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Axial Segregation in Horizontally Vibrated Granular Materials: A Numerical Study

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Abstract

It is known that a horizontally vibrated binary mixture in a tapered and inclined channel segregates axially, with the two species moving to the opposite ends of the channel. In general, the parameters that affect the segregation process include the forcing frequency and its amplitude, the constituents' mass and size, and the taper and inclination of the channel. The ultimate goal here is to locate those parameters that are most significant to the segregation process, thereby providing control variables for practical applications. However, owing to the complexity of the problem, as a first step to better understand the physics behind this phenomenon, we undertake three dimensional molecular dynamics simulations of a horizontally vibrated mono-disperse granular particles in a tapered and inclined channel. Though at this stage, the immediately addressed problem is of more relevance to the granular material industry, it is envisaged that tools developed to understand this process will ultimately have wide applicability to granular systems, occurring in both natural contexts and in geotechnical engineering.

Keywords: *molecular dynamics, granular materials, segregation*

1. Introduction

Granular materials are ubiquitous. In everyday life, we come across many things that count as granular materials, like wheat, corn flakes, rice, coal etc. These materials possess peculiar properties that are not displayed by the conventional substances, e.g., they may behave like solids, liquids or gases depending upon applied external conditions (Jaeger *et al.*, 1996). In addition, there are many other phenomena unique to these substances. It is observed that granular mixtures tend to segregate into their constituent species, when vibrated externally. A common example is the '*Brazil-nut Effect'* (Rosato et al., 1987) in which a large particle separates to the top, when a collection of small particles and a large particle is vibrated vertically. However, under different conditions the same big particle sinks to the bottom of vertically shaking container, thereby demonstrating the '*reverse Brazil-nut Effect*' (Shinbrot and Muzzio, 1998; Shinbrot, 2004). It is not always the case that particles segregate only in the vibrating direction. There are systems, in which particles segregate in a direction transverse to the direction of vibration (Levanon and Rapaport, 2001; Rapaport, 2001). This is also a feature of our system. Because segregation plays a very important role in the granular material industry, significant effort has been invested to understand this phenomenon. It is important to emphasize that any insight and/or tools that we may develop while investigating the present problem, will transfer seamlessly to problems that are of a more geophysical nature. Segregation is as important a process in nature, as it is in the industry, with common examples being avalanches and pyroclastic flows. In a geotechnical context, granular drains and granular laboratory samples frequently segregate.

It is observed that a granular mixture segregates axially in a horizontally vibrated channel, which is slightly inclined to the ground. This channel has a zigzag internal profile (see Fig. 1) whose effect is the segregation of light and heavy particles in up and down directions, respectively. Typically, a mixture of heavy and light grains is poured into the centre of the channel (see Fig. 1) which, as shown, is vibrated in a direction perpendicular to the channel's axis. It is observed that the heavy and light grains move towards the lower (A) and higher (B) ends, respectively. The separation achieved is nearly faultless.

As the reader will appreciate, the segregation process described above is a complicated one, due not only to the presence of two different species and their mutual interactions, but also with the channel's complex geometry. In order to ultimately arrive at the simplest model that captures the essential features of this segregation phenomenon thereby identifying important control parameters, we proceed by breaking the problem into a series of

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simple testable hypotheses.

We begin by first conjecturing that the channel's Christmas-tree pattern is really a concatenation of small trapezoidal chambers as shown in Fig. 1, with each chamber acting as a micro-sorter.

The sorting itself is hypothesized to be a result of the competition between gravity, which pulls material down towards the lower narrow end of the trapezium, and the collisional momentum transfer from the tapered walls that is biased upwards. The subject of this paper is to explore the behaviour of a monodisperse aggregate in a tapered and inclined chamber (as shown in Figs. 2 and 3) that is vibrated perpendicular to its axis.

We undertake three-dimensional Molecular Dynamics (MD) simulations (Allen and Tildesley, 1987; Poschel and Schwager 2005; Rapaport, 2004) to follow the dynamics of a monodisperse collection of spheres in a tapered and slightly inclined channel, as shown in Figs. 2 and 3. We explore the effects of vibration amplitude, friction coefficient, and the channel's inclination on the flow of grains at various driving frequencies. This will help identify important parameters that may play a role when we investigate a binary mixture of grains.

