Size Segregation and Convection of Granular Mixtures Almost Completely Packed in a Thin Rotating Box

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We simulate size segregation in granular mixtures which are almost completely packed in a rotating drum. Instead of a 3D drum, we simulate a 2D thin rotating box which is almost completely packed with granular mixtures. The phase inversion of a radially segregated pattern which was found in a 3D experiment is qualitatively reproduced with this simulation. A global convection appears after a radial segregation pattern is formed, and this convection induces an axially segregated pattern.

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Granular materials exhibit some complex phenomena [1]. One example is size segregation which occurs by shaking or stirring them [4–11]. Mixtures of granular materials which are partially filled in a horizontally rotating drum also segregate by size. Some of the recent experiments of such a rotating drum have shown two types of segregation patterns [12,13]. One of them is radial segregation where large materials accumulate near the walls of a drum and small materials accumulate to the central region around the rotating axis. The other is axial segregation where the system evolves to form alternating bands, one of which is rich in small material and the other rich in large material. These phenomena have been explained by recent numerical and analytical studies [13–16]. Most of these studies explained such segregation by considering the difference of the dynamic angle of reposes between large and small materials at the flowing surface of a granular bed. For radial segregation, another experiment reported that the mixing state and the reverse segregation appear when the angular velocity of a rotating drum becomes large [17]. Here, the reverse segregation is defined such that small materials accumulate near the walls of the drum and large materials accumulate to the central region around the rotating axis.

Recently, radial and axial segregation were observed in an experiment of a horizontally rotating drum which was almost completely packed with granular mixtures [18]. Moreover, as explained in the following, phase inversion between two types of radial segregation patterns takes place when w, the angular velocity of the rotating drum, passes through a critical value [19]. When $Aw^2 < g$, large particles accumulate near the wall of the drum and small particles accumulate to the central region. On the contrary, small particles accumulate near the wall of the drum and large materials accumulate to the inner region of the drum like the reverse segregation when $Aw^2 > g$. Here, A is the radius of the drum, and g is the acceleration of gravity. In this system, there is little surface flow because the drum is almost completely packed with granular mixtures. Thus, previous numerical and analytical studies which have taken into account the difference of the dynamic angle of reposes between large and small materials cannot explain these phenomena. In this paper, we discuss the mechanism of such segregation and phase inversion phenomena in a rotating drum almost filled with granular mixtures. First, we reproduce experimental results with a simple simulation. Second, we make an analytical study of the phase inversion phenomena between two types of radial segregation.

In order to simplify the simulation, we set the following situation. Instead of a 3D drum the radius and the width of which are, respectively, A and B, we use a 2D box which rotates along a horizontal axis with the length $2A$ and the width B. Here, the length of the 2D box corresponds to the diameter of the 3D drum. The rotation axis of this box is the line of half length A, and this box rotates with angular velocity w (Fig. 1). Our setup of the 2D thin box simulation is not the direct reflection of the 3D experiment. However, we believe it catches the intrinsic dynamics in the almost filled drum with little surface flow which plays an important role in the half-filled drum. In other words, this is the simplest system with which one can look into the detailed dynamics of particles in bulk. We employ the following particle model, which is one of the simplest models of granular dynamics [2,3]. The equation of motion of the ith particle is

$$\ddot{\mathbf{x}}_i = -\sum_{j=1}^{N} \theta(r_i + r_j - |\mathbf{x}_i - \mathbf{x}_j|) \times \{\nabla V(r_i + r_j - |\mathbf{x}_i - \mathbf{x}_j|) + \eta(\mathbf{v}_i - \mathbf{v}_j)\} + \mathbf{F}_i^{\mathrm{ex}}, \tag{1}$$

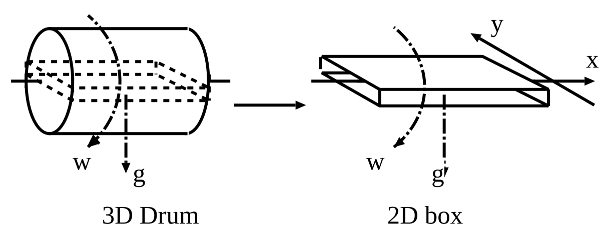

FIG. 1. Illustration of 2D rotating thin box.

$$V(r_i + r_j - |\mathbf{x}_i - \mathbf{x}_j|) = \frac{k}{2}(r_i + r_j - |\mathbf{x}_i - \mathbf{x}_j|)^2. \tag{2}$$

