A molecular dynamics simulation of segregation behaviours of horizontally vibrated binary granular mixture*

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This paper performs the two-dimensional, soft-sphere molecular dynamics simulations to study the granular segregation in a binary granular mixture with the same size but different density in the container with the sawtooth base under horizontal vibration. The segregation phase diagram is presented in the acceleration-frequency space. When the acceleration is high enough to result in relative motions of the particles, the system can be in various states (mixed state, vertical and horizontal segregation state), which depend on both acceleration and frequency. Due to the sawtooth base there is stratified flow effect besides density effect. The density effect raises the light particles. The stratified flow drives the particles in the upper levels to the right and the particles in the lower particles to the left, resulting in the appearance of the left segregation state. The left segregation state can be changed to the right segregation by changing the shape of the sawtooth. As the vibration frequency increases, the stratified flow effect becomes weaker and weaker, so at high vibration frequencies the vertical segregation state appears instead of the left segregation state.

Keywords: granular systems, segregation, molecular dynamics methods

PACC: 6475, 7115P, 4610

1. Introduction

Granular materials are composed of many solid particles, which are fundamentally different from any other type of matters, such as solid and liquid.[1] Of the many phenomena that granular matter presents under external excitation, one can observe the formation of clusters,[2,3] avalanches,[4,5] pattern formation,[6] surface waves,[7,8] and segregation.[9−16] Vibration-induced segregation of granular particles is one of the topics which has great application potential and has attracted the attention of many physicians and other scientists. Rosato *et al.*[9] showed that large particles in bi-disperse granular mixtures move to the top of the bed, which is the so-called Brazil nut effect (BNE), while the opposite one, known as reverse BNE that is, large particles sink into the granular bed, has also been observed.[11,13]

Granular media display a wide range of behaviour when vertically vibrated upon an asymmetric sawtooth-shaped base. In the experimental realization the grains is contained in a narrow annular region between two upright cylinders (this case is thus essentially two dimensional), Farkas *et al.*[17−19] observed the occurrence of horizontal flow. They found that the resulting material flow depends on the number of layers of particles and the driving frequency: under certain conditions increasing the layer thickness leads to a reversal of the current; the horizontal transport reverses with increasing frequency; the onset of horizontal transport as a function of dimensionless acceleration occurs gradually in a manner reminiscent of a phase transition. These results have also been confirmed by the simulations. Rapaport *et al.*[20,21] numerically produced stratified flows that large and small particles are horizontally driven in opposite directions which also depends on the elasticity of the grains. Thus under vertical vibration the ratchet base may result in two species of grains moving in opposite directions. Wambaugh *et al.*[22] numerically studied ratchet-induced segregation and transport of non-spherical grains. They demonstrated layer-by-layer variation in the average velocity as well as layer segregation of species and showed that horizontal separation of the species can be achieved by using the geometry. Distinct from the above saw-tooth base under

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vertical vibration, Gallas *et al.*[23] produced the similar horizontal flow in a flat base by combining horizontal and vertical base vibration. This result suggests that the sawtooth base under horizontal vibration can lead to the stratified flows, but it is not studied. Based on the above results, we think that in a bi-disperse granular system with the sawtooth base under the horizontal vibration there are three kinds of different states (mixed state, vertical and horizontal segregation state), which depend on the region in the huge control parameter space in which the system is located. Among these control parameters are the density ratio, the direction of vibration, the amplitude and frequency of the vibration of the system, the mechanical properties associated with particle collisions and so on.

2. Computation method

Our computer simulation is based on a two-dimensional, soft-sphere molecular dynamics method.[24] When spherical particle i collides with particle j, there are both normal and tangential forces acted on particle i by particle j. The normal contact force is determined by a damped and nonlinear spring model,

$$F_{\mathrm{n},ji} = k_{\mathrm{n}}\delta_{\mathrm{n},ij}^{3/2} - \gamma_{\mathrm{n}} m_{\mathrm{eff}} v_{ji}, \tag{1}$$

where $k_{\mathrm{n}} = Y\sqrt{r_i r_j/(r_i + r_j)}$ and Y is the Young modulus for collisions between grains of radii r_i and r_j, $\delta_{\mathrm{n},ij}$ is the normal overlap, γ_{n} is the normal dissipation parameter, ν_{ji} is the normal direction of velocity and $m_{\mathrm{eff}} = m_i m_j/(m_i + m_j)$ is the effective mass of spheres with masses m_i and m_j. The tangential contact force is determined by a linear spring in series with a frictional sliding element model:

$$F_{\mathrm{s},ji} = \mathrm{sign}(k_{\mathrm{s}}|\delta_{\mathrm{s},ij}|, \mu|F_{\mathrm{n},ji}|), \tag{2}$$

where $\delta_{\mathrm{s},ij}$ is the tangential overlap, k_{s} is the tangential spring constant and μ is coefficient of friction. The mechanical and environmental simulation parameters are listed in Table 1.

