Segregation of large granules from close-packed cluster of small granules due to buoyancy

Xian-qing Yang,[1,*] Kun Zhou,[1] Kang Qiu,[1] and Yue-min Zhao[2]
[1]*College of Science, China University of Mining and Technology, Xuzhou 221008, China*
[2]*School of Chemical Engineering and Technology, China University of Mining and Technology, Xuzhou 221008, China*
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Segregation of large granules in a vibrofluidized granular bed with inhomogeneous granular number density distribution is studied by an event-driven algorithm. Simulation results show that the mean vertical position of large granules decreases with the increase of the density ration of the large granules to the small ones. This conclusion is consistent with the explanation that the net pressure due to the small surrounding particle impacts balances the large granular weight, and indict that the upward movement of the large granules is driven by the buoyancy. The values of temperature, density, and pressure of the systems are also computed by changing the conditions such as heating temperature on the bottom and restitution coefficient of particles. These results indicate that the segregation of large granules also happen in the systems with density inversion or even close-packed cluster of particles floating on a low-density fluid, due to the buoyancy. An equation of state is proposed to explain the buoyancy.

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I. INTRODUCTION

Granular matter is composed of many pieces of grains that can move independently. In the past two decades, it has attracted a large amount of research attention [1], and is becoming one of the most active research fields. In addition to its importance in industries and its ubiquitous existence in nature, this is attributed to the unique properties of granular matter. While the granular matter shares many properties with solids, liquids, or gases, it cannot be simply classified as anyone of them, i.e., it should be considered as an additional state of matter in its own right. Therefore, beyond the standard statistical mechanics, hydrodynamics, or traditional solid mechanics, unique theoretical ideas are required.

Segregation phenomena exist extensively in granular materials of different species. For instance, in a vibrated granular system, depending on subtle variations in physical conditions, large particles can rise to the top, sink to the bottom, or show other patterns. The first two are known as "Brazil Nut effect" [2] and "anti-Brazil Nut effect," respectively.

Many experimental, numerical, and analytical techniques have been applied to probe segregation. For a recent review, see Ref. [3]. The underlying reason for segregation is the dissipative nature of the granular matter, arising from the frictional forces among grains. Nevertheless, segregation has been shown to be a complex phenomenon [1]. Many factors, associated with external physical conditions or particle-specific properties, can play significant roles in segregation. These factors include the frequency and amplitude of vibration [4–11], the nature of interstitial air, the size [2,4,6,7,10,12–14] and size distribution of granular particles [11,15], the shape of particles [16], and other properties such as density [13,14,17–25], elasticity [11], and others such as the nature of interstitial air [20,21,26]. As a consequence, albeit the Brazil Nut effect has been observed for decades, a completely satisfactory explanation still seems absent [3,27].

A variety of mechanisms has been proposed for segregation. The corresponding theoretical models include the void filling [2], the arching [4], the inertia [18,22,25], the global convection models [5], and the condensation models [25], etc. Naturally, each of these models involves a number of assumptions. While these assumptions may be plausible in some cases, they can be invalid in other cases. For instance, the "void filling" mechanism, which states that the upward movement of large particles in the Brazil Nut effect is due to the higher probability of the void filling by small particles, neglects the function of global-convection motions that can be important in some cases [5].

Recently, segregation was investigated in the dilute vibrofluidized regime [14]. In contrast to the dense regime where enduring contacts of multiple particles dominate, particles in vibro-fluidized granules are sufficiently agitated such that the main particle interactions are two-particle collisions and sustained contacts rarely occur. Using the discrete element computer simulations, Shishodia and Wassgren investigated an intruder model system in a two-dimensional vibrofluidized bed [14]. The large particle, namely the intruder, was observed to rise approximately to an equilibrium height and then fluctuate about that height. The equilibrium height was measured as a function of a variety of parameters, including the vibration amplitude, the mass density ratio of the intruder to the surrounding small particles, and the diameter ratio, etc. Instead of the mechanism mentioned in the previous paragraph, it was reported that segregation can be explained by a balance between the intruder weight and the net granular pressure, or "buoyant" forces within the vibro-fluidized bed. The quantitative agreement of the theoretical predictions and the simulation results is more or less satisfactory.

