region to a real reactor, or whether the Archard model is appropriate for modeling wear due to rapid collisions between pebbles. A precise match would also depend on the particular procedure to be employed for pebble reinsertion. Because of this, it was chosen to focus on the wear in the bulk below a height of $z_w$. The values of $z_w$ for the four simulation geometries are given in Tab. 2.

Figure 5 shows snapshots of the full-size, 3:1, and 6:1 simulations with $\mu = 0.35$ after approximately 20% of the pebbles have been drained, where the pebbles have been colored according to the amount of wear they have experienced in the region $z < z_w$. In the full-size geometry it can be seen that the pebbles in the bulk experience very little wear. This agrees with the results of Sec. 3, where this region was shown to be in plug flow with very little rearrangement, and hence very little pebble slip. In the boundary layers of slower flow, a significant amount of pebble wear is visible as the pebbles slide past one another. A large amount of wear is also visible in the converging region of flow above the exit pipe, as expected, since a large amount of pebble slip must occur. In general, the patterns of wear are qualitatively similar for the 3:1 and 6:1 geometries, although since the boundary layers of slower velocity take up a larger fraction of the reactor, there is a smaller region of plug flow where pebbles experience very little wear. At all scales, the plots are qualitatively similar for different values of friction.

The information used to generate Fig. 5 can also be used to calculate total wear production rates for each simulation, by computing the total wear and dividing by the total simulation length. These values are presented in Tab. 4, and are divided into wear production for $z < z_w$ (Tab. 4(a)) and for $z \geq z_w$ (Tab. 4(b)). In each table, the wear production from pebble–pebble contacts and pebble–wall contacts are shown. If the wear coefficient $k/p_m$ in Eq. 3 for the pebble surface is known, then the total dust production rate from the pebbles can be calculated by multiplying it by the sum of the pebble–pebble and pebble–wall rates. If the wear coefficient for the wall surface is known, then the total dust production rate from the walls can be calculated by multiplying it by the pebble–wall rates only.
Figure 5: Snapshots of pebble drainage in the (a) full-size geometry, (b) 3:1 geometry, (c) 6:1 geometry and (d) tall 6:1 geometry, all making use of a friction coefficient of $\mu = 0.35$. The snapshots are shown after the 672.5 $\tau$, 80 $\tau$, 30 $\tau$, and 30 $\tau$ respectively from the initiation of drainage, identical to the snapshots shown in Fig. 1. Each pebble is colored according to the amount of wear it experiences under the Archard model, being measured in units of work. Wear is not recorded for pebbles above $z > z_w$, to avoid counting a large amount of wear due to mixing in the reinsertion region.
Figure 6: (a) The average wear accumulated by a single pebble draining through each simulation geometry, as function of friction coefficient $\mu$. Only wear accumulated in the region $z < z_w$ is considered. Solid lines represent the average pebble–pebble wear and dashed lines represent the average pebble–wall wear. In (b), the average wear values are multiplied by the geometrical scaling factor, showing an approximate collapse. (Due to its different properties, the tall 6:1 simulation is omitted from this graph.)
Table 4: Wear production rates for each simulation geometry and each value of friction, given in units of $md^2/τ^3$.

Wear for (a) the bulk of the geometry where $z < z_w$ and (b) the reinsertion region where $z ≥ z_w$ are given separately. In entries in both of the tables, the first figure is due to pebble–pebble wear, while the second figure in brackets is due to pebble–wall wear.

By dividing each of the values in Tab. 4(a) by the corresponding pebble flow rate, the average wear that a pebble accumulates during one cycle of the reactor (not including wear for $z ≥ z_w$) can be calculated—these amounts are plotted in Fig. 6(a). In all cases, our calculated measure of wear is larger at lower values of friction, since lower friction allows for more tangential displacements between pebbles. However, it is worth noting that since the measure of wear is based entirely on tangential displacements and forces, it does not take into account that for smoother materials the wear coefficients are likely to be lower. Despite complex differences in the flow patterns that are seen at the different simulation scales, Fig. 6(a) highlights a surprisingly simple result: across all values of friction, the average pebble wear in the 3:1 simulations is approximately a third of that in the full-size simulations, and the average pebble wear in the 6:1 simulations is approximately a sixth of that of the full-size simulations. This can be seen more clearly in Fig. 6(b), where the wear production rates are multiplied by the geometric scaling factor, and an approximate collapse is visible. In Fig. 6(a), the data points for the tall 6:1 simulation are similar to those for the full-size simulation, although with slightly more pebble–wall wear and slightly less pebble–pebble wear. For all four geometries, there is a marked increase in the pebble–wall wear for $µ = 0.2$, which is in agreement with Fig. 2(c) where the slip velocity for $µ = 0.2$ is significantly larger.

