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SEGREGATION IN SHEARED GRANULAR MEDIA – EFFECTS OF INTRINSIC PARTICLE PROPERTIES SUCH AS SIZE, DENSITY AND SHAPE

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Abstract. When granular media which have different size, density, shape or even frictional properties flow they will tend to segregate. This is of fundamental scientific interest but also has significance in a variety of industries including mining, pharmaceuticals, food processing as well as for natural phenomena such as landslides. Here we consider segregation that occurs when a granular mixture is sheared, such as when it flows down along an inclined slope. A partially filled cylindrical drum is being slowly rotated about its axis (which is perpendicular to gravity) is a popular test-bed to examine sheared granular segregation. Here we consider simulation (Discrete Element Method, DEM), experiment and continuum theories in order to understand the segregation that occurs.

Using DEM simulations we can clearly determine the underlying causes of segregation which intimately depend on intrinsic particle properties such as their size, density and shape. We compare these DEM simulations with both experiments and continuum theories, for a number of these properties, and find very good agreement. It will be shown that segregation arising from differences in particle size is the strongest, with stable asymptotic states being reached after only one or two cylinder rotations. Density segregation is the next strongest followed by segregation due to particle shape. The underlying physical mechanism leading to segregation is different in each of these properties. We compare and contrast these mechanisms in detail.

1 INTRODUCTION

Mixing and segregation of granular mixtures is encountered in a variety of industries including minerals, polymer, food and pharmaceuticals processing. In some cases the sample is required to be as homogeneous as possible while any flow, vibrations or shear of the granular mixture will oppose this. On the other hand, in some circumstances separation of the mixture into its constituent parts is required so that one must understand how to harness the inherent segregation and maximise its rate and extent to attain the final goal. Experimentally it is known that any differences between the individual, constituent particles such as particle size, density, shape or frictional properties can lead to granular segregation when the mixture is forced into motion [1]. Thus these intrinsic (particle-scale) properties control the macroscopic differences observed in the mixtures.

Although granular segregation is significant to a wide range of industries and applications and also is itself of scientific interest, it is still incompletely understood. For example, there is no set of continuum equations that can describe the segregation in detail, as there is for the Navier-Stokes equations for liquids (Meir et al, 2007). This is not surprising considering the individual particles themselves behave differently depending on their intrinsic properties (as mentioned above). How a cubical shaped particle moves down a sloped surface is quite different to how a spherical particle does.

In this work we focus on the effect of shear on granular mixtures. Shear occurs in a variety of scenarios such as Couette flow, Poiseuille flow or even flow of particles down an inclined surface. In this study we focus on sheared flow which occurs in a cylindrical tumbler roughly half-filled with a granular mixture. This particular set-up has been the focus of much experimental [2-8], theoretical [9-16] and simulations [17-21]. The cylinder is oriented with its axis perpendicular to the gravity vector and is rotated slowly (1-5 revs per minute) about this cylindrical axis. To focus on the particular physical mechanisms that underlie the granular segregation it is usual for the granular mixture to be made up of two distinct particle types, which is called a *binary mixture.* We consider in detail radial segregation of the mixture, i.e. segregation in a radial direction within a plane perpendicular to the cylinder axis.

A useful dimensionless number which is commonly used to characterize the flow regime for this particular set-up is the Froude number, defined as $Fr = \omega^2 R/g$, where ω is the rotational speed of the cylinder, R is the cylinder radius and g the magnitude of gravity. For the relatively slow cylinder rotations we consider here (mostly 1 rev/min), the flow is in the rolling regime. This means particles predominantly roll once the main flow in the cylinder has been established and the particle bed remains contiguous. Much faster rotational speeds lead to particles becoming separated spatially from the main bed.

In this paper we describe DEM simulations for this slowly rotating tumbler. One tracks individual granular particles, which are subject to a soft collision interaction model, and the entire granular segregation process that evolves is close to the true physical evolution. We shall show this is true by comparison with experiments. We shall also compare the DEM results with continuum models for granular segregation.