In the work of Shishodia and Wassgren, the spatial distribution of the surrounding small particles was considered to be homogeneous. However, the inhomogeneity of spatial distributions of particles in vibrofluidized granules occurs more frequently than homogeneity. The density inversion and one of its limiting cases, the close-packed floating clusters, were

*E-mail: xianqyang@sina.com.cn

reported in both simulations [28–31] and experiments [32–34]. There is no guarantee that, although plausible, the buoyancy mechanism is mainly responsible for segregation in a vibrofluidized bed in which the small particles are nonuniformly distributed. In particular, the theoretical methods in Ref. [14], which were used to calculate the equilibrium height of the intruder, have to be adjusted or improved. A systematic investigation seems justified.

The organization of the present paper is as follows. In Sec. II, we employ the event-driven (ED) algorithm [35] to simulate the intruder model system in a two-dimensional vibrofluidized bed. The granular particles are fluidized by a rapidly vibrating bottom plate, which, together with the gravity field, results in an inhomogeneous vertical distribution of the small particles. Various quantities, including the equilibrium height of the intruder(s), the granular temperature, the granular pressure and its gradient, are measured or calculated. Section III presents a theoretical model for the segregation phenomena observed in Sec. II; a comparison of the theoretical prediction and the simulation results is made. A brief discussion is given in Sec. IV.

II. SIMULATIONS

The simulated granular materials consist of N_1 disks of diameter $d_1=2$ mm and N_2 disks of $d_2=6$ mm; the corresponding mass densities are denoted as ρ_1 and ρ_2, respectively. The present work focuses on the case $N_1 \gg N_2$, i.e., the intruder model system. The particles are restricted to move in the x-y plane, with gravity acceleration g acting in the negative y direction. They are placed within a frictionless infinitely high well with width $L_x=0.2$ m in the x direction; a driving base is located at $y=0$ in the vertical direction. The fluidized state of the particles is obtained by colliding with the vibrating bed that oscillates with high frequencies and small amplitudes: there is no other direct coupling between the vibration bed and the collective granular motion. Thus, instead of specifying frequency and amplitude for the oscillating bed, one can characterize the extent of vibrofluidization by a granular temperature for an immobile bottom plate (the definition of the granular temperature will be given later), say T_0. Immediately after colliding with the base, the velocity of a particle is given from a Maxwell distribution with temperature T_0 (measured in the units of energy). Then, the kinetic energy is gradually lost by inelastic hard-core collisions with other particles and with the walls of the well. The particle-particle and particle-wall coefficients of restitution were set identical, and are denoted as r.

First, we simulated granular of $N_1=1200$ and $N_2=20$. The restitution coefficient was set at $r=0.90$ and the temperature of the bottom plate was $T_0=1.44$. The density of small particles was taken as $\rho_1=1.0$ g/mm^2, and ρ_2 was varied. Initial simulations of about 1×10^4 collisions per particle are discarded for the transients to die out. For ratio $\rho_2/\rho_1=0.4$, 1.0, and 2.0, the corresponding typical configurations of the particles are shown in Figs. 1(a)–1(c), respectively. These suggest that the relative vertical positions of the larger particles (intruders) to those of the smaller ones (host particles) depend on their mass-density ratio ρ_2/ρ_1. For $\rho_2/\rho_1<1$, the Brazil Nut Effect occurs, namely, the intruders float to the top; for $\rho_2/\rho_1>1$, the intruders sink to the bottom, the anti-Brazil Nut Effect; for $\rho_2/\rho_1=1.0$, the larger particles almost stick around the middle of the well. Figures 1(a)–1(c) also show that the vertical distribution of small particles are not homogeneous: near the bottom and the top of the bed they are dilute while they are rather dense in the middle of the bed. As the number of the intruders is small enough, effects of the intruders on the distribution of the small particles can be neglected. Thus, the inhomogeneity is independent of the presence of the intruders.

