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Effect of Thermal Convection on Density Segregation in Binary Granular Gases with Dissipative Lateral Walls *

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Molecular dynamics simulations are employed to investigate the effect of thermal convection induced only by dissipative lateral walls on density segregation of the strongly driven binary granular gases under low gravity conditions. It is found that the thermal convection due to dissipative lateral walls has significant influence on the segregation intensity of the system. The dominant factor in determining the degree of segregation achieved by the system is found to be the relative convection rate between differing species. Moreover, a qualitative explanation is proposed for the relationship between the thermal convection due to dissipative lateral walls and the observed segregation intensity profiles.

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Granular materials defined as collections of macroscopic particles with dissipative interactions between particles, when exposed to external vibrations, can exhibit a variety of novel behaviors,[1] such as pattern formation,[2] convection,[3,4] and segregation.[5] Among these phenomena, the most relevant process to industrial application may be the granular segregation. The granular systems composed of two or more distinct particle components may spontaneously separate into their individual constituents.[6] Having no analogy in molecular materials, the granular segregation remains incompletely understood. The degree of the segregation, to which bi-disperse or poly-disperse mixtures may exhibit, is significantly dependent on the differences in particle size,[7] density,[8] inelasticity[9] or shape.[10] More recently, the bulk-buoyancy-driven convection (BBD TC) has been demonstrated to be another factor influencing the degree of segregation in strongly driven systems.[11,12] Through extensive research on the segregative processes, a reasonable level of comprehension of the mechanism influencing the degree of segregation within granular mixtures in the presence of gravity has been achieved. However, systematic study to reveal the fundamental factor, on which the degree of the granular segregation depends within the granular mixtures under low-gravity condition, is still surprisingly lacking.

Very recently, Pontuale *et al.*[13] experimentally showed that in highly fluidized granular systems, an outgoing energy flux always originates at a dissipative wall,[14] yielding in a horizontal temperature gradient induced by dissipative lateral walls (DLW), which leads always to a granular thermal convection (DLW TC). The convective flow induced by DLW is oriented downward at the walls and upward in the center of the system, which becomes important under low gravity conditions. In contrast, as the total number of particles or the gravity become larger and larger, the two DLW TC cells appear to move toward the lowest corners and occupy a smaller and smaller region, up to a point, which could hardly be noticed.[13] Their work reveals that DLW TC is essentially different from BBD TC and BBD TC is not the only mechanism able to generate convection in granular gases. Inspired by their work, using molecular dynamic simulations in this study, we aim to investigate how the thermal convection due to DLW TC may influence the intensity of the segregation in highly fluidized binary granular gases whose components are equally sized but differ in their densities (i.e., mass) and dissipative properties, subjected to the low gravity. The results of this work not only reveal the significant effect of DLW TC on the granular segregation of the binary granular gases under low gravity, but also show the degree of segregation achieved by the mixtures possibly controlled by altering the relative convection intensity between differing species within the mixtures.

The system is a binary granular gas of N smooth hard spheres moving in a cuboidal box which is vibrated sinusoidally in the vertical (z) direction from the bottom. The gravitational force acts along the negative z direction. The two species are chosen to have equal diameters $d = 3\,\text{mm}$ and unequal density $\rho_1 = 2500\,\text{kg}\cdot\text{m}^{-3}$ for species 1, $\rho_2 = 7900\,\text{kg}\cdot\text{m}^{-3}$ for species 2, respectively. The width, depth and height dimensions of the cuboidal box are $L_x = 20d$, $L_y = 20d$ and $L_z = 132d$, respectively. The bottom wall of the cuboidal box oscillates with frequency f and peak amplitude A. The average squared velocity of the vi-

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brating bottom wall defined as $v_0^2 = (A2\pi f)^2/2$ helps setting the energy and velocity units in the following. The relatively large size of the particles means that effects due to interstitial air can be safely ignored.[15]

In our system, the particles are subjected to the gravity $g_l \in [0.016g, 0.2g]$, where g is the Earth's gravity acceleration. In theoretical research,[16,17] it is shown that when $g \to 0$ the BBD TC instability requires a larger and larger wavelength to develop. Therefore, at a given width and depth of our system, unstable perturbations cannot appear and the BBD TC is sufficiently suppressed because of low gravity. The frequency and amplitude of vibration are varied in the range $f \in [20, 60]$ Hz) and $A \in [1.2, 4.5]$ mm, respectively. The rescaled maximum acceleration is $\Gamma = A(2\pi f)^2/g_l \in [10, 4070]$. We use $N = 2000$ ($N_1 = N_2 = 1000$), which yields the observed local variations of the packing fraction η reaching up to ∼5% at the lowest value of ε_w (the restitution coefficient of the lateral walls) and the highest value of g_l, i.e., we are always in the dilute regime, thus the event-driven algorithm is available for the system.