As the DEM procedure we use has been well documented previously (see [7,19-21]) we do not delve into it in any of this detail. However, we mention here a few important points about the variant used. Collisional forces are modelled with a soft contact model. Particles are allowed to overlap a certain amount, Δx and normal and tangential relative velocities (v_n and v_t respectively) determine the interaction forces via a linear spring and dashpot model. Since shape is one of the intrinsic properties considered we need to not only model spherical particles but also non-spherical ones which are given by the equi-axis super-quadric equation:

$$x^n + y^n + z^n = a^n \qquad (1)$$

For $n = 2$ this equation gives spheres of radius a, but as n increases the particles become more blocky in shape until as $n \rightarrow \infty$ the particle is a cube of side length $2a$.

2 DENSITY SEGREGATION

For granular mixtures composed of particles with different density (but same size and all are spherical) after around 2 rotations of the cylindrical tumbler a core of denser particles forms surrounded by a corona of less dense particles (see Fig. 1) form. As the cylinder rotates, particles are bought to the top of the upper flowing particle surface. The main segregation occurs in this upper region of the particle bed, where the denser particles sink into the core region, while the less dense ones flow down along the inclined free surface to the bottom of the inclined surface. This segregation mechanism is called *buoyancy*. Figure 1a shows the experimental results for this case (glass and lead particles) where the lead particles (dark grey) have migrated to the core of the particle bed and glass particles (light grey) migrate close to the cylinder walls. Figure 1b shows the corresponding DEM results also after 2 cylinder rotations. The small protruding rectangular ridges on the cylinder walls were included with the intention to mimic macroscopic surface roughness and prevent the rigid body slipping of the whole granular bed against the wall. This type of segregation state forms when (predominantly) all particles have a similar size. The similarity between experiments and DEM is apparent.

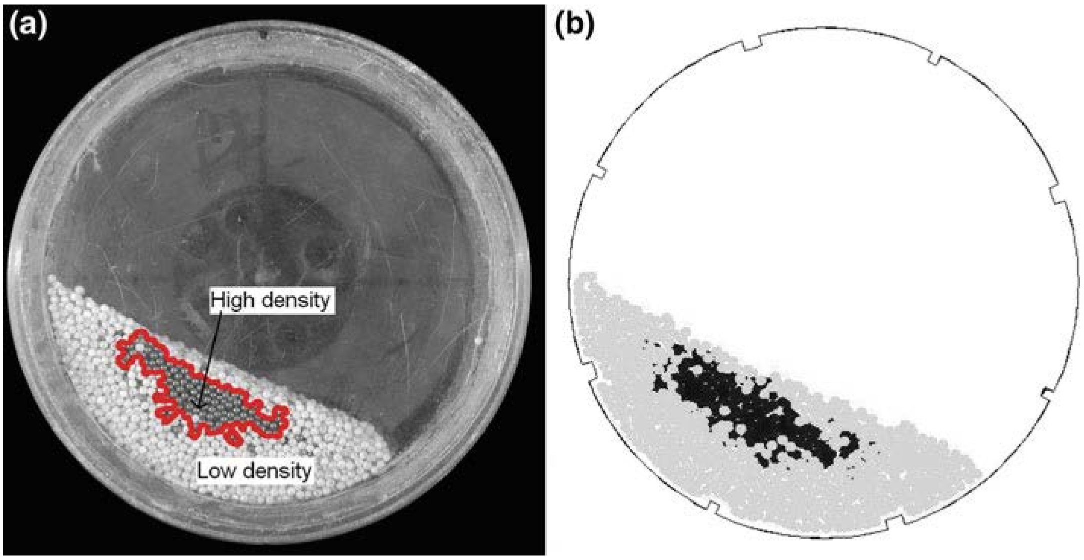

Figure 1. Particle distributions for density segregation for a cylinder fill fraction of 0.3 after 2 revolutions of the tumbler. a) Experimental result, and b) DEM result (Pereira et al, 2011). The red line in the experimental photo is used to calculate radial segregation fractions.

To make this comparison more quantitative, the normalized radial area is used. It is calculated as follows for both experiments and DEM. Snapshots of the particle distribution are taken at (small) regular time intervals (0.0625 revs). After two revolutions a boundary is defined around the main core of heavy particles (see red curve in Fig. 1a). This asymptotic boundary is subsequently superimposed on all earlier states, for both the experiment and the simulation, to determine the proportion of heavy particles currently enclosed within this boundary. The normalized radial area is defined as the number of heavy particles within the red boundary divided by the total number of particles.

