Abstract

Molecular dynamics simulation is used in studying the appearance of axial and radial segregation in a horizontal revolving drum containing a mixture of two different kinds of granular particles. As with real granular matter, the nature of the segregation is parameter dependent; for example, radial segregation can be transient or long-lasting, and axial bands can merge. Simulations displaying the different kinds of behavior are described.

1. Introduction

Understanding the mechanisms responsible for many of the surprising features of granular matter remains a challenge. The fact that the behavior often differs substantially from atomistic systems means that little theoretical help is available in trying to understand the dynamics of granular matter. Segregation is perhaps the most prominent of these features; the ability of granular mixtures to segregate into their individual components, despite a lack of entropic or energetic benefit, makes this a particularly worthy subject for study. Granular separation and mixing are central to a variety of types of industrial processing; the ability to either cause or avoid segregation can be central to the viability of such processes. There are economic benefits to be gained from a systematic understanding of the complexities of granular flow at a level comparable to fluid dynamics; the outcome would be improved reliability and efficiency. Consequently, considerable effort has been invested in exploring these phenomena, but, in the absence of theory, much of the progress [1, 2, 3, 4] involves computer simulation.

Experiments on rotational segregation employ a horizontal cylindrical drum revolving at constant rate and partially filled with a mixture of two granular species. Under suitable conditions the mixture spontaneously segregates into axial bands of alternating composition. The relevant parameters include the nature of the granular particles themselves, ranging from the most familiar forms of granular matter such as sand, through various organic products, plastic and glass beads, to metal ball bearings. The particles have a broad range of elastic and frictional characteristics, and the material can be in a dry or wet (slurry) state. Other parameters include the drum diameter and length, the rotation rate, the relative fractions and sizes of the granular components, and the fill level. In marked distinction to fluid systems, there are no known scaling relations that allow this parameter space to be reduced, and there is little guidance available for predicting the outcome of an experiment involving some unexplored combination of parameters.

The most direct observations address the structure of the upper surface [5], while more elaborate studies examine the interior using, for example, noninvasive magnetic resonance imaging (MRI) [6, 7, 8]. An additional effect occurs entirely beneath the surface, namely radial segregation, which produces a core rich in small particles extending along
the length of the drum. Radial segregation occurs early in experiments starting from a uniformly mixed state, and may or may not persist once axial segregation appears. Axial band formation might be regarded as a consequence of this core intermittently bulging by an amount sufficient to reach the outer surface [7]. The axial band patterns can also exhibit time dependence; an example of such behavior involves coarsening, in which narrower bands gradually merge into broader bands [9]. Further discussion of the experimental history appears in [7, 10, 11]. More recent results showing the richness of the segregation effect and its dynamics in dry and/or wet mixtures (slurries exhibit behavior that is similar in many respects, despite the lubricating role of the fluid medium) are described in [12, 13, 14].

Direct modeling of the dynamics of granular particles employs the same computational methods used in molecular dynamics simulation of atomistic systems. There have, however, been very few simulations of granular particles in a revolving drum exhibiting axial segregation. The first of these was an early, rather limited treatment [15]. This was followed by a broader study [11], in which the formation of multiple axial bands was demonstrated, and various aspects of the segregation phenomenon, such as band merging, were investigated. The most recent study was [16], which differed from the earlier work insofar as the choice of interactions was concerned. It was found to exhibit both axial and radial segregation, the latter feature not having been reproduced correctly in the previous study. The present report focuses on several key aspects discussed in that paper.

2. Granular models

The models used for granular simulation are generally based on spherical particles whose resistance to overlap is expressed in terms of a continuous potential [17, 18, 19]. In addition to this excluded-volume repulsion, particles are subject to forces designed to replicate the effects of inelasticity and friction. There are limitations to the accuracy of such models, with one empirical measure of success being the degree to which the essence of the phenomenon under study is captured.

Consider a pair of particles $i$ and $j$ with diameters $d_i$ and $d_j$. The repulsive force between particles depends linearly on their overlap

$$ f_r = k_r (d_i - r_{ij}) \hat{r}_{ij} \quad r_{ij} < d_i, \quad (1) $$

where $r_{ij} = r_i - r_j$ is the particle separation, $r_{ij} = |r_{ij}|$, and $d_{ij} = (d_i + d_j)/2$ is the effective diameter; in [11] the repulsive part of the Lennard-Jones interaction was used. Dissipative forces act for the duration of each collision. The first of these is velocity-dependent damping

$$ f_d = -\gamma_n (\hat{r}_{ij} \cdot v_{ij}) \hat{r}_{ij} \quad (2) $$

that depends on the component of relative velocity $v_{ij} = v_i - v_j$ parallel to $r_{ij}$; $\gamma_n$ is the normal damping coefficient, assumed the same for all particles. The total normal force is $f_n = f_r + f_d$. Details of the force parameters are given in [16].