The rest of the paper is organized as follows. In Sec. 2, a

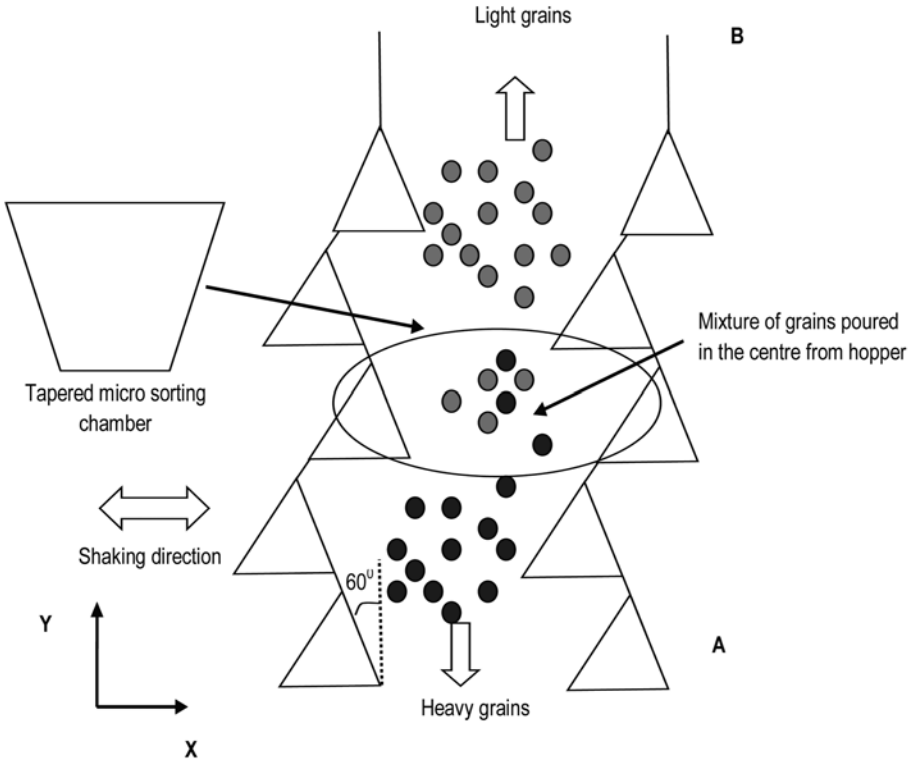

Fig. 1. The Geometry of a Segregating Channel in an Actual Grain Sorter (End A is at lower elevation than end B.)

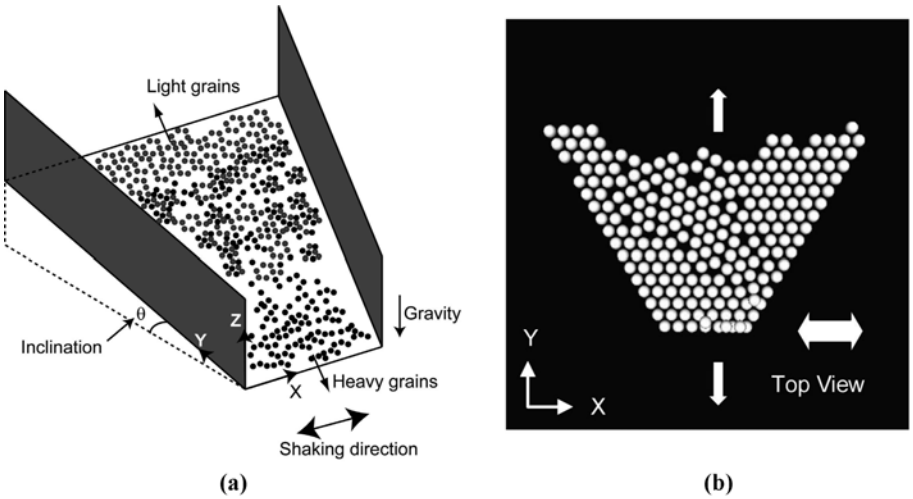

Fig. 2. (a) Three Dimensional View of Shaking Channel, (b) Initial Configuration of Grains in the Simulation