The collisions between particles are treated with normal restitution coefficients. The normal restitution coefficient for lateral walls and topmost wall are taken as ε_w. For intraspecies particle collisions, the normal restitution coefficients are chosen to be $\varepsilon_{11} = 0.96$ and $\varepsilon_{22} = 0.92$, respectively. For collisions of interspecies, the elasticity is taken as $\varepsilon_{12} = (\varepsilon_{11} + \varepsilon_{22})/2 = 0.94$. The equations describing the dynamics, which follow from instantaneous, binary and momentum conserving, for the particle–sidewall, particle–bottom-wall and particle–particle collisions, can be written as

$$\boldsymbol{v}_i' = \boldsymbol{v}_i - (1+\varepsilon_w)(\boldsymbol{v}_i \cdot \hat{\boldsymbol{e}}_n)\hat{\boldsymbol{e}}_n, \quad (1)$$

$$v_{i,z}' = 2v_w - v_{i,z}, \quad (2)$$

$$\boldsymbol{v}_{i,j}' = \boldsymbol{v}_{i,j} \pm (1+\varepsilon_{\alpha\beta})\frac{m_{i,j}}{m_i + m_j}[(\boldsymbol{v}_j - \boldsymbol{v}_i)\cdot\hat{\boldsymbol{n}}]\hat{\boldsymbol{n}}, \quad (3)$$

where v_i is the velocity of particle i, v_w is the velocity of the bottom wall, $v_{i,z}$ is the z vertical component of the velocity of particle i, $\hat{e}_n$ is the unit normal vector perpendicular to the sidewalls, $\hat{n}$ is the unit center-to-center vector between the colliding pair i and j, and $\alpha, \beta = 1, 2$ corresponding to index of the species to which the particle i or j belongs. Note that we have taken the tangential restitution coefficient for particle–particle and particle–wall collisions as unity, as well as the normal restitution coefficient for particle–bottom wall collisions. One problem with the event-driven simulation is that a sphere may collide more and more frequently with the sidewall as the horizontal component of its momentum is dissipated. To avoid the inelastic collapse,[18] which has been observed in simulations of the bulk granular system, we inject a small amount of energy in the horizontal direction when the horizontal velocity falls below a cut-off value. This condition arises infrequently and its handling in this way has no discernible effect on the results. All the resultant data are collected until a steady state has been achieved in the system.

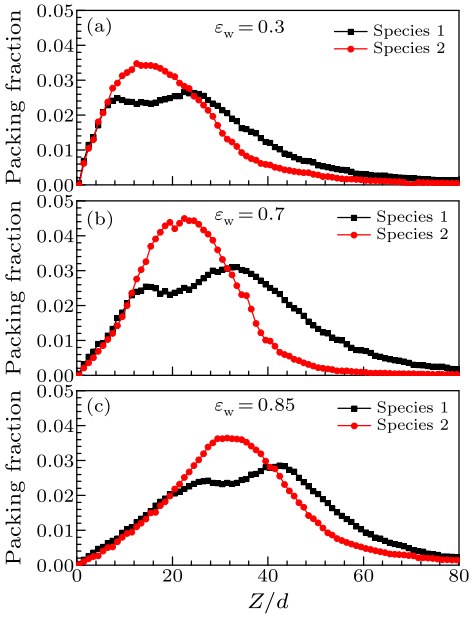

Fig. 1. Comparison of packing density profiles in the vertical direction for the binary granular gases with different dissipative sidewalls corresponds to (a) $\varepsilon_w = 0.3$, (b) $\varepsilon_w = 0.7$ and (c) $\varepsilon_w = 0.85$, where $N_1 = N_2 = 1000$, $\varepsilon_{11} = 0.96$, $\varepsilon_{22} = 0.92$, $\varepsilon_{12} = 0.94$, $g_l = 0.016g$, $A = 1.8$ mm, and $f = 50$ Hz.