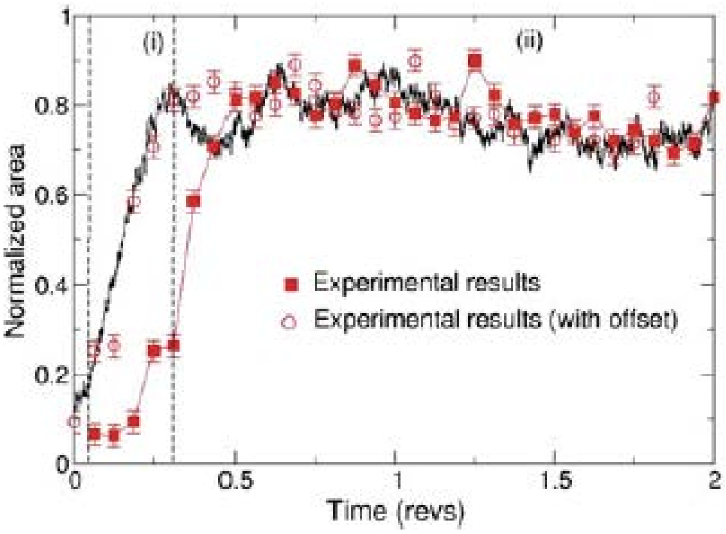

Figure 2. Radial segregation measure as a function of time (revolutions). The symbols are from experiment and the black line from DEM.

The evolution of the radial normalized area for both the simulation and experiment are shown in Fig. 2. The simulation exhibits a rapid increase (within 0.3 revs, region i) to around 0.8. After this (region ii) it tends to fluctuate about 0.75 and after two rotations has the value of 0.82. The comparison of the radial normalized area between simulation and experiments is excellent. Both show distinct temporal regimes in the segregation process. In the initial, rapid segregation regime, both simulations and experiments grow at the same rate and over the same period of time. Once they enter the equilibrium regime, they both show fluctuations of similar amplitude about their similar mean (plateau) values and have final values which are very similar. The main difference between simulation and experiments is when the initial slope failure occurs. For simulations this occurs earlier than for the experiments. In Fig. 2 we have also displayed the experimental results with a time offset of −0.1875 revs to account for the different time of flow initiation. With this offset accounted for the comparison is extremely good. The reason for this timing difference is that the DEM particle bed achieves it first failure much earlier than does the experiment. We postulate that this is due to particle shape – the DEM particles are exactly spherical while the experimental particles are fairly round but not exactly spherical. It is well known that spherical particle roll much more easily than even slightly non-round particles and a heap of such particles will form a stronger structure in contrast to spherical particles. Hence it is not surprising then that in DEM simulations, failure of the granular bed occurs earlier than in experiments. It is important to note though that the small shape differences do not affect the nature of the flow or segregation once initial slope failure has occurred.

Comparisons for other fill levels have also made, showing good overall agreement between DEM and experiments [7]. In these DEM simulations, the Froude number and the density ratio between the particle pairs was also systematically varied in order to study the functional dependence of the density segregation on these factors. A significant amount of density segregation is possible only for Froude number less than around 10^{-3}. Above this value, too much energy is supplied to the granular bed (from the cylinder rotation) which inhibits density segregation. The buoyancy mechanism is observed to become dominant over particle diffusion for density ratios above 2 leading to strong segregation of the particle bed.

3 SIZE SEGREGATION

Consider next binary granular mixtures which differ only in their size (the particles densities are the same and their shapes are spherical). Segregation of the granular mixture occurs via a mechanism known as *percolation* whereby the smaller particles percolate down through the gaps between the larger particles. Although this effect has probably been known for many centuries it was first detailed for granular mixtures undergoing vibration and termed the Brazil nut effect [22]. Although vibration and shear flow differ somewhat in the details of their dynamics, the flowing top layer of the granular bed provides sufficient relative motion between particles to induce percolation of the smaller particles. For mixtures where particles differ in size only we obtain a core of small particles surrounded by a corona of large particles (see Fig. 3).