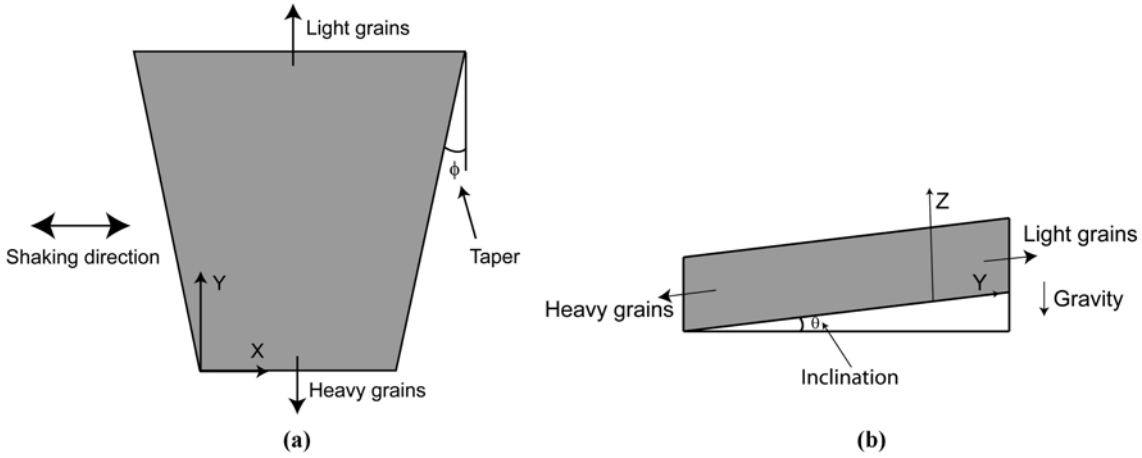

Fig. 3. Geometry of the Shaking Channel (a) Top View (b) Side View (Looking along the vibration axis)

complete description of the force schemes and parameters employed in the Molecular Dynamics simulation is provided. Simulation results are discussed in Sec. 3, and we close with outlines of future and ongoing work.

In passing, we mention that segregation is often a multi-component phenomenon, while our system involves only two species. However, we believe that the computational framework, able to address two components, will with minor modification be also able to handle more species.

2. Simulation Methodology

We model contact between spheres through a Lennard-Jones potential (Allen and Tildesley, 1987; Rapaport, 2002). A cut-off distance is introduced to model the fact that no interaction takes place between non contacting grains. The Lennard-Jones force within the cut-off range between particles located at $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$, with diameters σ_i and σ_j, is

$$\boldsymbol{F}_{LJ} = \frac{48\varepsilon}{r_{ij}}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - 0.5\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]\hat{\boldsymbol{r}}_{ij}, \tag{1}$$

where $\boldsymbol{r}_{ij}=\boldsymbol{r}_i-\boldsymbol{r}_j$, $r_{ij}=|\boldsymbol{r}_{ij}|$ and $\sigma_{ij}=0.5(\sigma_i+\sigma_j)$ is the mean diameter of two particles, and ε is depth of the potential well. We take the cut off distance to be $r_{cut}=2^{1/6}\sigma_{ij}$. Fig. 4 illustrates the geometry of two colliding particles.

During collisions, dissipation is accommodated by introducing a normal and a tangential dissipating force (Rapaport, 2004). The former is given by

$$\boldsymbol{F}^{n}_{damp} = -\gamma_n(\hat{\boldsymbol{r}}_{ij}\cdot\boldsymbol{v}_{ij})\hat{\boldsymbol{r}}_{ij}, \tag{2}$$

where $\boldsymbol{v}_{ij}=\boldsymbol{v}_i-\boldsymbol{v}_j$ is the relative velocity between two colliding particles, and γ_n is the normal damping coefficient. The normal force on the particles along $\hat{\boldsymbol{r}}_{ij}$ thus becomes

$$\boldsymbol{F}^{n} = \boldsymbol{F}_{LJ}+\boldsymbol{F}^{n}_{damp}. \tag{3}$$

There are cases when the normal force between two grains comes out negative (Zhang and Whitten, 1996; Poschel and Schwager, 2005) which should not happen, as dry granular particles don't attract each other. To avoid this situation, we set normal force to zero whenever it becomes negative. The tangential damping force is taken to be

$$\boldsymbol{F}^{t} = -\min(\mu|\boldsymbol{F}^{n}|, \gamma_t|\boldsymbol{v}^{t}_{ij}|)\hat{\boldsymbol{v}}^{t}_{ij}, \tag{4}$$

where γ_t is a tangential damping coefficient, μ is the friction coefficient, $\boldsymbol{v}^{t}_{ij}$ is the component of relative velocity in the direction of the common tangent of two contacting particles and is given by

$$\boldsymbol{v}^{t}_{ij} = \boldsymbol{v}_{ij}-(\boldsymbol{v}_{ij}\cdot\hat{\boldsymbol{r}}_{ij})\hat{\boldsymbol{r}}_{ij}-\left(\frac{\sigma_i\boldsymbol{\omega}_i+\sigma_j\boldsymbol{\omega}_j}{\sigma_i+\sigma_j}\right)r_{ij}, \tag{5}$$

where $\boldsymbol{\omega}_i$ is the angular velocity of the i^{th} particle. $\boldsymbol{F}^{t}$ is the tangential force along the direction of the common tangent of two colliding particles. The above damping force is simply a less singular version of the classical dry Coulomb friction model, and