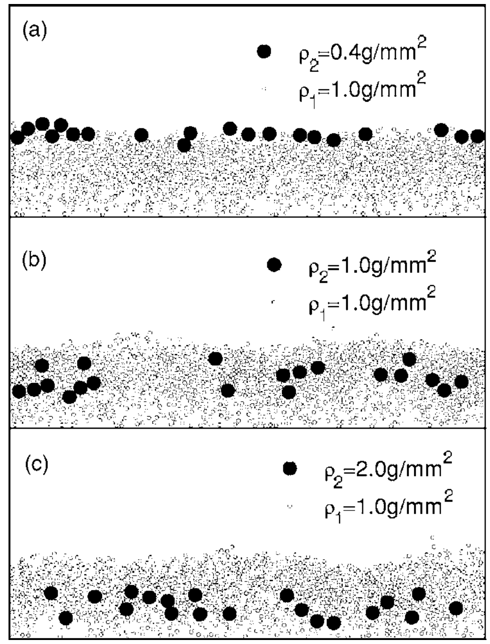

FIG. 1. Three typical configurations of a bed with $N_1=1200$ and $N_2=20$ for different values of $\rho_2/\rho_1=0.4$ (a), 1.0 (b), and 2.0 (c). The restitution coefficient $r=0.90$, and the base temperature $T_0=1.44$. The data are obtained after 10^4 collisions pre-particle.

The time-averaged vertical positions of the intruder particles and those of the host particles were measured. The ratio $\langle y_2\rangle/\langle y_1\rangle$ is shown in Fig. 2(a), as a function of the ratio ρ_2/ρ_1. This indicates that the ratio $\langle y_2\rangle/\langle y_1\rangle$ is a monotonically decreasing function of $\langle\rho_2\rangle/\langle\rho_1\rangle$. For $\rho_2/\rho_1=1$, the value of the ratio $\langle y_2\rangle/\langle y_1\rangle$ is roughly 1. Only for rather large (or small) values of ρ_2/ρ_1 do the intruders sink to the bottom (or rise to the top) of the bed. In comparison of these results with those in Refs. [14,24,36], we conclude that the segregation of intruders from the inhomogeneously distributed host particles is also driven by buoyancy: balance of the gravity force and the "buoyant" forces owning to the interparticle collisions. Nevertheless, a quantitative theory is still desired, since the distribution of host particles is no longer uniform as in Refs. [14,24,36].

Next, for a quantitative description of the inhomogeneity of the host particles, we simulated the vibrofluidized bed with $N_2=0$, i.e., the absence of the intruder. To obtain the number density of small particles, we divide the two-dimensional box into several small domains in the y direction and then calculate the number of small particles in every