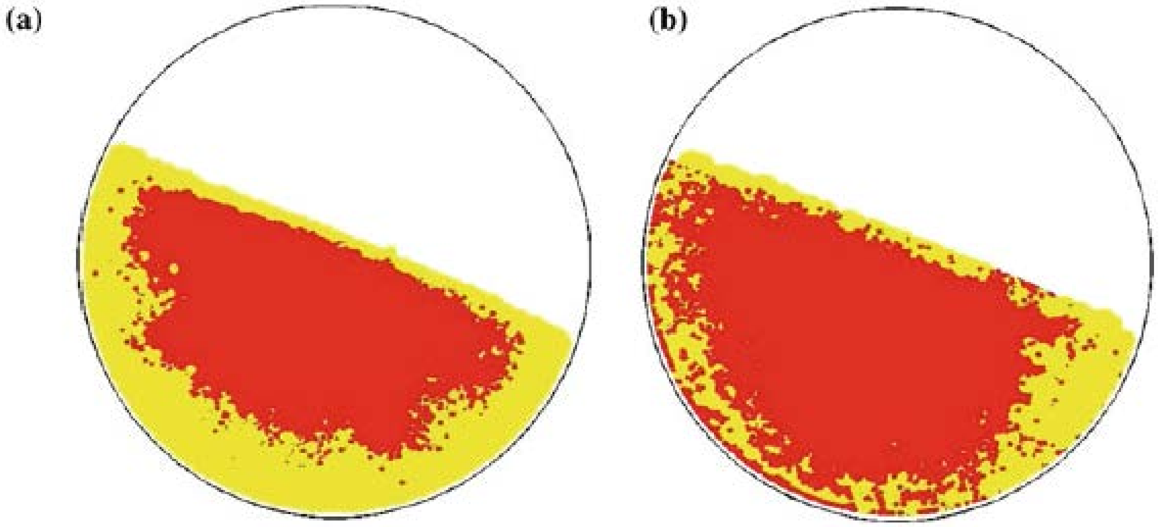

Figure 3. Equilibrium distribution of particles after 5 revolutions for different size (same density and spherical) binary granular mixture. Yellow represents large particles while red represents smaller particles. a) 1 mm and 2 mm diameter particles, and b) 1 mm and 4 mm diameter particles.

Figure 3a shows the segregation pattern after 5 rotations of the cylindrical tumbler for particles with a size ratio of 2 (ratio of radii). Here we see quite pure segregated states evolve with the small particles occupying a core region (which is almost pure red) and the large particle forming a corona region (almost pure yellow). However, note when the size ratio increases to 4 then the large particle region becomes less pure than occurs for a size ratio 2. This counter-intuitive result comes about from the fact that now the small particles are so small they have percolated to the bottom of the container, through the corona region. To understand the difference between the two cases, one should recognize that particles are packed together well in the coronal region. So for size ratio 2, this packing prevents “leakage” of smaller particles from the core into the corona, while for size ratio 4, even this close packing is not small enough to prevent small particles leaking through the pore network from the core to the corona.

Segregation of ternary granular mixtures (i.e. three different sets of particle sizes) was also modelled via DEM [19]. For example, Fig. 4 shows the segregated mixture after 5 cylinder rotations. Here we have used particle diameters 1 mm (blue), 2 mm (red) and 3 mm (yellow). As one might anticipate the smallest particles (blue) might migrate to the inner core, and the largest particles (yellow) migrate to the corona while the intermediate sized particles (red) are more or less found in between the other two. For different combinations of particle sizes, this segregation behaviour remains broadly similar for the smallest and largest particles, but the behaviour of the intermediate size particles is found to depend on their size ratios to the other two sizes and can accordingly be more dispersed through one or other of the two regions, see for example Fig. 4b for particle sizes 1, 2 and 4 mm.