Transverse frictional damping acts at the point of contact to oppose sliding

$$ f_s = -\min(\gamma_s [v_{ij}^s, \mu_s (|f_n|)] ) \hat{v}_{ij}^s \quad (3) $$

where the relative transverse velocity of the particle surfaces at this point is

$$ v_{ij}^s = v_{ij} - (\hat{r}_{ij} \cdot v_{ij}) \hat{r}_{ij} - \left( \frac{d_i \omega_i + d_j \omega_j}{d_i + d_j} \right) \times r_{ij} \quad (4) $$

and $\omega_i$ is the particle angular velocity. The value of $v_{ij}^s$ depends on the particle types $c_i$ and $c_j$, and $\mu_s^{c_i c_j}$ is the static friction coefficient.

In a model of this type there is no true static friction, but a way of overcoming this limitation is to introduce a tangential restoring force that acts during the collision and depends on the cumulative relative displacement at the point of contact [17, 18, 20]

$$ f_s = -k_s \int_{(coll)} v_{ij}^s(\tau) \, d\tau \quad (5) $$
where the integral is evaluated as a sum of vector displacements during contact; the magnitude of \( f_i \) is also limited by \( \mu \| \bar{f}_{\text{int}} \| \). In addition, to avoid occasional unrealistically large displacements, if \( |u_i| > 0.1 \) (an arbitrarily chosen limit) it is reset to zero. This history-dependent force was not present in [11]. The total transverse force is \( f_i = f^t_i + f^r_i \).

The drum wall and end caps are treated as rough and smooth boundaries respectively. The interaction of particles with the curved boundary (together with gravity) drives the system, so this force includes the same components as the interparticle force. To minimize spurious effects associated with the end caps, only \( f^t_i \) acts there. Further details concerning the interactions (with the exception of \( f_i \)) appear in [11], together with a discussion of the friction coefficients and the particle-wall force computations. The runs are begun from a uniformly mixed initial state. Other aspects of the simulation follow standard molecular dynamics procedures [21].

The time-dependent axial segregation, \( S_a(t) \), is evaluated from binned counts along the axis weighted by relative particle volume \( (b') \)

\[
S_a = \frac{\langle |b| n_b(q) - n_s(q) \rangle_q}{b'n_b + n_s}
\]

where \( n_b(q) \) and \( n_s(q) \) are the number of big and small particles in a slice (width \( \approx 2.5 \)) centered at \( q \) along the axis, \( \langle \cdots \rangle_q \) denotes an average over all slices, and \( n_b \) and \( n_s \) are the totals. Binned counts are less suitable for evaluating the radial segregation, \( S_r(t) \); instead, a measure based on the mean-square radial distance of each type of particle from its center of mass is used

\[
S_r = \frac{\langle (r^2_b - \langle r^2_b \rangle)^2 \rangle - \langle (r^2_s - \langle r^2_s \rangle)^2 \rangle}{\langle r^2 \rangle^2 - \langle r \rangle^2}
\]

where \( \langle r_b \rangle \) and \( \langle r_s \rangle \) denote the mean distances of big and small particles from the axis, and \( \langle r \rangle \) the overall mean. These quantitative measures of segregation augment direct observation.

3. Results

Due to the very nature of the segregation effect, not all of its features are readily quantifiable. A global summary of pattern development is provided by \( S_a(t) \) and \( S_r(t) \), Eqs. (6-7), but these lack detailed information concerning the bands. The use of space-time plots provides a more detailed picture, since they show the relative populations, weighted by particle volume, in appropriately oriented slices; for the axial plots slices are normal to the drum axis, while for the radial plots the slices are parallel to the upper free surface. Even more detailed information can be extracted from snapshots of the entire system, in which particular subsets of particles can be selected for viewing; images of this kind reveal interior organization analogous to that observed experimentally with MRI. An even richer visual approach employs animated recordings showing the full temporal development of the system; an animation of this type consists of an extended series of snapshots, recorded at regular intervals throughout the run.

The three runs discussed here are the first three listed in [16]. In each the filling density is 0.3, and the relative big particle size \( b = 1.8 \); the volume fractions of big and small particles are equal. In run #A the drum length \( L = 240 \) and diameter \( D = 40 \), for a total of \( N = 71600 \) particles, and angular velocity \( \Omega = 0.2 \); run #B has \( L = 360, D = 30, N = 57600, \Omega = 0.1 \); run #C has \( L = 160, D = 40, N = 47300, \Omega = 0.1 \). The run lengths, expressed in terms of drum revolutions, \( n_r \), are 1620, 2630 and 1800, respectively.

In view of the extensive simulations involved, it is interesting to note the computational performance. For run #C, and a partly parallelized computation running on a dual 3.6 GHz Intel Xeon workstation, the simulation proceeds at a rate of approximately 23 000 time steps/hr, equivalent to 1.8 revolutions/hr; some of the runs therefore extend over several weeks.

Fig. 1 shows the axial and radial space-time plots for run #A. Radial segregation appears very early in the run and a core of small particles persists throughout, although the outer layer rich in big particles disappears from the radial plot once axial banding begins; after the 12 axial bands have formed the pattern appears stable, with no hint of any future change.