4.2. Correlations in pebble wear

Figure 7(a) shows a scatter plot of each pebble’s radial position as it passes $z = z_w$ versus the total amount of wear it accumulates from $z = z_w$ before reaching the exit pipe, for the 3:1 simulation with $µ = 0.35$. The plot shows a large amount of correlation between these two variables, with a high probability that a pebble reinserted close to the wall will experience more wear. In the previous section, it has been observed that the bulk of pebble wear appears close to the walls, and since there is relatively little horizontal pebble motion in most of the reactor geometry, a pebble’s wear
is strongly influenced by its initial radial coordinate. In an experimental facility, this may provide a method of controlling how the pebbles are worn: reinserting more heavily worn pebbles in the center of the reactor will lead to a more even distribution of pebble wear, whereas reinserting these pebbles near the reactor wall provides a method of generating and testing extreme cases of wear. Figure 7 shows a plot of pebble wear versus the residence time, defined as the time needed for a pebble to travel from \( z = z_w \) to the exit pipe. Again, a high degree of correlation can be observed, with an almost linear relationship between the two variables.

As shown in Figs. 7(c) and 7(d), similar correlations are also present in the tall 6:1 geometry with \( \mu = 0.35 \). However, unlike the 3:1 geometry, it was found that there was a significant evolution in the data points over the duration of the simulation. Pebbles passing \( z = z_w \) during the first two complete cycles of the simulation (\( 0 < t < 1727\tau \)) are shown in a different color, and have fairly large spread of wears and residence times. However, later in the simulation the points are separated...
into two clusters corresponding to interior pebbles and pebbles adjacent to the wall. It is likely that this evolution in behavior is connected to the increase in boundary organization discussed in Sec. 3, which happens over a similar timescale.

4.3. Spatial distribution of wear

In addition to recording on a per-pebble basis, the wear contributions are also recorded in the $rz$ plane, by binning them into a square grid with spacing $d/(10\sqrt{2})$. Figure 8 shows plots of wear for the 3:1 simulations with $\mu = 0.2, 0.5, 0.8$. This figure concentrates on wear by the pebbles themselves, by counting the wear contribution at each pebble–pebble contact twice, and the wear contribution at each pebble–wall contact once. The three plots are qualitatively similar, with the amount of wear being largest near the walls and in the converging region of flow above the orifice. A large amount of wear is also visible at the top of the packing where the pebbles are
introduced, which was discounted in the above analysis. The three plots differ considerably in overall magnitude, with the lower values of friction leading to more wear. A lower value of friction leads to less resistance to tangential slip, and thus more wear should be expected.

Figure 9(a) shows a close-up of the wear generation rate for the 3:1 simulation with μ = 0.35. Close to the wall, there are bands of high wear generation that arise due to the pebbles being ordered into layers as shown in Fig. 3. The bands are divided into two families: one family is due to wear between layers and appears rather blurred, and the second family is due to wear within each layer and appears more focused, particularly for the layer of pebbles adjacent to the wall. A large amount of wear is visible with the wall, although at the interface between the cylinder and the funnel, a small part of the wall experiences no wear since pebbles cannot come into contact with it. In addition to wear, a local measure of porosity is computed, as the probability that a given location will not be covered by a pebble. The center of each square bin in the rz plane corresponds to particular values of r and z, which define a circle in three-dimensional space. The arc length of this circle that is covered by pebbles can be calculated. Porosity is then defined as the fraction of the circle that is not covered by pebbles, time-averaged over the duration of the simulation. Figure 9(b) shows a close-up of the porosity for the 3:1 simulation with μ = 0.35. The ordering of pebbles at the reactor walls creates channels of high porosity, which are particularly well-defined close to the reactor wall, with variations from 17% in the first pebble layer to 73% in the space between the first and second layers—these observations are in good agreement with previous studies (du Toit, 2008). Recent
CFD studies have shown that the gas flow through pebble packings has complex localized features (Lee et al., 2007; Hassan, 2008; Wu et al., 2010), that are not captured by a coarse-grained porous media model. The significant correlations between porosity and the regions of high dust generation may therefore need to be taken into account in determining the transport of dust.