Figure 1 shows the packing fraction in the vertical direction of individual species as a function of sidewall dissipation corresponding to $\varepsilon_w = 0.3$ (Fig. 1(a)), $\varepsilon_w = 0.7$ (Fig. 1(b)) and $\varepsilon_w = 0.85$ (Fig. 1(c)). All the parameters other than ε_w are kept to be constant. The packing fraction of each species, analyzed by binning the simulation box into horizontal slabs of height $1d$, is the ratio of the volume occupied by particles of individual species to the volume of each horizontal slab. As observed for the packing fraction profiles in Fig. 1, along the z direction, the packing fraction shows a maximum at some given height. Such a maximum shifts toward the base as ε_w decreases, which is consistent with the density profiles observed in the previous experimental work.[13] The notable and somewhat counter-intuitive feature of Fig. 1 is that the system becomes most segregated for the intermediate sidewall dissipation corresponding to $\varepsilon_w = 0.7$, while the system becomes better-mixed with the more dissipative sidewalls corresponding to $\varepsilon_w = 0.3$ or the less dissipative sidewalls corresponding to $\varepsilon_w = 0.85$. It is interesting to note that the observed degree of segregation displays no monotonic dependence on the dissipation of the sidewalls. Meanwhile, the degree of segregation of the system may be altered by varying the inelasticity of the lateral walls without changing

any other system parameters. Here comes the question: is the sidewall dissipation indeed the key feature to vary the degree of segregation of the system?

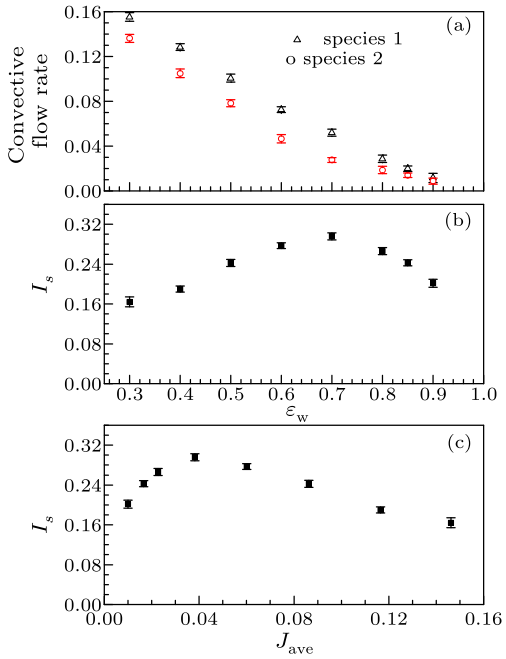

Fig. 2. (a) The convective flow rate of individual species and (b) the segregation intensity as a function of the restitution coefficient of the sidewalls ε_w for the bi-disperse granular gases. (c) The segregation intensity versus the average convective flow rate of the system. The simulation conditions are $N_1 = N_2 = 1000$, $\varepsilon_{11} = 0.96$, $\varepsilon_{22} = 0.92$, $\varepsilon_{12} = 0.94$, $A = 1.8$ mm, $f = 50$ Hz ($v_0 = 399$ mm/s), and $g_l = 0.016g$. The convective flow rates are rescaled by v_0.

In the case of the thermal convection induced by DLW TC present in this study, the thermal convection is always observed and the sidewall dissipation has a significant influence on the convective motion within the system.[13] The convective flow rates rescaled by v_0 for each particle species with various ε_w are shown in Fig. 2(a). To study the convection profiles of the system, we divide the bi-disperse system into a series of equally sized 3D cubic bins with length 3 mm ($1d$). Then the time-average velocity vector and number density for each species in each bin are calculated. The convection strength, quantified by the convection flow rate J, is calculated as the average of the vertical velocity component of particles through the vertical height of the convective center where the horizontal velocity components of particles are zero. The convective flow rates obey[19]