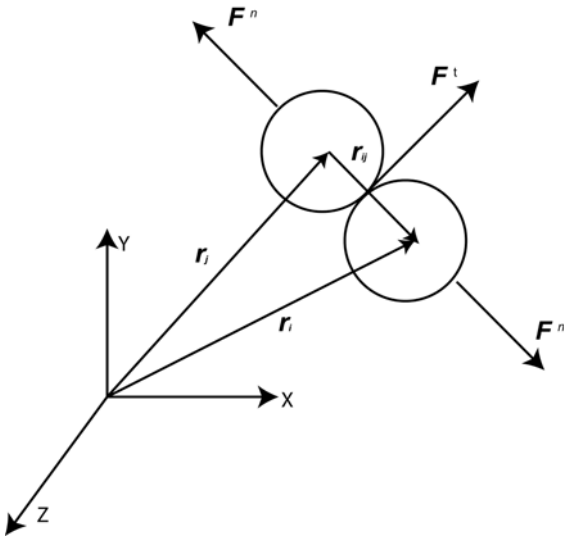

Fig. 4. Contact between Two Particles

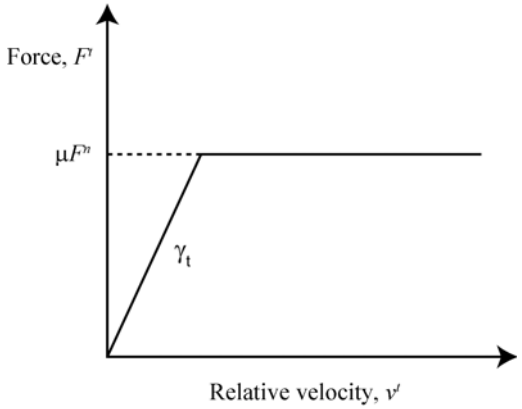

Fig. 5. Coulomb Friction Model: A Limiting Friction Force to Prevent Sliding between Particles

is shown in Fig. 5.

A similar approach is adopted to model the interaction of particles with the channel's surface and walls. When a grain comes within the cut-off range of a wall, a virtual particle is created at the foot of the perpendicular dropped from the colliding grain on to the wall (see Fig. 6).

This construction ensures that the radial force experienced by the incoming grain is indeed normal to the wall, as should be the case. Here we assume that this virtual particle has similar properties to the ones in the mixture, however, this is a simplifying but not necessary assumption. The colliding grain now interacts with the wall particle according to the collisional framework developed above.

Several simulation runs were carried out employing 216 particles. The initial configuration is first generated by arranging the particles in a lattice above the channel, and then allowing them to fall under gravity (Poschel and Schwager, 2005). This was done by running the simulation separately. The initial configuration thus generated was stored, and each subsequent simulation was carried out with this same arrangement, and zero initial velocities.

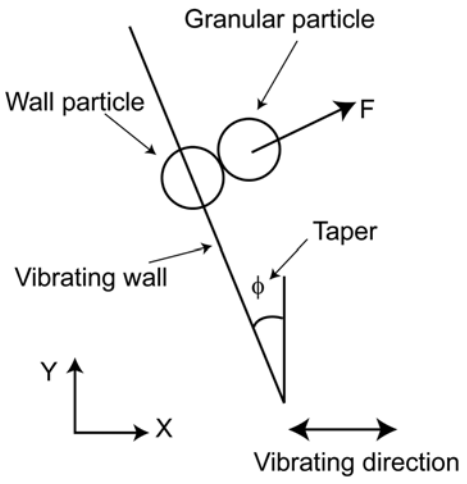

Fig. 6. Grains' Interaction with System's Boundary Wall

Now we list the different computational routines employed in our simulation. The Leap-frog integration algorithm (Allen and Tildesley, 1987) is utilised for numerically following the grain's velocities and positions. The Metropolis Algorithm (Metropolis *et al.*, 1953) is used for inserting particles into the channel to compensate for grain's lost from the channel's ends. Particles are inserted by randomly placing them in a fixed volume at some height above the channel's surface. By this process we balance the influx and the efflux, thus maintaining steady state.