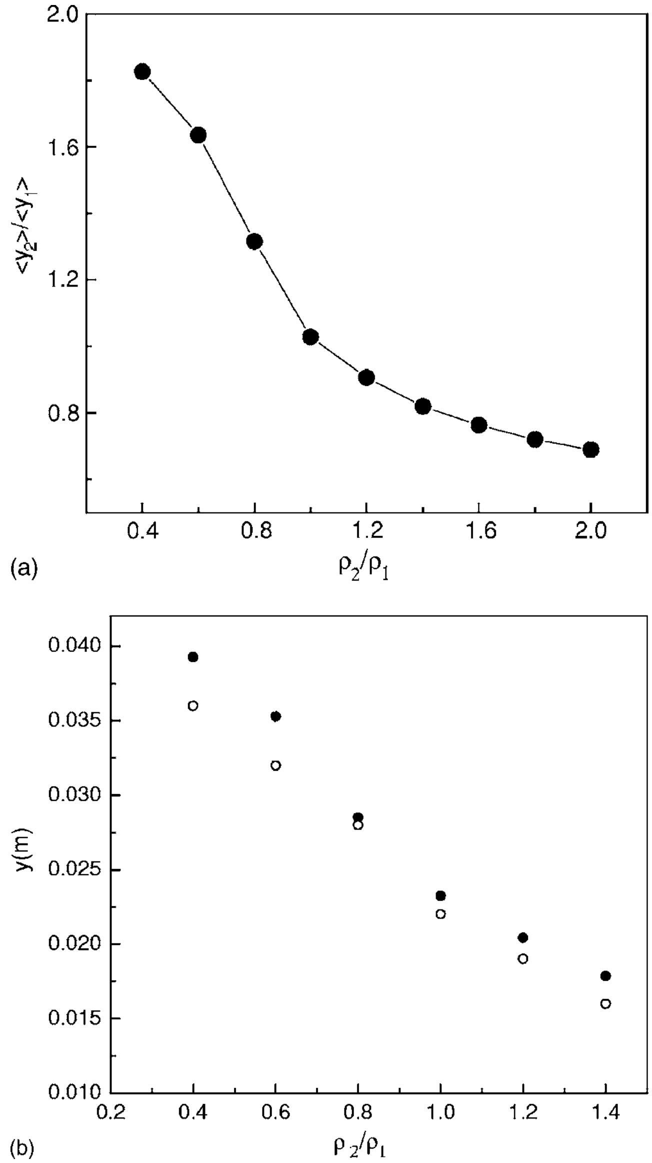

FIG. 2. (a) The ration $\langle y_2/y_1\rangle$ as a function of the density ratio ρ_2/ρ_1 for $d_2/d_1=3.0$. The restitution coefficient $r=0.90$, and the base temperature $T_0=1.44$. The data are obtained after 10^4 collisions per particle. (b) compares vertical positions of intruders obtained by Eqs. (6) and (7) (open circle) with the simulations (solid circle). The restitution coefficient $r=0.90$, and the base temperature $T_0=1.44$. The data are obtained after 10^4 collisions per particle.