$$J = \frac{1}{2n_b}\sum_{i=1}^{n_b}|v_z^i|, \tag{4}$$

where v_z^i is the vertical velocity component corresponding to the ith bin, and n_b is the number of bins falling within the horizontal slice through the vertical height of the convective center. As shown in Fig. 2(a), the convective flow rates for each species, rescaled by v_0, are observed to decrease monotonically with increasing ε_w, following the general trend displayed in the previous experiment.[13] However, the difference in J between individual species which initially increases with ε_w before passing through a maximum and decreasing for relatively large ε_w, clearly shows no monotonical dependence on ε_w. Having studied how ε_w affects the convective flow rate, we now turn to explore how the convective flow rate J may influence the segregation profiles of the system. The segregation intensity I_s, quantifying the degree of segregation, is defined as the standard deviation of the compositions of samples and is calculated by[20]

$$I_s = \left[\frac{1}{N_b - 1}\sum_{i=1}^{i=N_b}(\phi_i - \phi_m)^2\right]^{1/2}, \tag{5}$$

where N_b is the total number of equally sized 3D bins, ϕ_i is the number concentration of the single species in the ith bin, ϕ_m is the mean concentration of the system. The number concentration ϕ_i of the single species in the ith bin is calculated as the fraction of the particle number of the specified species to the total particle number in the ith bin. Thus $I_s = 0$ represents a perfectly mixed system and $I_s = 0.5$ indicates a completely segregated system. The segregation intensity I_s as a function of ε_w is illustrated in Fig. 2(b). It is observed that I_s initially increases with ε_w before passing through its maximum value at $\varepsilon_w = 0.7$, and then decreases with ε_w. Comparing Fig. 2(a) and Fig. 2(b), it is clearly revealed that the system becomes more segregated as the difference in J between species becomes more pronounced, while a decrease in I_s can be attributed to increasingly equilibrated convective flow rate of dissimilar species. In addition, the segregation intensity as a function of the average convective flow rate J_{ave} of the system is shown in Fig. 2(c). The average convective flow rate is also rescaled by v_0. The notable feature of this graph is that I_s shows surprisingly no monotonic dependence on the average convective flow rate of the system, which one might expect from the previous study,[11,12] meanwhile, it is also not dependent on either of the individual convective flow rate for each species. In a word, in comparison of Figs. 2(a)–2(c), it seems that the key element impacting the degree of segregation is the difference between the two species' convective flow rates. Such a relationship between the disparity in J of species and the segregation intensity can be explained by the fact that the heavier particles are less likely to be dragged into the convective flow.[21] When the convective flow is weak in the system corresponding to $\varepsilon_w = 0.9$, both the heavy and the light particles are rarely dragged into the convective stream, leading to a small disparity between the convective flow rates for

each species which induces a small degree of segregation. In the system of very strong convection for small ε_w (for example, $\varepsilon_w = 0.3$), as both the heavy and light particles undergo significant convective motion, the difference between the convective flow rates for each species is also small, leading once again to a small degree of segregation. However, when the convective strength is relatively moderate corresponding to $\varepsilon_w = 0.7$ in the system, the lighter and less dissipative particles exhibit relatively prominent convective motion while the heavier and more dissipative particles are relatively undisturbed.[22] This different convection motion displayed by the two species results in the greatest separation of particle species.

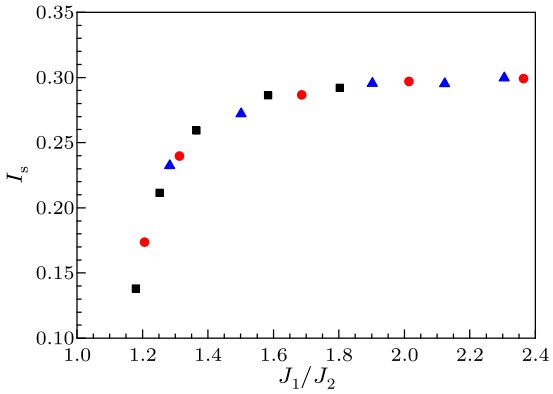

Fig. 3. Segregation intensity I_s as a function of the ratio of convective flow rates J_1/J_2 for species 1 (light particles) and species 2 (heavy particles) of the larger system. Variation of J_1/J_2 is induced by varying ε_w (solid squares), the driving strength of vibration of the system (solid circles) or the value of gravity (solid triangles). The simulation conditions are $N_1 = N_2 = 1000$, $\varepsilon_{11} = 0.96$, $\varepsilon_{22} = 0.92$, and $\varepsilon_{12} = 0.94$.