For more generality we non-dimensionalize the length by the diameter s of the sphere and time by (Rapaport, 2002).

$$t^{su} = \sqrt{\frac{g\sigma}{10}} \tag{6}$$

where g is a scaling factor. For value $g=5$ and diameter 3.175 mm used in simulation, one time unit corresponds to approximately 0.04 s. Thus, a frequency of 10 Hz corresponds to a non-dimensional value of 0.4.

We next describe the channel's physical characteristics. The side wall's height (along the Z direction) is taken to be infinite. The upper and lower cross-sectional width of the channel is taken to be 30 and 8 particle diameters, respectively. The channel's taper is kept fixed at 30 degrees, however, the inclination is varied.

Validation tests were conducted to check the code's accuracy, and also the dependency of system response on the force model. A channel with parallel side walls (see Fig. 7) is vibrated horizontally. Interaction between the grains is modelled by employing the Hertzian contact force model (Johnson, 1985) and the Lennard-Jones potential. Flow rate of particles is plotted against vibration frequency in both cases, as shown in Fig. 8. We observe that the variation in flow rates from ends A and B, for both force models, almost coincide, so that the net flow rate is nearly zero. This shows that the system's behaviour is independent of the force model, and also gives us confidence in the correctness of our code. The flow rate from one end, say A, of the channel is measured by the ratio of the number of particles leaving the system from that end per unit time to the total number of particles in the system. The net flow rate is the difference between the flow rates of particles from both ends.

In addition to the above tests, we employed our code to recover the results of an experiment (see Fig. 9) due to Blair and Kudrolli (2003). In their experiment, a collection of balls is vibrated in an inclined direction. Because this is a similar set-up to our problem, their experiment provided a good testing ground for our code. The density profiles obtained, as shown in Fig. 10, have the same qualitative form as observed by Blair and Kudrolli (2003). Quantitative difference is due to our utilizing rubber balls in our simulations instead of the steel balls that they employed in their experiment. This is because the very high stiffness of steel makes computation ill-conditioned with steel balls. Further, fluctuations seen for simulations done at higher inclination and larger system size is due to the errors associated with the averages. To obtain more accurate values for big system size, a large number of

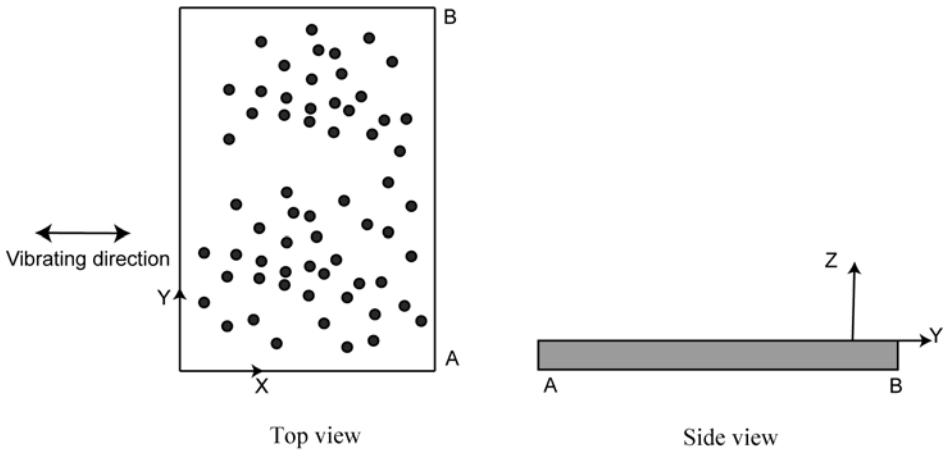

Fig. 7. Geometry of a Horizontally Vibrated Channel with Parallel Side Walls Employed in the Simulation (Channel is open at ends A and B, and not inclined to the ground.)