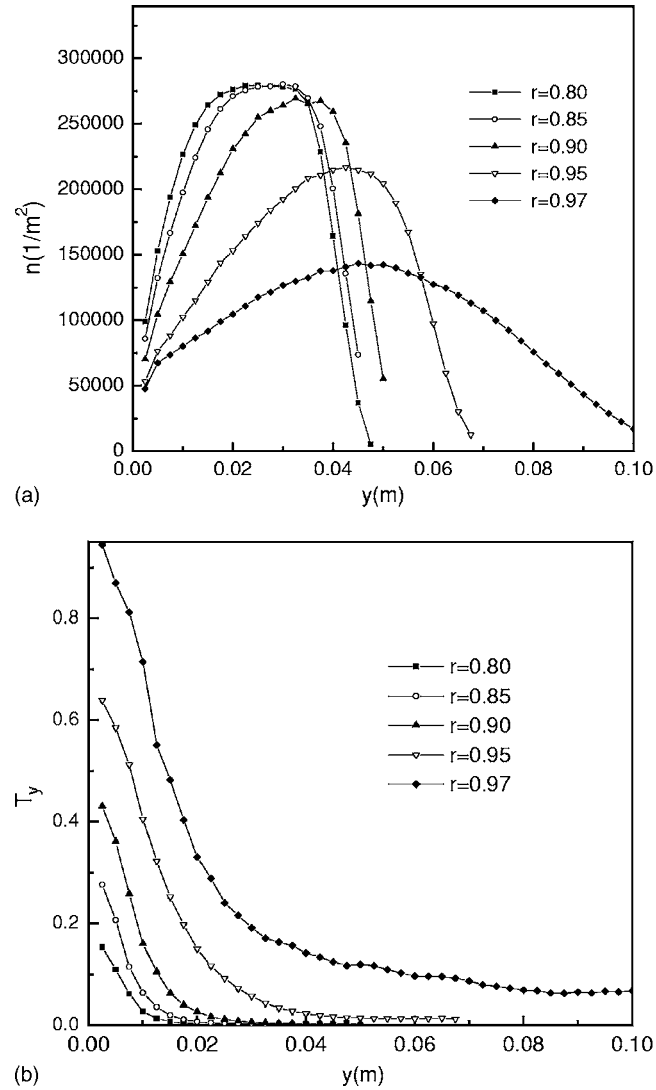

FIG. 3. (a) The particle number density $n(y)$ versus the height y with different restitution coefficient r. The particle diameter d $=2$ mm, density $\rho=1.0$ g/mm^2, the base temperature $T_0=2.25$, the number of particle $N=2000$. (b) shows that the granular temperature T_y (scaled by units of energy) versus the height y with different restitution coefficient r. The particle diameter $d=2$ mm, density ρ $=1.0$ g/mm^2, the base temperature $T_0=2.25$, the number of particle $N=2000$.

small domain. Let n denote the number density of the small particles. Further, the granular temperature of particles as the height increasing within the bed was calculated to characterize granules in the vibrofluidized limit. We define the granular temperature T of the particles as

$$T_{x,y}=\frac{m}{2}(\langle v_{x,y}^2\rangle-\langle v_{x,y}\rangle^2), \tag{1}$$

where $v_{x,y}$ is the velocity of the small particles in the x direction or the y direction and the angular brackets represent the statistical average over configurations arising from different initial particle distributions. Owning to the vector nature of the velocity, the temperature T is not a scalar in vibrated systems either, and equipartition of energy is not observed [33]. Therefore, T_x and T_y are not equal. Here, we focus only on velocity in the y axis and obtain the temperature in the vertical direction T_y. Figure 3 shows the number density of particles and the granular temperature as a function of the height y. As expected, the particles are not homogeneously distributed: dilute on the top and at the bottom of the well, and dense in the middle. Namely, the particle density inversion is observed. But, granular temperature exhibit different behavior: T_y decreases with the height monotonically. Therefore, in the case of uniformity of the small particles and monotonically decreasing of granular temperature, we would wonder why the value of ratio $\langle y_2\rangle/\langle y_1\rangle$ shows linearly decreasing, as seen in Fig. 2(a).

As buoyancy dominates, net pressure is from particle collisions in the vertical direction. Suppose there is a number of horizontal walls which do not exist actually and are only considered as test surfaces, and collisions between particles and the walls are elastic. If a particle with vertical velocity v_y touches the wall, the difference of the momentum of the particle after and before the collision is

$$-m_i v_y - m_i v_y = -2m_i v_y, \tag{2}$$

and the impulse of particle exerted by the wall in the vertical direction is $2m_i v_y$, according to the second law. To calculate the collisional vertical stresses, let us consider the number of particles colliding with one wall locating at y_l in a time interval Δt. We define an average vertical velocity $\bar{v}_y$ of particles within the region $[y_l - d, y_l + d]$, where d denotes the radius of the small particles, thus the average time interval is $\Delta t = d/\bar{v}_y$. If colliding with the wall, particles above the wall satisfy

$$v_{iy} < 0, \quad y_l < y_{iy} < y_l + |v_{iy}\Delta t|, \tag{3}$$

and particles below the wall have

$$v_{iy} > 0, \quad y_l - |v_{iy}\Delta t| < y_{iy} < y_l. \tag{4}$$

Therefore, the total impulse of particles exerted by the wall is $\Sigma 2m_i v_{iy}$, where the summation is over all collisions occurring in time Δt. Then, the net force acting in the vertical direction reads

$$F = \frac{\sum 2m_i v_{iy}}{\Delta t}, \tag{5}$$

and the net pressure in the vertical direction is

$$P = \frac{F}{L_x}. \tag{6}$$

On the basis of the above equation, one can compute the distribution of the net pressure within the bed. Figure 4 shows the pressure versus the height y, which suggests that the pressure distribution is also inhomogeneous. The pressure increases rapidly with the increase of the height y in the region where the value of the height is below about 0.015 m; while the value of the height is above about 0.015 m, net pressure decrease monotonically with the increase of the height. As we know, the pressure distribution given here is different from that obtained in a vibrofluidized bed where the pressure increases with increasing depth from the free surface of the bed and reaches a maximum at the floor [14]. In the work of Shishodia and Wassgren, two modes including the "streaming" mode and the "collisional" mode have been taken into account because the systems investigated there have flow states. But, here we only consider collisions between particles.