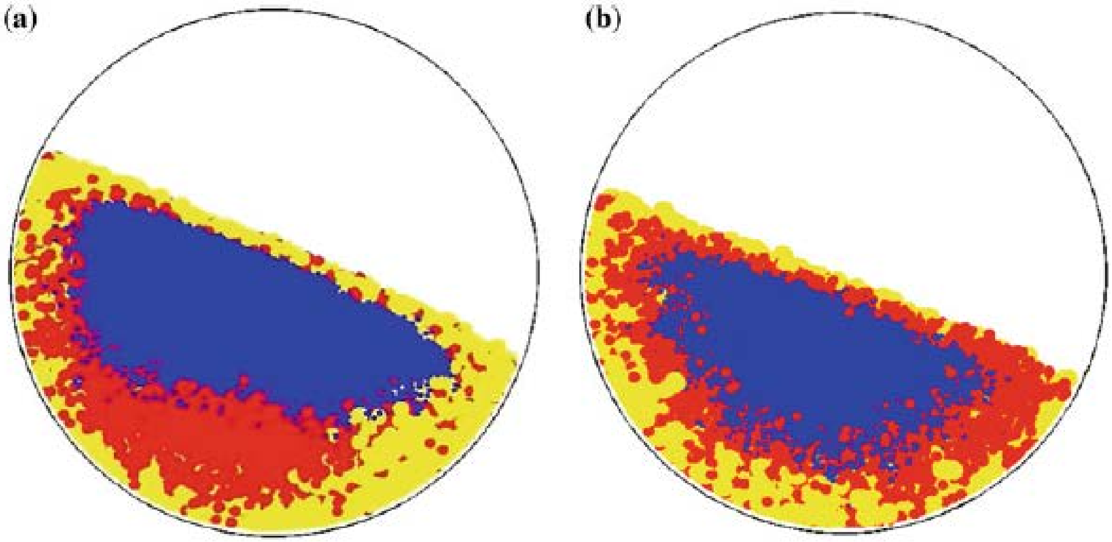

Figure 4. Equilibrium distribution of particles (after 5 revolutions) for a ternary granular mixture of different sizes (but with same density and spherical) particles. Yellow represents the largest particles, blue represents the smallest particles and red are intermediate sized ones. a) Particle diameters are 1 mm, 2 mm and 3mm, and b) particle diameters are 1 mm, 2 mm and 4 mm.

The amount of radial segregation was evaluated quantitatively by obtaining a (normalized) average of each particle type in 2 mm thick annuli from the cylinder centre, once equilibrium was established. This is shown in Fig. 5a, for a mixture with particle sizes 1, 2 and 3 mm. The smallest particle size has a peak close to the scaled radius of 0.2 (corresponding to the core) while the largest particles have a peak at scaled radius of around 0.95 (corresponding to the corona) with the intermediate size particles having a peak around scaled radius of 0.7 (which is in between the other two regions). To determine the strength of the competing mechanisms, one may compare this radial with the theoretical continuum model of Gray and Ancey [15]. While the details of the continuum model are too detailed to be given here, it focuses on the upper flowing (shear) layer and includes advection, diffusion (due to particle collisions) and segregation (due to particle size differences). The continuum model then involves four phenomenological parameters – a diffusion constant and three (binary) interaction terms which control segregation. These can be varied so that the segregation profile matches the DEM radial segregation profile (see Fig. 5b). The match between the two profiles is adequate which validates the dominant competing mechanisms (percolation and diffusion).