5. Stress

In addition to analyzing wear, the stresses experienced by the pebbles have also been examined, providing further information about the magnitude of the contact forces that the pebbles will encounter. In a particulate system, the stress tensor can be decomposed as $\sigma = \sigma^S + \sigma^K$, where $\sigma^S$ is the static stress and $\sigma^K$ is the kinetic stress (Silbert et al., 2001). Consider a small region with volume $V$, in which pebbles are labeled from 1 to $N$. The static stress is due to the forces between pebbles, and can be calculated according to

$$\sigma^S_{\alpha\beta} = \frac{1}{2V \sum_{i=1}^{N} \sum_{j \neq i} r_{ij}^\alpha F_{ij}^\beta + r_{ij}^\beta F_{ij}^\alpha}{2}$$  \hspace{1cm} (4)$$

where $\alpha$ and $\beta$ are coordinate suffixes, $r_{ij}$ is the separation vector from pebble $i$ to pebble $j$, and $F_{ij}$ is the force exerted on pebble $i$ by pebble $j$, which is taken to be zero if the pebbles are not in contact. The sum over $j$ also includes pebbles outside the small region. This equation is equivalent to the original formulation of Christoffersen et al. (1981) and has been employed in a variety of studies of dense granular flow (Depken et al., 2007; Rycroft et al., 2009a). The kinetic stress is given by

$$\sigma^K_{\alpha\beta} = -\frac{1}{V \sum_{i=1}^{N} m(v_i^\alpha - \bar{v}^\alpha)(v_i^\beta - \bar{v}^\beta)}$$  \hspace{1cm} (5)$$

where $v_i$ is the velocity of pebble $i$ and $\bar{v}$ is the average velocity of pebbles in the small region. It represents a contribution to stress due to pebble collisions and momentum, and is particularly significant in highly energized particulate systems like gases.

In the reactor simulations, the stresses have been computed in the $rz$ plane using square bins with side length $d$. The stress tensor is computed in the $(r, \theta, z)$ coordinate system. For each pebble under consideration, its velocity $v_i$, separation vectors $r_{ij}$, and forces $F_{ij}$ can be expressed in terms of the orthogonal basis $e_r, e_\theta, e_z$ at the pebble’s position, which are then made use of in the sums in Eqs. 4 and 5, and time-averaged over all available simulation snapshots.

One difficulty that occurs in the stress computation is choosing the volume $V$ to use in Eqs. 4 and 5. If pebbles are ordered randomly, then the volume can be simply chosen to be the volume of each stress computation region. However, as described in Sec. 3, the pebbles are persistently ordered into layers near the reactor walls, with Fig. 2(d) showing typical separations between layers of $0.8d$ to $0.9d$. Since the stress computation regions have width $d$, then depending on exactly how the layers are aligned, some computation regions may have two layers of pebbles within them and thus have significantly more pebbles than others. This may lead to an overestimate of stress, since the sums in Eqs. 4 and 5 will include a larger number of pebbles. In cases like this, the pebbles whose centers lie within this stress computation region will protrude into the neighboring computation regions. The
Figure 10: (a) The Voronoi cells for a particular drainage snapshot in the 6:1 geometry. Additional plane cuts are made to the Voronoi cells to approximate the cylindrical and conical sections of the reactor geometry. The exit pipe is not considered, and Voronoi cells for pebbles at the top of the packing are not shown. (b) A cutaway showing the Voronoi cells in a vertical slice through the container. (c) The Voronoi cells corresponding to three stress computation regions centered on \((r, z) = (3.5d, 20.5d), (4.5d, 14.5d), (1.5d, 7.5d)\). (d) Corrections to each stress computation region in the \(r_z\) plane for \(\mu = 0.35\), expressed as the ratio of the time-averaged Voronoi cell volume divided by the volume of the ring \(2\pi rd^2\).

A straightforward choice of \(V\) misses the fact that the pebbles in these computation regions effectively take up more volume than others.

To circumvent this issue the Voronoi tessellation can be employed. For a collection of particles in a domain, the Voronoi tessellation is defined by associating a Voronoi cell to each particle that consists of the space that is closer to that particle than any other (Okabe et al., 2000). In the absence of complex boundary conditions, Voronoi cells form irregular convex polyhedrons, whose faces are the perpendicular bisectors with neighboring particles. The Voronoi cells perfectly partition the domain. The Voronoi tessellation provides a method of computing a more accurate value of \(V\). For each stress computation region, the value of \(V\) is calculated as the volume of the Voronoi cells of the pebbles whose centers lie within that region. The computation of the Voronoi cells is carried out using the VORO++ software library (Rycroft, 2009; Voro++ website), which is well-suited to the task, since it computes Voronoi cells individually, from which it is straightforward to calculate their volumes. On the reference Linux desktop computer with 2.6 GHz Opteron processors, the library can compute approximately 40,000 Voronoi cells per second per CPU thread, which is fast enough that all pebble snapshots from all simulation runs can be analyzed in a reasonable time frame.