At equilibrium, the net vertical force acting on an intruder due to collisions with the surrounding particles will balance with the intruder' weight. Thus, equating the net pressure force with the weight gives

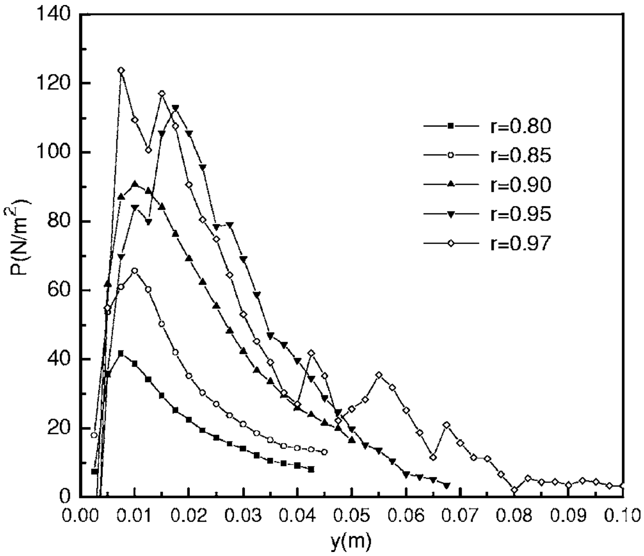

FIG. 4. The pressure P versus the height y with different restitution coefficient r. The particle diameter $d=2$ mm, density $\rho=1.0$ g/mm^2, the base temperature $T_0=2.25$, the number of particle $N=2000$.

$$Pd_2 = m_2 g, \tag{7}$$

where m_2 and d_2 are the mass and the diameter of the intruder, respectively.

In the vibrofluidized limit, it is plausible that the presence of some intruders does not change the pressure distribution of host particles. Then, Eqs. (5)–(7) yield the equilibrium position of the intruder, as long as the density ρ_2 is given.

On the other hand, the pressure distribution given by Eq. (6) in the case of density inversion can be checked by calculating the equilibrium position of the intruder. As shown in Fig. 4, there are two heights at which the net pressure force balances the intruder weight. But, near the bottom of the bed, that is $y < 0.015$ m, granular temperature is very high, and particles are very dilute, as seen in Fig. 3, therefore the position of the intruder below about 0.015 m becomes unstable due to intensive perturbation of surrounding small particles to the intruder. The stable position of the intruder is only above the height about 0.015 m. For given density of intruder particles, according to Eq. (7), the net pressure balancing the weight of the intruder can be obtained. Therefore the expected equilibrium positions of the intruder corresponding to the net pressure can be estimated with the aid of Fig. 4.

Figure 2(b) compares the equilibrium positions of the intruder particles predicted by the net pressure, with the equilibrium positions found in simulations with different density ratios between large intruder particles and small host particles. As shown in Fig. 2(b), open circles correspond to the equilibrium position of the intruder particles predicted by Eqs. (6) and (7), and solid circles represent the equilibrium positions of the intruders obtained from simulations. One can see that the agreement between simulations and the net pressure predictions is very good. The near linear dependence of the equilibrium position on the density ratio occurs due to the approximately linear varies of the net pressure with the height.