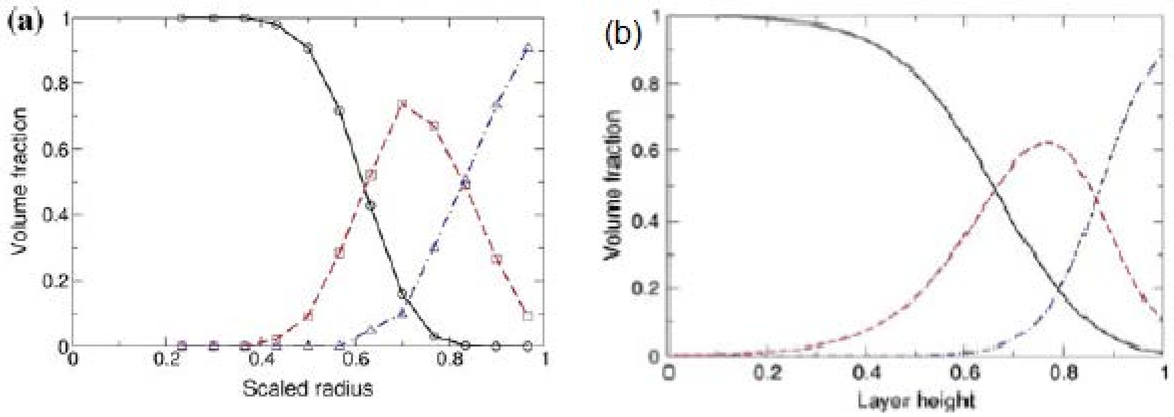

Figure 5. a) DEM volume fraction (of different sizes) as a function of distance from the cylinder centre (averaged over the axial direction) for the ternary mixture in Fig. 4a (1, 2 and 3 mm diameter particles). Circles – smallest particles, squares – intermediate particles, triangles – largest particles. Curves are guides for the eye. b) Results from Gray and Ancey's (2011) continuum model for different particle size mixtures. We have chosen he four coefficients so that the result is close to that shown in Fig. 5a. Black solid curve – largest particles, red dashed curve – intermediate particles and blue, dot-dashed curve – smallest particles.

4 SHAPE SEGREGATION

Now consider a binary granular mixture where particles differ only in their shape (their sizes and density being the same, with particles having the same *a* value in Eq. 1). Here we use particles which are either spherical or blocky (i.e. with an *n* value in Eq. 1 which is greater than 2). Figure 6 shows the segregation pattern for a binary granular mixture of particles of different shape after 9 rotations of the cylinder. In Fig. 6a we have a core of more blocky particles ($n = 4.55$, red) and a corona of spherical particles (blue). However, in contrast to size and density segregation we see that the boundary between the two particle types is quite diffuse, with red particles still distributed throughout the blue region and vice-versa. For a granular mixture with a higher ratio of *n* values (see Fig. 6b) it is now observed that the core and corona regions are more pure (here the red particles have an *n* value of 10.05, while the blue particles are spheres).

While the buoyancy mechanism underlies density segregation and percolation underlies size segregation, what gives rise to the segregation in the case of shape? We postulate that this relates to *flowability* of each particle shape [21]. As the cylinder rotates, the two types of particles are transported up to the top of the inclined free surface layer. At this point both sets of particles are at the same height, and so have the same amount of gravitational potential energy. As they begin their descent down along the flowing layer, the spherical particles travel faster than do the more blocky particles. The more blocky particles dissipate their available potential energy more quickly and so both travel more slowly and come to rest earlier within the flowing layer. At this point, other particles (mainly spherical ones) flow over them burying them at the bottom of the current shear layer. Over repeated passes through the shear layer the blocky particles move progressively towards the center to form a core region for the particle bed. Meanwhile the spherical particles which on average dissipate their potential energy more slowly have higher flow speeds in the surface shear layer and are typically able to reach the bottom of the slope and build up against the wall of the cylinder.

They are then transported around the cylinder, via rigid body rotation of the main bed. This shape segregation occurs within the top, flowing layer and provides a downward dynamic pressure in a continuum interpretative sense that causes them to migrate towards the core.