The studied granular materials consist of 700 heavy particles with density ρ_{h}, and 700 light particles with density ρ_{l}. These particles are the same with diameter and are placed within a rectangular container of height, 50 mm, and width, 180 mm. The base of container contains many sawteeth of height 6 mm, with an asymmetry such that the right edge of each tooth is vertical. The sawtooth base is constructed from a set of particlelike balls positioned to produce the required profile, these balls oscillate horizontally in unison to produce the effect of a sinusoidally vibrated base. The balls themselves interact with the particles using the same force laws as above, their diameters are d and the distance between centres of balls is half of this value. The vibration frequency f and dimensionless acceleration $\Gamma = A(2\pi f)^2/g$ are used as control parameter, where A is the vibration amplitude and g is the gravitational acceleration. Here we change the range of frequency from 5.0 to 80.0 Hz and the range of acceleration from 1.1 to 5.0.

Table 1. Baseline parameters used in the simulations.

number of heavy particles (HP), N_{h}	700
number of light particles (LP), N_{l}	700
HP, LP diameter, d	1.0×10^{-3} m
LP density, ρ_{l}	1.31×10^{3} kg·m^{-3}
normal Young modulus, Y	8.35×10^{6} N·m^{-2}
normal dashpot coefficient, υ_{n}	4.112×10^{3} s^{-1}
tangential spring stiffness ratio, k_{s}	5.904×10^{3} N·m^{-1}
friction coefficient, μ	0.2
time step, Δt	2.0×10^{-6} s

3. Discussion and simulation results

We first describe the effect of density ratio on the segregation behaviour in a container with a sawtooth base under horizontal vibration of fixed frequency and dimensionless acceleration. The sawtooth base contains 20 sawteeth. Initially, all particles are simultaneously released from random positions, which can cause particles to form uniform mix. Figure 1 presents a numerical snapshot of particle distribution showing two different states for the mixture with different density ratio at $\Gamma = 4.0$ and $f = 15.0$ Hz. The heavy and light particles mix together and are not segregated for the case of density ratio $\rho_{\mathrm{h}}/\rho_{\mathrm{l}} = 1.5/1.31$ (shown in Fig. 1(a)), when the density ratio $\rho_{\mathrm{h}}/\rho_{\mathrm{l}} = 9.44/1.31$ heavy particles congregate to the left side of container and the light ones congregate to the other side (shown in Fig. 1(b)). The former is denoted as a mixed state (MS) and the later is referred to as a left segregated state (LSS). These two states are steady. In order to explore the quantitative density-ratio dependence of these states, the separation degree of a binary mixture is quantified by the horizontal segregation parameter,

$\Delta x = \dfrac{2(x_{\rm l} - x_{\rm h})}{x_{\rm l} + x_{\rm h}}$, where $x_{\rm h}(x_{\rm l})$ is the average horizontal coordination of heavy (light) particles. So that $\Delta x \approx 0$ denotes that heavy and light particles mix together and are not segregated, when $\Delta x > 0$ the heavy particles are in the left side of container, and $\Delta x < 0$ corresponds to the heavy particles gathering to the right side. Figure 2 shows that the segregation parameter Δx as a function of the density ratio $\rho_{\rm h}/\rho_{\rm l}$ at $\Gamma = 4.0$ and $f = 15.0$ Hz. We can clearly see that horizontal segregation parameter Δx increases fast as the density ratio increases and it approaches the saturation value at higher density ratio. This is as expected, when the density ratio approaches to 1 (i.e, the disappearance in the difference of particles) the segregation phenomenon disappears, the larger the density ratio is, the easier the appearance of segregation behaviour is.