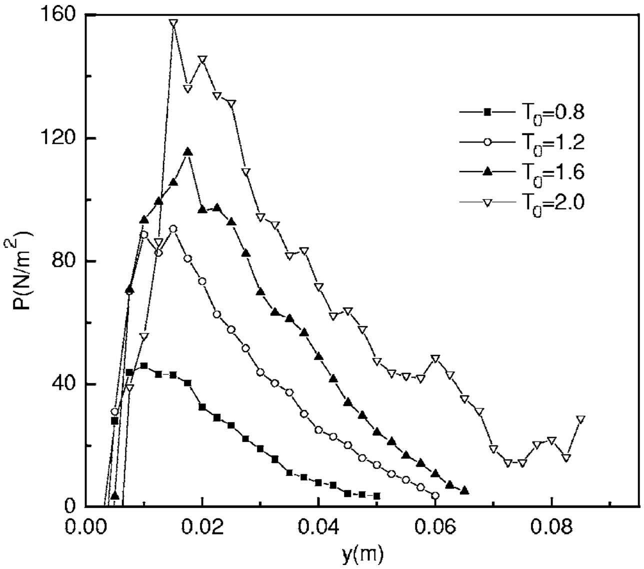

FIG. 5. The pressure P versus the height y with different values of the base temperature T_0. The particle diameter $d=2$ mm, density $\rho=1.0$ g/mm^2, the restitution coefficient $r=0.95$, the number of particle $N=2000$.

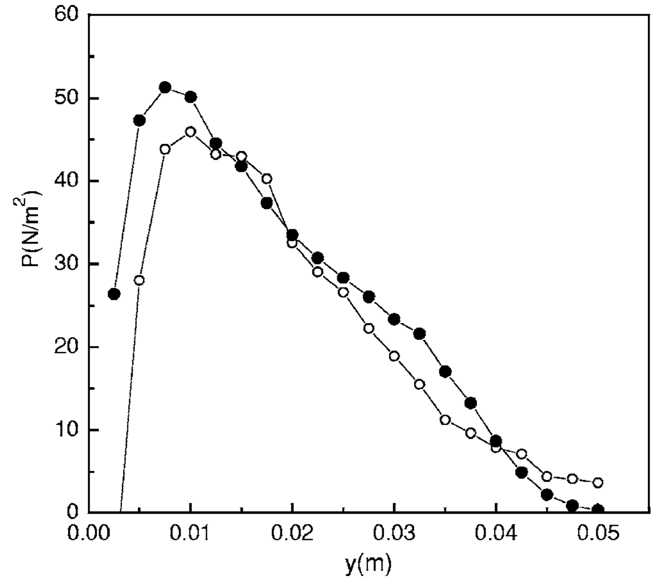

FIG. 6. The pressure P versus the height as predicted by the EOS (open circle curve), and obtained by simulations (solid circle curve) with $N=2000$ of particles with diameter $d=2$ mm, density $\rho=1.0$ g/mm^2, $r=0.95$ and the temperature at base $T_0=0.64$.

Figures 3 and 4 also show the particle number density n, the granular temperature T_y, and the net pressure distributions by changing restitution coefficient of granular r. In Fig. 3(a), the particle number density increases with the increase of the height y, to a maximum, and then decrease with further increase of height y. The particle number density inversion happens. As the restitution coefficient r is suppressed, the value of $n(y)$ increases for a fixed height y, and the height y of the highest number density shifts toward the left. Moreover, Fig. 3(a) shows that the maximum value of $n(y)$ increases when r is reduced. When the value of r is about or below 0.85, the maximum value of $n(y)$ does not further increase. In this case, a close-packed cluster occurs. the granular temperature T_y is shown in Fig. 3(b), which suggests that the value of T_y is the highest on the base, and monotonically decreases with the height. Further, as expected, the value of T_y ascends when r is enhanced. Figure 4 shows the net pressure as a function of y for several values of r: the value of the pressure monotonically decreases with that of y. Thus, if an intruder is placed in the system, the equilibrium position rises with the decrease of its density; in the case of the close-packed cluster, the intruder can rise across the top if its density is sufficiently small.

Figure 5 shows the net pressure $P(y)$ for several values of the base temperature T_0. It is suggested that, for a given height y above a certain value, increasing T_0 would raise the value of the pressure P. Further, the granular temperature T_y and the impulse of particle collisions increase when T_0 goes up, because more energies can be obtained from the environment. As a result, the net pressure obtained from Eq. (6) increases with the increase of the base temperature. Therefore, when an intruder is in the system, its equilibrium position will rise with the decrease of its density, because of a balance between the intruder weight and the net granular pressure.