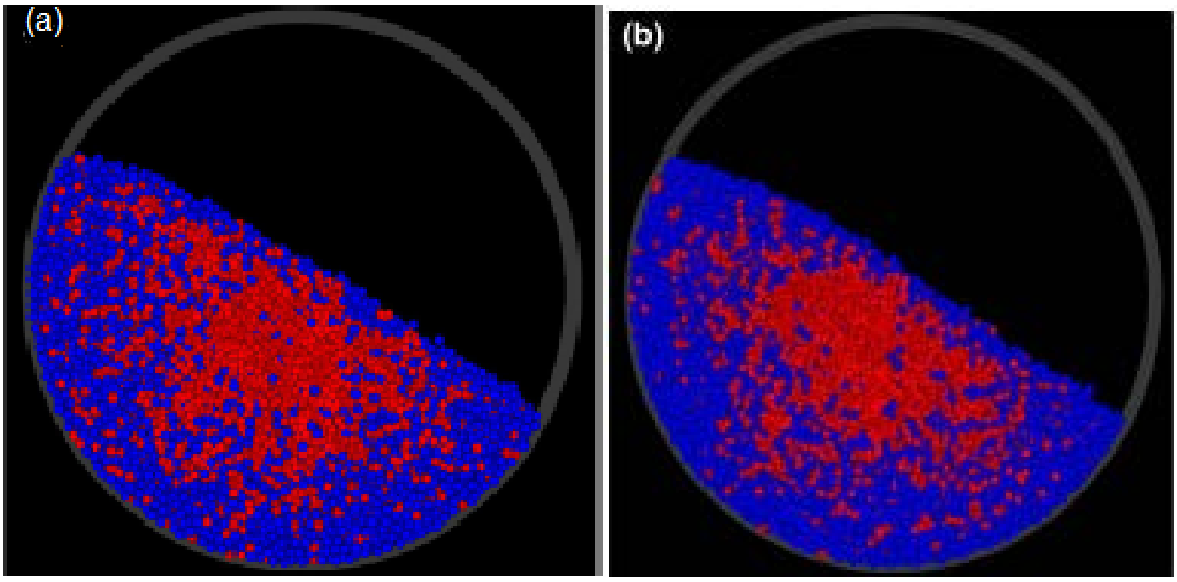

Figure 6. Particle distribution for binary mixture where particles only differ in their shape after 9 revolutions. a) spherical (n = 2) shown as blue and rounded cubical (n = 4.55) shown as red, and b) spherical (n = 2) shown as blue and sharp cubical (n = 10.05) (red).

The operation of this segregation mechanism was demonstrated by evaluating the surface layer speeds of the two particle types (spherical and blocky). At each time step during a DEM simulation, we evaluated (using only particles in the upper flowing layer): (i) the percentage of time that spherical particle had a speed greater than the blocky particle, (ii) the average differential in speed between the two particle types, and (iii) the average spread (standard deviation) in the average differential speed between the two particle types. The results are shown in Fig. 7 (with the left axis showing the percentage of time and the right axis showing the average differential speed) for four different shape ratios. For small shape ratio, the spherical particles 60% of the time have a larger speed than the blocky particles but at large shape ratio this increases to about 95% of the time. The speed differential (spherical particle speed – blocky particle speed) is 1.8 mm/s (with a spread of 6.6 mm/s) at the smallest shape ratio (of 1.25) but rises to 23.4 mm/s (with a spread of 13.6 mm/s) for the largest shape ratio (of 4.95) considered. These clearly indicate that for significantly blocky particle (i.e. large n) not only do the spherical particles *consistently* travel faster down the flowing layer than the blocky particles, they do so with a *significantly* larger surface speed. These differences then control the deposition location on the slope for each shape which drives the inward migration of the blockier particles.