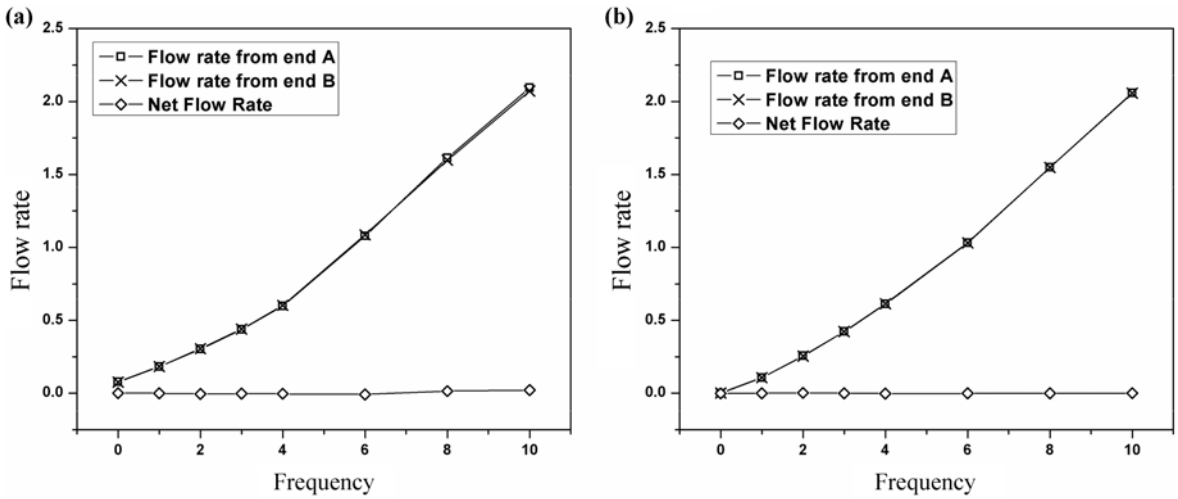

Fig. 8. Flow Rate of Particles in a Horizontally Vibrated Channel with Parallel Side Walls, Not Inclined to the Ground (The contact between grains is modeled by employing the (a) Lennard-Jones Potential, and the (b) HertziaN Contact Force Model. Vibration frequency is in Hz.)

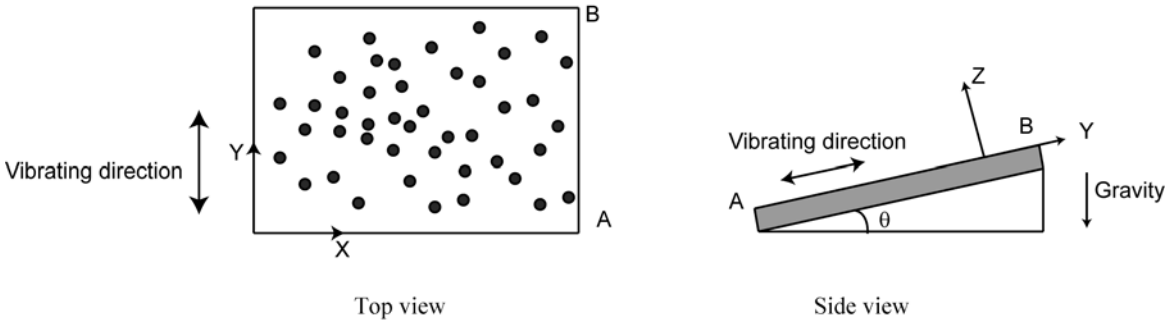

Fig. 9. Experimental Setup of Blair and Kudrolli (2003), cf. Fig. 1 (Top (B) and bottom (A) ends of vibrating plate are closed, i.e., there is no influx or efflux of grains in the system.)

sampling is required. We defer an in depth analysis of system size effect for a future investigation. Other than this, we successfully tested our code along the lines suggested in Asmar *et al*. (2002).

3. Results and Discussions

Fig. 11 shows the variation of net flow rate with the frequency at different vibration amplitudes, and a fixed friction angle $\alpha =$ 26.56°, so that the friction coefficient $\mu = \tan\alpha = 0.5$. We note that