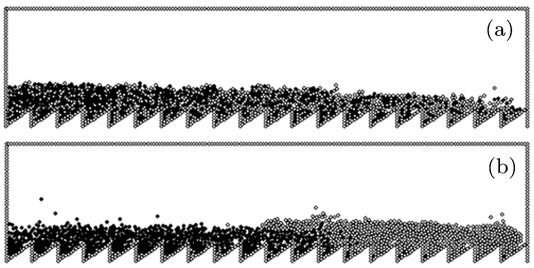


Fig. 1. The snapshot of the segregated state of binary granular mixtures at $\Gamma = 4.0$ and $f = 15.0$ Hz: (a) the density ratio $\rho_{\rm h}/\rho_{\rm l} = 1.5/1.31$; (b) the density ratio $\rho_{\rm h}/\rho_{\rm l} = 9.44/1.31$. The light and heavy particles are denoted by gray and black disks, respectively.

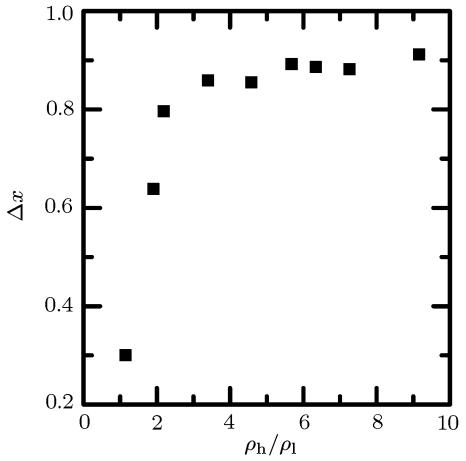


Fig. 2. The segregation parameter Δx as a function of the density ratio $\rho_{\rm h}/\rho_{\rm l}$ at $\Gamma = 4.0$ and $f = 10.0$ Hz.

As we know, the properties of external vibration have an essential role in selecting the final segregation state. For example, large particles stay in the upper layer of the granular bed at low vibration frequency, then sink into the granular bed at a certain depth as the frequency increases, but rise up again at high frequency.[25] As expected, the segregation state in our present system exhibits the obvious dependence of the frequency. The segregation parameter Δx is plotted against vibration frequency for a given value of $\rho_{\rm h}/\rho_{\rm l} = 8.31/1.31$ in Fig. 3. The segregation parameter Δx first increases sharply with vibration frequency f, and arrives at its saturation value at $f = 20-35$ Hz, then decreases and approaches to 0. That is, in much low frequency region the heavy and light particles mix together. As the frequency increases, the heavy particles congregate to the left side of container and the light ones congregate to another side forming the LSS. At higher frequency, the horizontal segregation phenomenon disappears, but a vertical segregation state (VSS) appears: the light particles move up and form a pure layer in top of the system, the heavy particles and part of light particles stay at the bottom, which is consistent with previous experimental studies of vertically vibrated binary granular mixtures.[26]

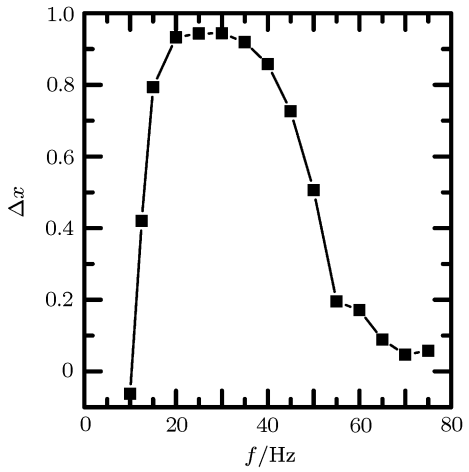


Fig. 3. The segregation parameter Δx as a function of the frequency f at $\rho_{\rm h}/\rho_{\rm l} = 9.44/1.31$ and $\Gamma = 4.0$.