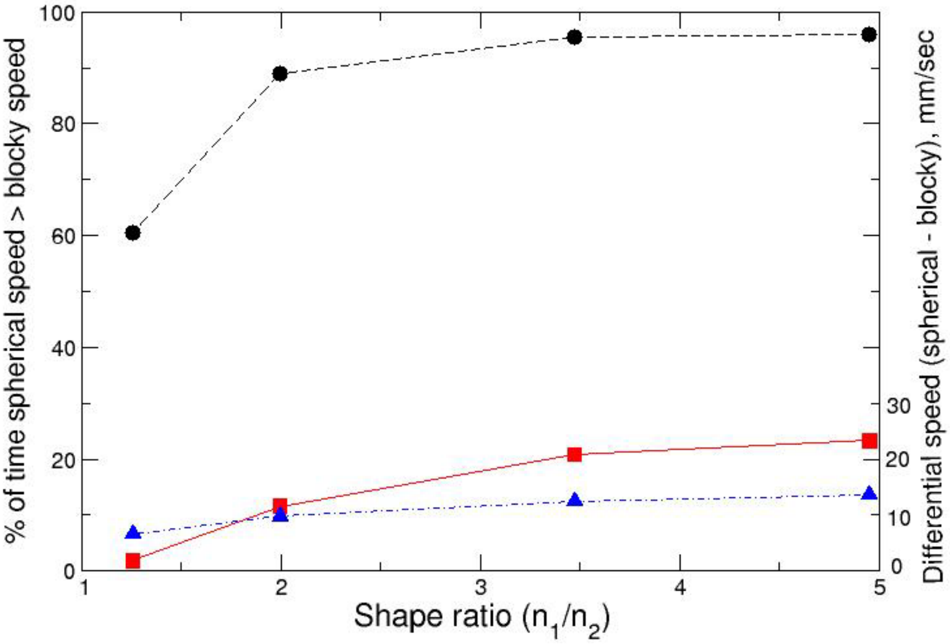

Figure 7. Difference in speeds between the two particle shapes (spherical and blocky) in the top, surface layer as a function of the shape ratio. The black circles are the percentage of time the spherical particles have a larger speed than the blocky particles (left axis). The red squares are the average differential speed in the surface layer between spherical and blocky particles and the blue triangles are the spread in average differential speed (right axis). Curves are drawn as guides for the eye.

5 COMPARISON BETWEEN DENSITY, SIZE AND SHAPE SEGREGATION

These DEM simulations have been not only able to determine the stable segregation patterns for granular mixtures which may differ either in particle density, size or shape but also other quantitative information. Here we can summarise the main outcomes as follows

- Size segregation appears to be the strongest of the three segregation mechanisms, closely followed by density segregation and both are much stronger than shape segregation. It was found that size segregation could lead to relatively pure core and corona regions, but only for a small range of particle size ratios – the ratio of radius of the big particles to small particles should be less than approximately 3. If the particle size ratio is greater than 3, leakage occurs which limits the segregation extent.
- Density segregation generally increases monotonically with particle density ratio. In shape induced segregation one never obtains pure regions of either particle type.
- The kinetics of segregation are equally fast for size and density segregation and slow for shape segregation. It takes of the order of 10 cylinder rotations before the (asymptotic) steady state is reached for shape segregation, while for the other two mechanisms it takes only 2-4 rotations. This correlates with the strength of segregation (above).
- For shape segregation the interface between regions is typically rather diffuse while it can be quite well defined for the other two.

- Segregation occurs *along* the top, flowing layer for shape segregation, while for size and density segregation it occurs *through* this top layer.

6 CONCLUSIONS

Intrinsic, micro-scale particle properties have been shown to play a vital role in the segregation of granular mixtures. Three specific properties have been studied in this work – those being particle density, size and shape. Each has a corresponding physical mechanism which underlies the granular segregation process that it drives. These are buoyancy for mixtures of different density, percolation for mixtures of different size and flowability for mixtures of different shape. In fact the last mechanism of flowability should also applies to particles with different surface roughness. Surface roughness has two contributions – macroscale roughness (which typically is described as being the shape of the particle) and microscale roughness (which is interpreted as the particle friction). So in a mixture of particles with different surface roughness, it would be expected that the rougher particles would segregate to the inner core.

The three segregation mechanisms have been compared and we have seen that size and density segregation are the strongest, with the segregation typically occurring within 2-3 cylinder rotations for this system. They also lead to fairly pure segregated regions (small or dense particles in the core and large or less dense particle in the corona). In contrast, shape segregation is much weaker, with a core of the more blocky particles and corona of the spherical particles forming after 5-10 cylinder rotations. Here the interface between segregated regions remains quite diffuse with many blocky particles dispersed in the corona and vice-versa. Whilst both density and size segregation evolve by particles moving through the upper surface, flowing layer shape segregation occurs when particles move with different speeds along this upper surface layer.

We have compared selected results with experiments and found excellent agreement. Some results were compared with continuum theory, so as to identify the strength of macro-scale mechanisms, and with appropriate choices of the phenomenological constants we have been able to achieve satisfactorily agreement between theory and simulations. The DEM technique has been shown to be ideal in understanding micso-scale details of granular segregation. For example calculation of the surface layer velocities for the different particle types can be readily done virtually, but with much more difficulty in experiments

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