Here, θ is the Heaviside function, N is the total number of particles, k and η are, respectively, the elastic constant and the dumping coefficient, and $\mathbf{x}_i(x_i, y_i)$, $\mathbf{v}_i(v_{x_i}, v_{yi})$, and r_i are, respectively, the position, velocity, and radius of the ith particles. The elastic constant k and the dumping coefficient η are related to the coefficient of restitution e and the collision time t_{col}, the time period during collision [20], which are determined in the ideal two bodies collision. In this model, the effect of particles' rotation is neglected. We regard the rotating axis as the x axis ($y = 0$), and the length direction (radius direction for 3D drum) as the y direction in this simulation. $\mathbf{F}_i^{\mathrm{ex}}$ is the external force which directly acts on the ith particle not by collision. Since gravitation and centrifugal force work on each particle, $\mathbf{F}_i^{\mathrm{ex}}(F_{x_i}^{\mathrm{ex}}, F_{y_i}^{\mathrm{ex}})$ is given as follows:

$$F_{x_i}^{\mathrm{ex}} = 0, \tag{3}$$

$$F_{y_i}^{\mathrm{ex}} = y_i w^2 - g\sin(wt). \tag{4}$$

The above equations are calculated with the Euler's scheme. The time step δt is set small enough such that δx, the displacement of the ith particle during δt, does not exceed a given value. We set $2A = 7.43$, $B = 24.0$, $t_{\mathrm{col}} = 0.05$, e between a pair of particles is 0.99, and $g = 3.0$. Moreover, boundaries of box $|x| = A$ or $|y| = B$ are given as the viscoelastic walls with $e = 0.95$. The total number of particles is $N = 750$, the ratio of particle numbers between large and small particles is 1:4, the ratio of average radius between them is 2:1, and a 10% polydispersity for large and small particles' radius is given. The packing density, which is defined as (the area of region occupied by particles)/(the area of 2D box), is estimated to be about 84%. It means this system is not completely packed. In practice, the movement of the center of the mass of particles appears through the rotation process in our simulation. However, the distance of this movement from the average position is almost the same as the average radius of small particles, which is small enough compared to A. Hence, this system is regarded as an almost completely packed system. Because of such polydispersity and the movement of the center of mass of particles, each particle in the system barely moves.

We pack particles at random at the initial condition [Fig. 2(a)] and simulate with several values of w. Figures 2(b)–2(d) are typical patterns of radial segregation for (b) $w = 0.5$ ($Aw^2 < g$), (c) $w = 0.9$ (Aw^2 is a little larger than g), and (d) $w = 1.2$ ($Aw^2 > g$). Figure 2(b) indicates that large particles accumulate near the wall of a drum ($|y| = A$) and small particles gather around the central region when $Aw^2 < g$. Figures 2(c) and 2(d) indicate small particles accumulate near the wall of a drum and large particles accumulate to the central region when $Aw^2 > g$. In Fig. 2(c), the region in which large particles distribute is wide for the radial direction compared to Fig. 2(d). These results qualitatively correspond to the experimental results of a rotating drum which is almost completely packed with granular mixtures [19]. The patterns illustrated in Figs. 2(c) and 2(d) are stable, whereas the pattern like Fig. 2(b) evolves into the pattern like Fig. 3(c). This is because the fluctuation of large particles' concentration in the axial direction grows up slowly as follows. Now, we consider the case that the direction of gravity is the negative direction in y. It means that $y = -A$ corresponds to the bottom of a box. Near the bottom of the box, the region in which large particles are packed exists. Above this region, the region in which small particles are rich exists. For convenience, we name the boundary between these two regions the *S-L* boundary. Because of the fluctuation of large particles' concentration near the bottom, *S-L* boundary has finite inclination. Small particles on this slope cannot invade the region in which large particles are rich because large particles are packed densely. However, along this boundary, small particles can flow down. Then, the amount of small particles that flow in the $y < 0$ region is very small compared to that in the $y > 0$ region because particles in the $y < 0$ region are packed more densely than in the $y > 0$ region. Moreover, above the