To further investigate the effect of difference in J between species on segregation intensity, I_s as a function of the disparity in J between species with various ε_w is shown in Fig. 3. The disparity in J between species is characterized by the ratio J_1/J_2, where J_1 is the convective flow rate for light particles (species 1), and J_2 is the convective flow rate for heavy particles (species 2). It is more clearly demonstrated that the key parameter in determining the segregation intensity is the ratio J_1/J_2 rather than the average convective rate of the whole system. To further verify that the dominant parameter producing the segregation behaviors observed above is the ratio J_1/J_2 rather than the other parameters of the system, additional simulations are carried out by keeping ε_w to be constant but changing the driving frequency ($f \in [20, 60]$ Hz) and amplitude ($A \in [1.2, 4.5]$ mm) or gravity ($g_1 \in [0.012g, 0.2g]$) to vary the convective flow rates of two species. The resultant data are also shown in Fig. 3. The collapse of all data points onto a single increasing curve indicates that it is not the sidewall dissipation or driving parameters or gravity, but the relative convection rate between individual species being the primary factor in determining the degree of segregation displayed by our systems. The results presented here imply a possibility that the degree of segregation for highly fluidized granular mixtures may be indirectly varied through the adjustment of the driving parameters, dissipative properties of the sidewall of container or the effective value of gravity.

To test our observations in a larger system, additional simulations are performed using an increased system size. The width and depth of the larger system are increased to $40d$ and the total number of particles is set to 8000 to maintain the resting bed height constant. The segregation intensity versus J_1/J_2 for the larger system is displayed in Fig. 4. Despite the slight decrease in the absolute values of I_s, the observed trend of I_s versus J_1/J_2 of the larger system corresponds closely to our original system, supporting the idea that the phenomena observed here may be applicable in larger-scale, real-world systems, as well as further proving that J_1/J_2 is the dominant factor impacting the degree of segregation.

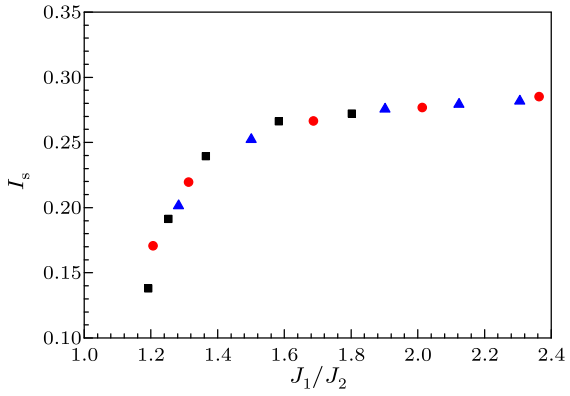

Fig. 4. Variation of the segregation intensity I_s with the ratio of convective flow rates J_1/J_2. Variation of J_1/J_2 is induced by varying ε_w (solid squares), the driving strength of vibration of the system (solid circles) or the value of gravity (solid triangles). The simulation conditions are $\varepsilon_{11} = 0.96$, $\varepsilon_{22} = 0.92$, and $\varepsilon_{12} = 0.94$.

In conclusion, molecular dynamics simulations are employed to elucidate the influence of the thermal convection induced only by dissipative lateral walls, on the extent of segregation displayed by the vertically vibrated bi-disperse granular gases under low gravity conditions. It is found that the dominant factor in determining the degree of segregation achieved by the system is the relative convection rate between individual species. Therefore, DLW TC has significant influence on the segregation intensity of binary granular gases under low gravity. The results of this work imply a possibility that the degree of segregation for highly fluidized granular mixtures may be indirectly adjusted through the variation of the driving parameters, dissipative properties of the sidewall of container

or the effective value of gravity. Moreover, we propose a qualitative explanation to the relation between the relative convection rate between individual species and the segregation intensity. Further theoretical investigation is needed to provide more quantitative predictions, as well as the experiments in microgravity.

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