III. A THEORETICAL MODEL

The above simulation results indicate that no mean flow of macroscopic grains exists in the system of density inversion or close-packed cluster. In this case, the molecular chaos assumption breaks down, and the Navier-Stokes granular hydrodynamics (NSGH) is not applicable. Recently, using free volume arguments in the vicinity of the hexagonal packing, Grossman *et al.* [30] derived an equation of state (EOS) $P=P(n,T_y)$, describing almost close-packed floating cluster. The EOS reads

$$P = nT_y \frac{n_c + n}{n_c - n}, \tag{8}$$

where $n_c = 2/(\sqrt{3}d^2)$ denotes the close-packing density, n is the particle number density, T_y represents the granular temperature, and P is the pressure. Then, a variant of the NSGH was proposed to describe the density inversion or the almost close-packed floating clusters [31]. A very good agreement between the number density obtained by this hydrodynamics and molecule dynamics (MD) simulations was obtained in Ref. [31]. Therefore, we believe that Eq. (8) is also suitable for characterizing our model.

Figure 6 compares the net pressure, predicted by the EOS (open circle curve), with the pressure obtained by simulations (solid circle curve) with $N=2000$ of particles with diameter $d=2$ mm, density $\rho=1.0$ g/mm^2, $r=0.95$ and the temperature at base $T_0=0.64$. Here we do not intend to work out the constitutive relations (CRs) proposed in Refs. [30,31], and only calculate the P by replacing $n(y)$ and $T_y(y)$ in Eq. (8) by simulations shown in Fig. 3. One can see that the agreement between the EOS and simulations is surprisingly good.

The results shown above indicate that the vibrofluidized steady state, considered in this work, has zero mean flow. Accordingly, in Sec. III, the method for computing the net pressure which only considers collisions between particles and ignore the "streaming" mode, is successful. Although the buoyancy dominate size segregation in both the model proposed by Shishodia and Wassgren and us, the origin of buoyant forces in our model is different from that in Ref. [14]. Thus, these results also indicate that buoyant forces which drive the size segregation come neither from differences in the local granular temperature [37], nor from convection triggered by the dynamically created temperature gradient [38], in presence of density inversion, or almost close-packed floating cluster. Instead, it is from particle collisions in the vertical direction.

IV. CONCLUSIONS

Size segregation of large granules from the small ones has extensively been studied in systems where the spatial distribution of the surrounding small particles is homogeneous. In this paper, we used an event-driven algorithm to investigate the size segregation of intruder large particles from small particles with an inhomogeneous particle number density. Simulation results exhibit that the mean vertical position of large granules decreases with the increase of the density ration of the large particles to the small ones. The pressure of granular system due to the surrounding small particle impacts has been calculated. One can see that the pressure decreases with the increase of the height. With the aid of the pressure, the equilibrium position of the intruders can be derived and gives an agreement with the simulation results. Therefore, the upward movement of the large granular is driven by the buoyancy.

The values of temperature, small particle number density, and pressure of the systems are also computed by changing the conditions such as temperature of the thermal base and restitution coefficient of particles. These results indicate that the segregation of large intruder granules also happen in the small surrounding particle systems with density inversion or even close-packed cluster of particles floating on a low-density fluid, due to the buoyancy.

The simulation results here indicate that an intruder will move to an equilibrium position within the bed such that the net pressure balances the particle weight. This conclusion looks like the results obtained in Ref. [14]. In fact, our model is different from one presented in Ref. [14]. In Ref. [14], an intruder moves to top in the homogeneous vibrofluidized bed. However, in this paper, we discuss that intruders are in the nonhomogeneous systems, even in the case of the density inversion or close-packed floating cluster. The cause of buoyant forces in our model is also different from that offered in Ref. [14]. On the other hand, only an intruder's equilibrium position can be predicted from the granular pressure profile. In the paper, the pressure profile cannot only be used to predict intruders' equilibrium position, but can be explained by an equation of state.

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