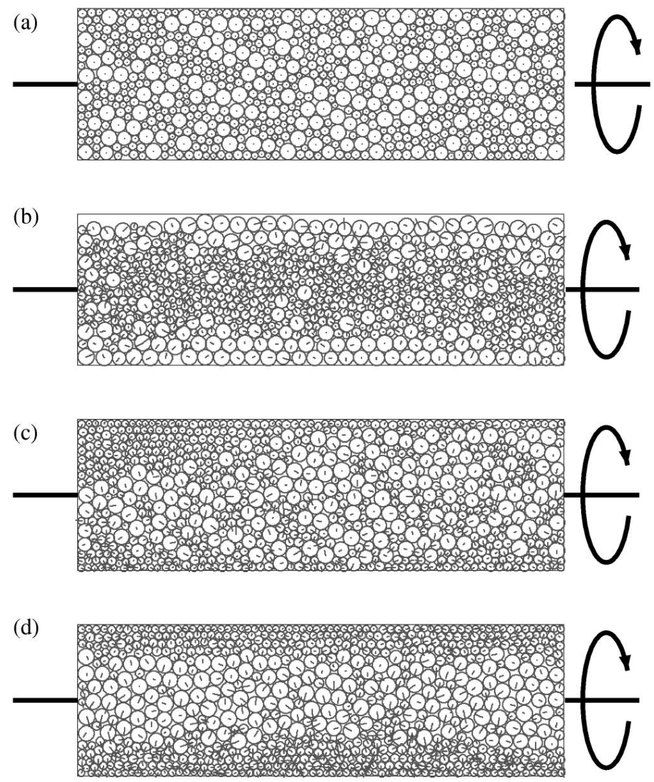

FIG. 2. Typical snapshots of (a) initial condition, and radial segregation patterns respectively (b) $Aw^2 < g$; (c) Aw^2 is a little larger than g; and (d) $Aw^2 > g$.

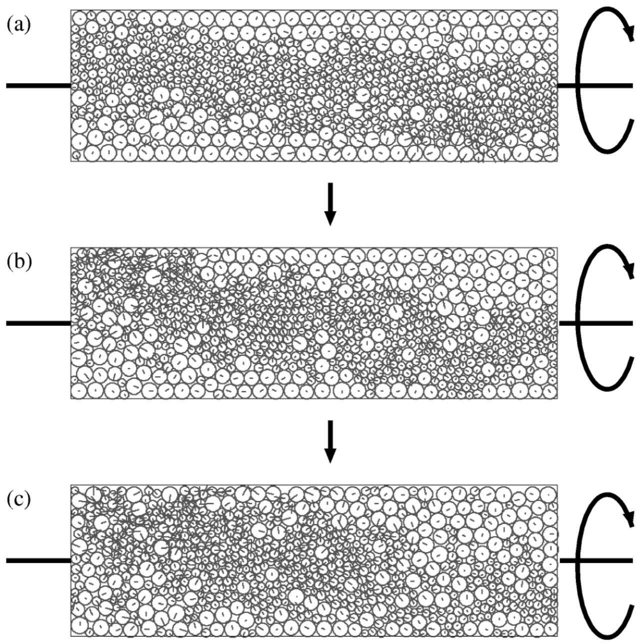

FIG. 3. Snapshots of fluctuation growth of large particles' concentration for axial direction [(a)→(b)→(c)], and typical axial segregation pattern (c).

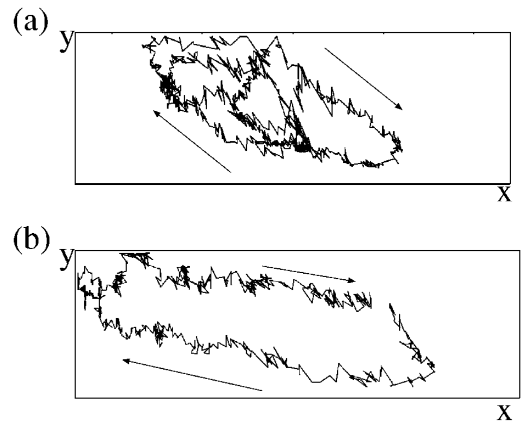

FIG. 4. Trajectories of sample particles for 1600 rotation times of box: (a) small particles, and (b) large particles.

region rich in small particles, the region rich in large particles exists again. We name the boundary between these two regions the *L*-*S* boundary. Large particles in this region cannot invade into the region in which small particles are rich because they cannot go through small voids which appear in the region rich in small particles. Because of friction working at the *L*-*S* boundary, however, some parts of the large particles in this region near the *L*-*S* boundary are dragged by the flow of small particles, which flow down along the slope of the *S*-*L* boundary. Thus, some of the large particles around the *L*-*S* boundary flow down along the boundary. Hence, the axial concentration of large particles in this region fluctuates and this fluctuation increases along the *S*-*L* boundary [Figs. 3(a)→3(b)→3(c)]. The direction of gravity periodically changes between the negative direction and the positive direction in y with the rotation of the box. Thus, the above-mentioned flow of particles all around the system forms global convection along the *S*-*L* boundaries as in Fig. 4. Furthermore, the convection makes the fluctuation of large particles' concentration increase, and changes the segregation pattern from the radial to the axial. Moreover, the axial segregation pattern is kept stable by the convection.