At the same time, we also studied the effect of dimensionless acceleration Γ on segregation behaviours and plotted a phase diagram in $\Gamma - f$ space for given value of $\rho_{\rm h}/\rho_{\rm l} = 9.44/1.31$ in Fig. 4. As can be seen from this figure, under different vibration conditions there exist five regions where the various effects (weak vibration, MS, LSS and VSS) are observed. For all frequencies, there is a low-Γ region ($\Gamma < 1.2$, weak vibration in this figure) where the particles stay at rest. Increasing acceleration ($\Gamma > 1.2$) results in rearrangements or movements of particles. But relative motions

of particles do not lead to the appearance of the segregation when the vibration frequency is relative low, so the system is still in the MS. When the frequency is increased, the segregation behaviour is observed. The LSS appears first, i.e., the transition from the MS to LSS takes place and this transition depends on both acceleration and frequency. When the frequency is further increased beyond 20 Hz, in the relative low acceleration region the system returns to the MS from LSS, while in the relative high acceleration regime the system changes to the VSS from LSS, both transitions depend on acceleration and frequency. When the system is in the VSS, increasing frequency or decreasing acceleration results in the transition from the VSS to MS. In our presently studied system five regions and four various states are observed. Therefore, there exist many state transitions, such as from the MS to LSS, from the LSS to VSS and from the VSS to MS, which are dependent on vibration parameters Γ and f. For example, when Γ is fixed to be 3, as frequency increases, we first observed the MS, then the LSS, after that the VSS and finally the MS again. These transitions depend on the acceleration and frequency.

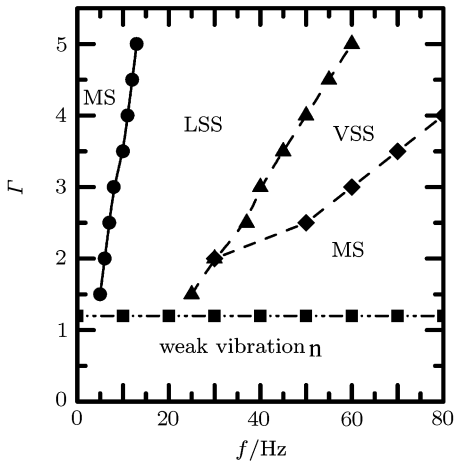


Fig. 4. Schematic phase diagram in Γ versus f space for the case of $\rho_{\rm h}/\rho_{\rm l} = 9.44/1.31$. MS: mixed state; LSS: left segregation state; VSS: vertical segregation state; Weak Vibration: $\Gamma < 1.2$, no relative motion of particles.

To seek the reason of leading to the granular segregation that shows the frequency-dependence behaviour, we study the height dependence of average horizontal velocity of particles in each layer along the ratchet $v = (1/N)\sum(v_i - v_{\rm base})$. To measure v the periodic boundary condition has been used in the simulated system, where there are 1400 light particles with density $\rho_{\rm l}$ and other conditions remain unchanged. Figure 5 shows that the average horizontal flow velocity as a function of height for given values of $\Gamma = 4.0$ at different frequencies. The velocity of particles in the horizontal direction is stratified in a certain frequency range, with the fastest moving layers located nearest to the ratchet floor. This result agrees with previous experimental[17,18] and numerical[17,20,22]studies of the system under vertical vibration. The vibration base with a sawtooth surface profile can produce stratified flows in opposite directions at different heights. We also find that the stratified flows depend on the frequency f: the stratified flows become weaker and weaker as the frequency increases and there is almost no flow at higher frequency. Figures 6(a)–6(c) present the snapshot pictures of distributions of heavy and light particles with $\rho_{\rm h}/\rho_{\rm l} = 9.44/1.31$ under horizontal vibration of $\Gamma = 4.0$ and $f = 35.0$ Hz at three times $t = 0.0$, 2000.0 and 8000.0 s, respectively. We can clearly see that, initially, these heavy and light particles mix together and are not segregated (shown in Fig. 6(a)), the lighter particles move to the top as the vibration lasts (shown in Fig. 6(b)), then top particles go to the right side of container but bottom particles go to another side, finally the light particles stay at the right side of container and the heavy ones at another side forming the steady LSS (shown in Fig. 6(c)). According to the results shown in Figs. 5 and 6, there are density effect and stratified flow effect in our simulated system with the sawtooth base under horizontal vibration. The density effect raises the light particles. The stratified flow drives the particles in the upper levels to the right and the particles in the lower particles to the left. As the vibration frequency increases the stratified flow effect becomes weaker and weaker as shown in Fig. 5, therefore at high vibration frequencies the VSS appears instead of the LSS.