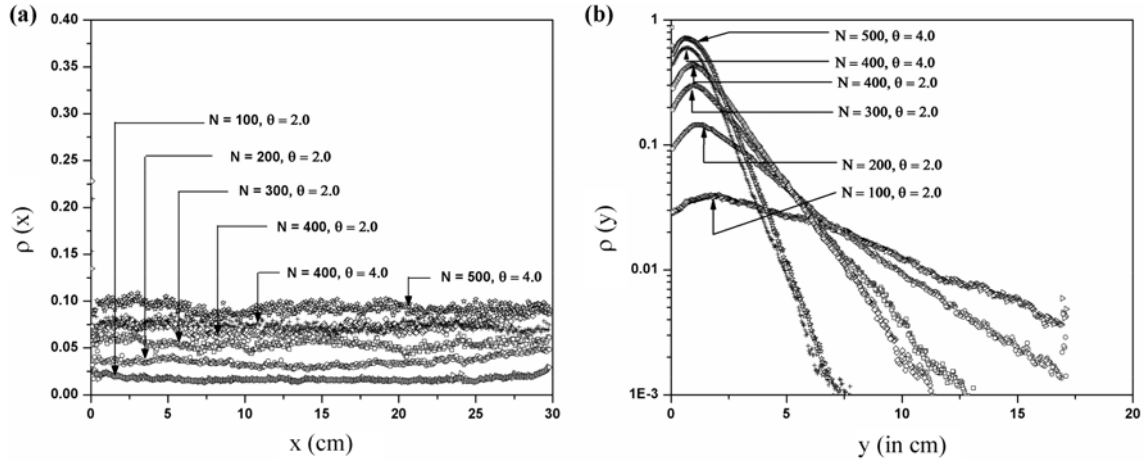

Fig. 10. (a) Density Profile of Grains on a Linear-linear Scale Transverse to the Vibrating Direction, (b) Density Profile of Grains on a Log-linear Scale in the Direction of Vibration

at low frequencies, most of the mass moves down. As the frequency increases, so does the amount of collisional upward momentum transferred to the grains by the channel's tapered walls. Thus, at higher frequencies the grains move upwards preferentially, so that the net flow rate becomes negative. We call the frequency at which flow reversal occurs, the critical frequency ν_{cr}. In Fig. 11, by extrapolating the curve for amplitudes less than 2.5 particle diameters, it is seen that the critical frequency decreases with an increase in the vibration amplitude A. This apparent behaviour is also expected as the physics suggests that the rate of upward collisional momentum should increase as $\nu^2 A$. An interesting feature in Fig. 11 is that there is a sudden drop in the net flow rate at a frequency of 0.1 and it remains almost constant until frequency of 0.15. We believe that this behaviour may be due to the mono-disperse spheres arranging themselves in a regular pattern at low frequencies. This allows long-range transfer of momentum from the walls, which increases the tendency of the mass to move upwards, thereby lowering the net flow rate. Beyond a frequency of 0.15, the net flow rate begins to increase with vibration frequency until it reaches a maxima. Subsequently it decreases again continuously. The frequency at which the net flow rate begins to decrease again is called the changeover frequency. It is clear from the Fig. 11 that the changeover frequency increases with the decrease in vibration amplitude. We believe that as the frequency increases, the regular arrangement of grains breaks down, and the system goes into a disordered state that is affected to a lesser extent by collisions with the channel's walls, subsequently leading to a decrease in the upward flow rate. This is reflected in an increase in the net flow rate between the frequency of 0.15 and the changeover frequency. However, as the driving frequency continues to increase, the upward movement must ultimately increase, and this does happen beyond changeover frequency. In other words, the ordered state of grains disappears completely after this changeover frequency. A more detailed analysis is required to study the behaviour of ordered/disordered state of the granular system. Also, calculations for appropriate correlations are needed to justify the phenomenon of systematic arrangement observed in the system, and we are in the process of doing so.

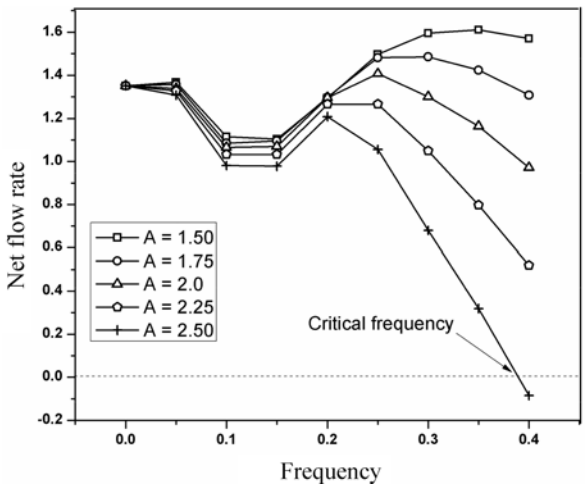

Fig. 11. Variation in the Net Flow Rate of Grains with Frequency at Different Vibration Amplitudes A (Friction angle (α) and channel's inclination (θ) is kept constant at 26.56° (μ= 0.5) and 2° respectively. Amplitude is in terms of particle diameters and a non-dimensional frequency of 0.4 corresponds to about 10 Hz. The net flow rate is the difference between the downward and upward flow rates of particles. Negative net flow rate indicates preferential upward motion and the net flow rate of one indicates that approximately 25 more grains are exiting the lower end per second compared to the upper end.)