The library also provides a mechanism for approximating the curved reactor walls by making
additional plane faces to the Voronoi cells. Figure 10(a) shows an example Voronoi tessellation for a 6:1 simulation snapshot with $\mu = 0.35$, where additional plane faces approximating the cylindrical wall and conical funnel are visible. The exit pipe is not considered in the analysis, since by default the library can only compute Voronoi cells as convex polyhedra, and would therefore encounter a problem at the obtuse internal angle at the funnel–pipe interface. Figure 10(b) shows a cutaway of the Voronoi cells through a central slice of the reactor, and Fig. 10(c) shows the pebbles and Voronoi cells corresponding to the stress computation regions centered on $(r,z) = (3.5d, 20.5d), (4.5d, 14.5d), (1.5d, 7.5d)$. The volumes of the Voronoi cells in each one of these rings can then be summed and time-averaged over all frames to find an appropriate value of $V$ for each stress computation region. Figure 10(d) shows an example of the computed values, which are normalized by the volume of the ring, given by $\pi d ((r + 0.5d)^2 - (r - 0.5d)^2) = 2\pi rd^2$. Variations of up to $\pm 25\%$ are visible, and are particularly noticeable in the region corresponding to $r = 3.5d$.

Once the stress tensors are computed, the pressure can be calculated according to $p = -\frac{1}{3} \text{Tr} \sigma$, and several plots are shown in Fig. 11 for the case when $\mu = 0.35$. In Figs. 11(a) and 11(b), the...
kinetic component of pressure, and total pressure, in the full-size geometry are compared. To relate them to the same color scale, the kinetic contributions have been multiplied by a factor of 500, confirming that they have an almost negligible effect. The only two regions where there is an appreciable contribution are the exit pipe and the reinsertion region, where values of 0.14 m/dτ^2 and 0.2 m/dτ^2 respectively are present.

Figure 11(b) shows that the pressure in the reactor initially increases as a function of depth from the top surface. At z = 80d on the central axis, about 90d from the top of the packing, the pressure is approximately 70 m/dτ^2. In Fig. 3, the average number density is approximately 1.2, and thus the density of the pebble packing is 1.2 m/d^3. For a fluid with this density, the pressure at z = 90d would be ρg(90d) = 108 m/dτ^2, which is somewhat larger. This should be expected, since stresses in granular materials behave very differently to fluids. In particular, in a phenomenon known as the Janssen effect (Janssen, 1895; Sperl, 2006; Ovarlez et al., 2003), the stresses in a tall granular
Figure 13: Profiles of pressure in the simulations on the central axis, as function of \( z \): (a) profiles for several full-size and tall 6:1 simulations and (b) profiles for the 3:1 and 6:1 simulations. The full-size profiles are averaged over the region \( r < 6d \), while the scaled profiles are averaged over the region \( r < 3d \).

column are known to saturate, instead of growing linearly as in a fluid, due to the frictional contacts with the side walls supporting the column’s weight. Below \( z = 80d \), the pressure increases sharply, in an arched band spanning the width of the container, below which the pressure decreases rapidly.

Figures 11(c) and 11(d) show plots of pressure in the 3:1 and 6:1 geometries with \( \mu = 0.35 \). The plots are scaled by factors of three and six respectively, as would be consistent with how hydrodynamic stresses would scale, and with these factors the three plots appear qualitatively similar. However, there are noticeable differences, with the arch above the exit pipe becoming progressively less pronounced, and stresses at the corner between the cylinder and funnel becoming progressively larger. In Fig. 12, plots of pressure are shown for several 3:1 simulations with different values of friction. Pressures are significantly larger in the simulations with lower values of friction, which is consistent with the Janssen effect, since it is harder for the weight of the packing to be supported by frictional forces with the wall. Higher pressures will also contribute to the larger amounts of wear that are seen in the simulations with low friction. It is also noticeable in Fig. 12 that the profiles of pressure across the width of the geometry are flatter for the lower values of friction, showing less variation in the radial direction, and are more similar to a hydrostatic pressure profile.