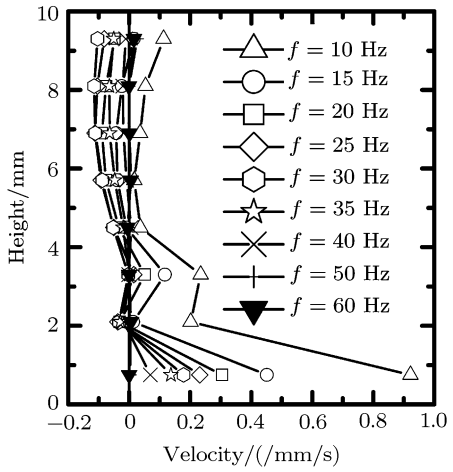


Fig. 5. The average horizontal flow velocity as a function of height for given values of $\Gamma = 4.0$.

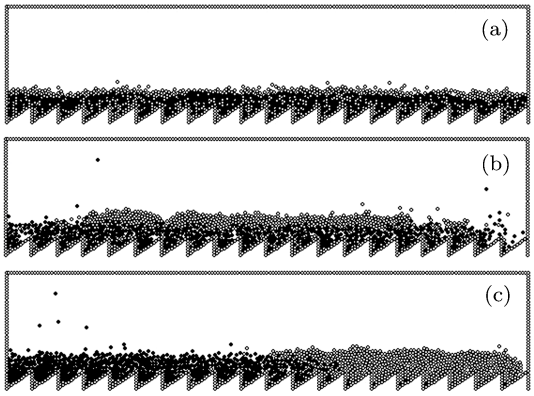


Fig. 6. The snapshot of the segregated state of binary granular mixtures for given value of $\rho_{\rm h}/\rho_{\rm l} = 9.44/1.31$, $\Gamma = 4.0$ and $f = 15.0$ Hz at different time: (a) $t = 0.0$ s; (b) $t = 2000.0$ s; (c) $t = 8000.0$ s. The light and heavy particles are denoted by gray and black disks, respectively.

No doubt, the shape of sawtooth has an effect on the direction of stratified flow under vertical vibration.[17,20] So, we performed a study of the same binary mixture in the container with different shapes of sawtooth. Here we change the sawtooth shape by changing the number of the sawtooth and fixing the height of the sawtooth (H). Figure 7 shows the segregation parameter Δx as a function of sawtooth number for the case of $\rho_{\rm h}/\rho_{\rm l} = 9.44/1.31$, $\Gamma = 4.0$ and $f = 15.0$ Hz. We observe that the value of Δx changes from negative to positive as the number of sawtooth increases, and when the number of sawtooth is about 16, the value of $\Delta x \approx 0.0$. That is, the horizontal segregation behaviour is dependent on the shape of the sawtooth. The system changes from the right segregation state to the left segregation state through the MS, where the number of sawtooth is about 16.

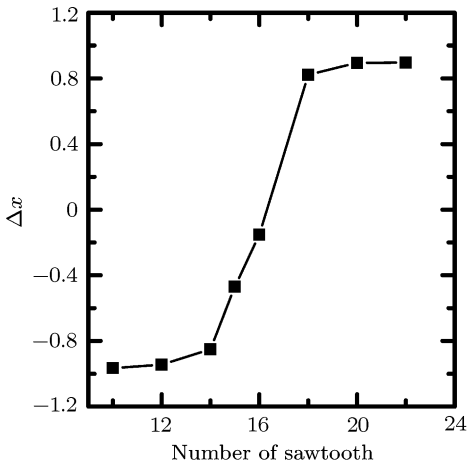


Fig. 7. The segregation parameter Δx as a function of number of sawtooth for given value of $\rho_{\rm h}/\rho_{\rm l} = 9.44/1.31$ at $\Gamma = 4.0$ and $f = 15.0$ Hz.

4. Conclusion

We have numerically studied the horizontally vibrated binary mixtures in a container with a sawtooth base. When the acceleration is high enough to result in relative motions of the particles, the system can be in various states (MS, VSS and horizontal segregation states), which depend on the region in the control parameter space. Therefore, there exist many state transitions, such as from the MS to LSS, from the LSS to VSS and from the VSS to MS, which are dependent on the acceleration and frequency. Due to the sawtooth base there is a stratified flow effect besides density effect. The density effect raises the light particles. The stratified flow drives the particles in the upper levels to the right and the particles in the lower particles to the left, which results in the appearance of the LSS. The LSS can be changed to the right segregation by changing the shape of the sawtooth. As the vibration frequency increases the stratified flow effect becomes weaker and weaker, so at high vibration frequencies the VSS appears instead of the LSS.

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