We next explore the effects of friction on the net flow rate by running several simulations at the fixed amplitude of 2.0 particle diameters, which is shown in Fig. 12. It is apparent from Fig. 12 that an increase in the friction leads to a lower net flow rate at a fixed vibration frequency. The qualitative behaviour of variation in the net flow rate with frequency is similar for all friction angles and consistent with our observations for net flow rate

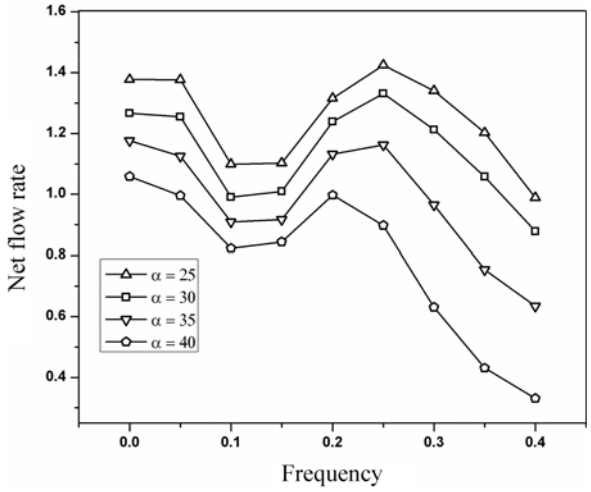

Fig. 12. Variation in the Net Flow Rate with Frequency for Different Friction Angles Keeping the Amplitude (A) Constant at 2.0 Particle Diameters and Channel's Inclination (θ) at 2° (Friction angle (α) is in degrees and a non-dimensional frequency of 0.4 corresponds to about 10 Hz.)

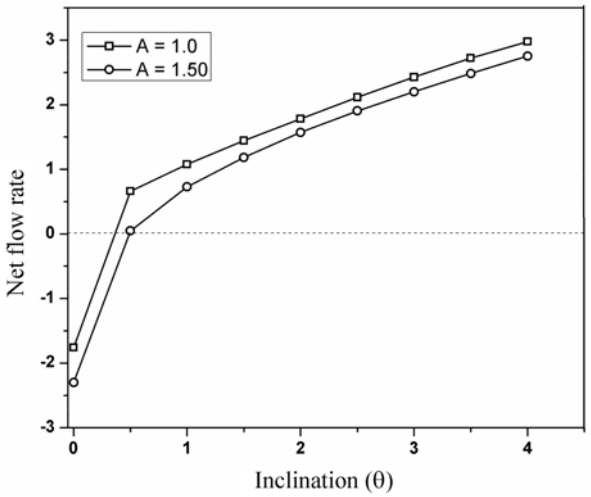

Fig. 13. Effect of Vibrating Channel's Inclination on the Net Flow Rate of Particles for Different Vibration Amplitudes at Constant Frequency of 0.4 (A non-dimensional frequency of 0.4 corresponds to about 10 hz. friction angle (α) is kept at 26.56° (μ=0.5) and inclination angle is in degrees.)

variation at different vibration amplitudes (see Fig. 11).

Finally, we explore gravity's role in this segregation process. Fig. 13 displays how the net flow rate varies with the channel's inclination (θ). As expected, the net flow rate increases, i.e., grains move down preferentially, with an increase in the inclination due to gravity's increased downward pull.

4. Conclusions

In this paper, we focussed on the effect of various parameters, i.e., amplitude A, frequency ν, inclination θ and the friction angle, on the net flow rate of mono-disperse grains vibrated in the slightly inclined tapered channel (see Figs. 1, 2, and 3). Based on our numerical simulations, following are our observations:

Critical frequency ν_{cr} is identified at which the net flow rate of the grains reverses. This critical frequency is seen to depend on the vibration amplitude and channel's inclination.

We also noticed that the dynamics of the system is very sensitive to inclination, indicating the need for its proper control.

We also observed several curious features that may be related to systematic arrangements. In the future, in addition to investigating the effects of taper, particle diameter and density, and packing fraction on the motion of mono-disperse spheres, we intend to simulate the dynamics of binary systems first in the trapezoidal geometry of Figs. 2 and 3, and then in the more intricate shape displayed in Fig. 1. This will test our earlier hypothesis regarding the geometry being simply a concatenation of micro-sorting chambers. Finally, efforts are underway to put in place an experimental set-up to corroborate and also provide insight into this problem.

Acknowledgements

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