Images of the final state of run #A appear in Fig. 2. The first is an oblique view of the full system showing the 12 alternating bands. The others are views looking down in a direction normal to the surface that show big and small particles separately. These interior views reveal that while the bands of big particles are not entirely separate, there are visible divisions between them, and that the bands of small particles are joined by a central core.
Figure 1: Axial and radial space-time plots for run #A: \( n_R = 1620, L = 240, L/D = 6 \); medium and dark gray (or red and blue in the color images) denote higher volume fractions of big or small particles. Time is along the horizontal axis, and the vertical axis measures axial or radial (the latter normal to the free surface) position.

Figure 2: Final state of run #A; the full system, and views showing just the big and small particles.
Fig. 3 shows the space-time plots for run #B. Here, unlike #A, radial segregation is a transient effect lasting less than 200 revolutions; furthermore, the early axial pattern is not maintained, and the initial 17 bands are eventually reduced to 11. During the latter portion of the run, extending over more than half its total length, there is no suggestion of further pattern change. Band coarsening is a well-known experimental result, with the band count falling roughly logarithmically with time [12], although the dependence can be more complicated than this [14].

Fig. 4 shows the final state of #B. Band separation is practically complete in this case, with essentially no misplaced big particles, and only the faintest remnant of a small particle core.

The development of axial and radial segregation for runs #A and #B is shown in Fig. 5. The graphs confirm that the preference for small particles in the core persists over the duration of #A, but not #B.

Fig. 6 shows run #C after 60 revolutions and exemplifies the kind of radial segregation that can develop. Here the complete system is shown, together with three narrow slices (of thickness 0.03L) at the midpoint and at a distance 0.1L from either end.

Two general observations concerning segregation emerge from these and other simulation runs. When radial
Figure 5: Time-dependent axial and radial segregation, $S_a$ and $S_r$, for runs #A and #B; time is expressed in drum revolutions.

Figure 6: Views of #C after 60 revolutions; the full system and three slices are shown.
segregation occurs it takes the form of a core of small particles surrounded by big particles; this is also the case experimentally, although in the simulations the core boundaries are not as sharp and the effect appears to develop more slowly. There is no preferred particle type near the end caps nor a tendency for bands to nucleate there; bands can form at different axial positions at different times; sometimes bond formation is almost simultaneous and sometimes not. Further aspects of the behavior, such as dependence on fill level, drum angular velocity, relative particle size, force constants, reproducibility under a minor change of initial conditions, and the behavior of systems started in a segregated state, are discussed in [16].

The configurational snapshots recorded during the runs enable post-run analysis of the motion of individual or selected groups of particles over extended intervals. Here we consider the merging of two bands of big particles, accompanied by the dispersal of the small particles from the disappearing middle band. A merge event of this type occurs in run #B (see Fig. 3) between revolutions 700 and 1200. The upper portion of Fig. 7 shows three views prior to the event, namely the full system, and the selected bands of big and small particles (the latter also revealing small particles that intrude into the big particle band, a detail hidden from the outside). The lower portion shows three views at the end of the event, namely the full system, and all the previously selected particles in their new positions, principally within the bands directly involved. Even though there is essentially no residual small-particle core at this stage of the run, small particles are able to migrate across the big particle bands more readily than the converse.

An interesting feature revealed by these images is that while the small particles are dispersed in both directions, more seem to have traveled to the right where the original band of big particles was somewhat narrower. An eventual goal for this kind of analysis is developing a capability for relating local organization and dynamics at the level of individual particles to the behavior at a scale where the collective nature of segregation is exhibited.

4. Conclusion

Simulations based on a simple particle-based model of granular matter have demonstrated the occurrence of both axial and radial segregation in a revolving drum containing a two-component granular mixture. The different forms of segregation observed are indicative of a large, complex parameter space, as is the case experimentally. To further explore the phase diagram and determine which parameters dominate in different regimes, a systematic study, including multiple realizations due to reproducibility issues, is required. The results suggest many questions of the “what if” type; of necessity, the answers will also have to await further work. The model itself is open to critical examination, in particular, how the components of the interparticle force influence the behavior, as well as the relevant ranges of the force parameters.
In theoretical fluid dynamics, stability analysis [22] is used to determine when symmetry breaking is advantageous. No analogous theory exists for granular segregation, and the question of what distinguishes the different segregation modes from one another, and from the uniformly mixed state, remains open; is it, for example, the ability to optimize energy dissipation, thereby ensuring the most efficient flow? The segregation band coarsening slows with increasing band width, and the states eventually reached have varying numbers of bands and degrees of pattern regularity; here the question is whether such patterns are stable, or are they slow transients on the path to even further coarsening? Another issue is the relation between the radial and axial segregation processes; are they independent phenomena that just happen to coexist, or does the former actually drive the latter? Finally, no attempt has been made to probe the underlying mechanisms beyond the exercise in particle tracking; if simulation can be shown to reproduce experiment reliably, then, in view of the level of detail provided, it may prove an important tool for exploring the complexities of segregation.

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