In order to discuss the phase inversion of the radial segregation pattern, we assume the following assumptions hold according to previous studies [4–11]. Compared to large particles, small particles can move more easily in a granular bed because they can move through smaller voids. It means that small particles are more directly drifted by external force than large particles. Then, we assume that small particles, compared to large particles, tend to move to the direction in which external force works. Large particles can also move through voids if their sizes are larger than that of large particles. Then, large particles tend to move to the low particles' density region in which such large voids tend to appear. By the use of these assumptions, the mechanism of the phase inversion of a radial segregation pattern is discussed. The force which works on each particle is given by Eqs. (3) and (4). We put $(X, Y) = (y\cos(wt), y\sin(wt))$. Here, the direction of gravitation is from $Y > 0$ to $Y < 0$. Now, the region in a drum is given by circle $X^2 + Y^2 \leq A^2$, and the region in which $F_i^{\mathrm{ex}} < 0$ for $y > 0$ and $F_i^{\mathrm{ex}} > 0$ for $y < 0$ are satisfied is given by the circle

$$X^2 + \left(Y - \frac{g}{2w^2}\right)^2 < \left(\frac{g}{2w^2}\right)^2. \tag{5}$$

For convenience, we name the former circle "circle 1" and the latter "circle 2." The external forces work toward the center of circle 1 on each particle in circle 2, and toward the circumference of circle 1 in another region in circle 1. Now, the movement of particles in the $Y < 0$ region seems quite small compared to that in the $Y > 0$ region because the packing of particles in the $Y < 0$ region is more dense than that in the $Y > 0$ region. Hence, we need to consider the movement of particles only in the $Y > 0$ region. When $Aw^2 < g$, circle 2 covers up to the circumference of circle 1 in $Y > 0$ (Fig. 5). It means that in most of the $Y > 0$ region, the external force works toward the center of the drum, so that small particles move toward the center of the drum. Because of the movement of small particles, a low density region appears near the uppermost position of the drum and large particles accumulate around there. On the contrary, when $Aw^2 > g$, circle 1 completely covers circle 2 (Fig. 5). It means that small particles in circle 2 move toward the center of the drum, and small particles out of circle 2 move toward the wall of the drum. Then, since low particle density space appears around the circumference of circle 2, large particles accumulate there.

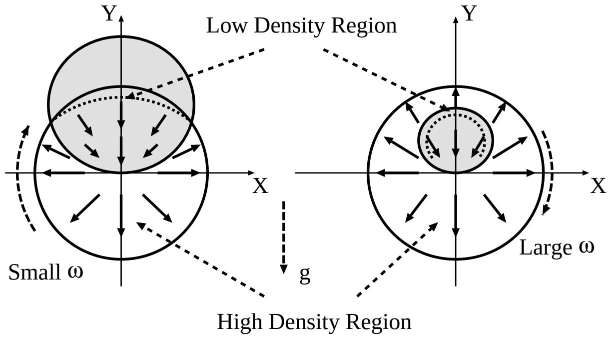

FIG. 5. Direction of external force and distribution of particle density. White circles are "circle 1," gray circles are "circle 2," and solid arrows indicate the direction of external force.

The length between the center of circle 1 and the farthest point on the circumference of circle 2 from the center of circle 1 is given by $\frac{g}{w^2}$. Hence, when $Aw^2 > g$, the annular pattern of the radius which is estimated to be about $\frac{g}{w^2}$ is formed by large particles. Thus, the relation between the angular velocity of the drum w and the radius $\bar{y}$ where large particles aggregate is given by

$$\bar{y} = A \left[w < \left(\frac{g}{A} \right)^{1/2} \right], \tag{6}$$

$$\bar{y} \sim \frac{g}{w^2} \left[w > \left(\frac{g}{A} \right)^{1/2} \right]. \tag{7}$$

The phase inversion angular velocity w_c is given by $w_c = (\frac{g}{A})^{1/2}$.

In this paper, by use of simulations and brief analysis, we discussed the radial segregation and axial segregation of granular mixtures which are almost completely packed in a horizontally rotating drum. By simulating a 2D horizontally rotating box, we reproduced two types of radial segregation patterns and the phase inversion between them, which have been found in previous experiments [19]. Furthermore, in this simulation, global convection was observed to appear after the radial segregation pattern was formed, and this convection caused the axial segregation pattern. Moreover, by use of the competition between gravitation and centrifugal force which depends on the angular velocity of a drum, we explained the phase inversion and found the critical angular velocity at which it takes place. By this discussion, we also derivate the annular pattern as the radial segregation pattern which appears in experiment [19]. We expect that the clear annular pattern appears also in the simulation if we use the system which includes a larger number of particles. This is a future issue. Moreover, in order to explain the phase inversion, we assumed that small particles, relatively, tend to move in the direction of external force and large particles move to the lower particle density region. The justification of this assumption remains to be made.

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