To investigate the friction dependence in more detail, vertical profiles of pressure were computed on the central axis at \( r = 0 \). Profiles for three full-size simulations are shown in Fig. 13(a) and have similar characteristics to Fig. 11(b), with the pressure slowly increasing as the depth of the packing increases, before rapidly peaking, and decreasing again as the exit pipe is approached. While the pressures appear to be somewhat larger for the lower friction values, the dependence is not straightforward, with the peak in pressure being largest for \( \mu = 0.5 \). Profiles for the tall 6:1 simulation are also plotted on the graph, and despite the depth of the packing being similar to the full-size geometry, the pressures are much smaller, rapidly saturating due to the Janssen effect. Previously, it was shown that the wear in the tall simulations was comparable to the full-size simulations, and since the pressures are much smaller, it must be the case that there is much more
Figure 14: Plots of stress tensor alignment for $\mu = 0.35$ and the (a) full-size geometry, (b) 3:1 geometry, and (c) 6:1 geometry. Each eigenvector of the stress tensor is plotted as a cylinder, the length of which is proportional to the square root of the magnitude of the corresponding eigenvalue. The largest eigenvalue is shown in magenta, the intermediate eigenvalue is shown in purple, and the smallest eigenvalue is shown in orange.

Figure 13(b) shows the pressure profiles for the 3:1 and 6:1 simulations. It can be seen that the pressures in the 3:1 simulation are significantly higher than in the tall 6:1 simulation, contrary to what would be expected in a fluid. For both the 3:1 and full-size simulations, the maximum value of pressure is located higher in the reactor as the friction coefficient is increased.

To obtain more information about the stresses, the alignment of the stress tensor throughout each simulation can be plotted, by computing its eigenvectors, which are referred to as the principal directions. Following a previously-used technique (Rycroft et al., 2009a), the eigenvectors can then be plotted with each scaled according to the corresponding eigenvalue. Figure 14 shows plots of the tensor alignment for the three simulations. In a wide granular material in the absence of side walls, the stress tensors would be expected to be aligned with the vertical direction, but here they form arches. This provides further evidence of the Janssen effect since it points to a significant $\sigma_{rz}$ component, capable of supporting the weight of the packing. Similar patterns in alignment are seen across the three different scales, although the stress tensor in the layer adjacent to the wall in the 6:1
simulation is more strongly aligned with the vertical direction.

6. Conclusion

Overall, the results suggest that flows in scaled geometries will bear some qualitative similarity to a full-size flow, but that there are many issues that make a precise quantitative match difficult. Perhaps the most significant issue is that the pebble length scale controls many features of the flow, with the boundary layers of slower velocity taking up proportionally much more space in the scaled geometries. Given that the boundary layers are of particular importance in the generation of wear, with the simulations showing that a large fraction of pebble wear is generated there, this may be a critical design issue. Furthermore the results show that flows in the scaled geometries may have fundamentally different features to full-size flows. This is particularly evident in the 6:1 geometries, where the entire flow becomes organized into layers and there is no homogenized central region. Ordering of the pebbles at the wall was also shown to occur in the 6:1 geometries, while largely being absent in the 3:1 and full-size simulations.

Nevertheless, the results highlight some general rules that may be useful in experimental design. It was shown that across the complete range of friction values that were considered, the average wear accumulated by a pebble during a single drainage cycle is roughly proportional to the geometrical scaling factor. Similarly, even though the stresses within the pebble packing are markedly different from those in a fluid, their overall magnitudes scale in a similar manner to a fluid, again being roughly proportional to the geometrical scaling factor. Both of these results may be somewhat contingent on the particular geometry considered, and only apply to the simulations where all dimensions are scaled equally. The tall 6:1 simulation exhibits very different behavior, with higher levels of wear, particularly pebble–wall wear, and lower stresses due to the Janssen effect.

The results can also be used to make some practical recommendations for constructing a scaled-down facility. For this, it is perhaps most useful to compare the 3:1 and tall 6:1 geometries, since they feature similar numbers of pebbles, which would likely make them comparable in cost. If the primary concern is total amount of dust generation, then the tall 6:1 geometry may be the most appropriate since the wear production rates are significantly higher. However, the 3:1 geometry gives a more faithful representation of the granular flow in a full-size reactor, recreating the region of plug flow in the bulk of the geometry, which is absent at the 6:1 scale. Also, while the pebble stresses in all of the scaled geometries are significantly lower than the full-size geometry, the 3:1 simulations exhibit somewhat larger stresses than in the tall 6:1 simulations. Given the importance of the pebble length scale in setting many features of flow, scaling down the pebble diameter may be another avenue worth considering.

Acknowledgments

C. H. Rycroft is grateful to L. E. Silbert for useful discussions about the computation of wear within the simulations. C. H. Rycroft was supported by the Director, Office of Science, Computational and Technology Research, U. S. Department of Energy under Contract No. DE-AC02-05CH11231.
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