

# DEM/CFD modelling of the deposition of dilute granular systems in a vertical container

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**Deposition of granular materials into a container is a general industrial packing process. In this study, the deposition behaviour of dilute granular mixtures consisting of two types of particles that were of the same particle size but different particle densities in the presence of air was numerically analyzed using a coupled discrete element method (DEM) and computational fluid dynamics (CFD). Bilayer granular mixtures with light particles at bottom and heavy particles at top were first simulated. It was found that the presence of air significantly affected the flow behaviour of the bilayer mixtures. For the system with a relatively low initial void fraction, the air entrapped inside the container escaped through the dilated zones induced due to the friction between the powder bed and wall surfaces. The escaping air streams entrained light particles that were originally located at the bottom of the granular system. Consequently, these light particles were migrated to the top of the granular bed at the end of deposition process. More light particles were migrated when the deposition distance was increased. For the system with a high initial void fraction, some light particles penetrated into the top layer of heavy particles and created a mixing zone. Deposition of random mixtures with different initial void fractions was also investigated and the influence of initial void fraction on the segregation behaviour was explored as well. It was found that the increase of void fraction promoted segregation during the deposition in air. It was demonstrated that, for granular mixtures consisting of particles of different air sensitivities, the presence of air had a significant impact on the mixing and segregation behaviour during the deposition.**

DEM, CFD, packing, deposition, mixing, segregation, air effect, dusting

Granular mixtures are common physical matters in nature and in various process industries, such as chemical, pharmaceuticals, food and powder metallurgy. They generally consist of particles with different physical properties, such as size, density and shape. The difference in particle properties can induce segregation that is referred to as a phenomenon in which a homogeneous granular mixture becomes spatially non-uniform in such a manner that the particles with the same physical properties congregate in the mixture during handling and processing<sup>[1]</sup>. It has been shown that segregation can be induced as a result of the differences in particle size<sup>[2–4]</sup>, density<sup>[5,6]</sup> and shape<sup>[7]</sup>.

Among all the properties which might cause segregation, it is well recognised that the difference in particle size was the most important factor in most situations<sup>[2–4]</sup>.

While an increasing amount of evidence showed that the density difference could predominate, especially during the flow of gas-solid systems<sup>[8–12]</sup>. Density induced segregation in binary granular mixtures subjected to vertical vibration was investigated by Shi et al.<sup>[8]</sup>, who observed that a layer of light particles emerged at the top of the powder bed after the vibration and the thickness of this top layer depended on the density ratio. Yang<sup>[9]</sup> simulated the vertical vibration of granular mixture using DEM and showed that the heavy particles tended to gather around the central region and the concentration of

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light particles was higher at the top compared with that of heavy ones. Nevertheless, Burtally et al.<sup>[10]</sup> found that the light particles could also segregate to the bottom due to the effect of air drag in the vibration experiments, and similar behavior was also observed by Zeilstra et al.<sup>[11,12]</sup> from numerical simulations using a hybrid granular dynamics-computational fluid dynamics method. Therefore, for gas-solid systems, the presence of gas can significantly affect the flow behaviour of the granular systems and subsequently the mixing and segregation behaviour.

Our recent study<sup>[13]</sup> revealed that the influence of the presence of air on the flow behavior of granular systems consisting of particles with different sizes and densities can be characterized using a dimensionless parameter  $\xi$  that is defined as

$$\xi = A_r \Phi_p, \quad (1)$$

where  $\Phi_p (= \rho_s / \rho_a)$  is the ratio of solid density  $\rho_s$  to the air density  $\rho_a$  and  $A_r$  is the Archimedes number for particle flowing in air and is given as

$$A_r = \frac{\rho_a (\rho_s - \rho_a) g d_p^3}{\eta^2}, \quad (2)$$

in which  $d_p$  is the particle diameter,  $\eta$  is the air viscosity and  $g$  is the gravitational acceleration. Granular materials are hence classified into two regimes with a critical value of the dimensionless parameter  $\xi_c = 9.56 \times 10^6$ : (i) air-sensitive ( $\xi < \xi_c$ ), for which the air has a significant effect on the granular flow; (ii) air-inert ( $\xi \geq \xi_c$ ), for which the effect of air is negligible. In the air-sensitive regime ( $\xi < \xi_c$ ), the sensitivity of powder flow to the presence of air is defined using an air sensitivity index  $\zeta$ ,

$$\zeta = 1 - \ln \xi / \ln \xi_c. \quad (3)$$

The smaller the value of  $\zeta$ , the less sensitive the powder is to the presence of air<sup>[14]</sup>.

In this study, the deposition of dilute granular systems consisting of powders with different air sensitivity indices ( $\zeta$ ) in a vertical container in the presence of air is simulated in 2D using the coupled DEM/CFD developed by Kafui et al.<sup>[15]</sup>. The mixing and segregation behaviour of the dilute granular mixtures in air and in a vacuum are explored.

## 1 Computational set-up

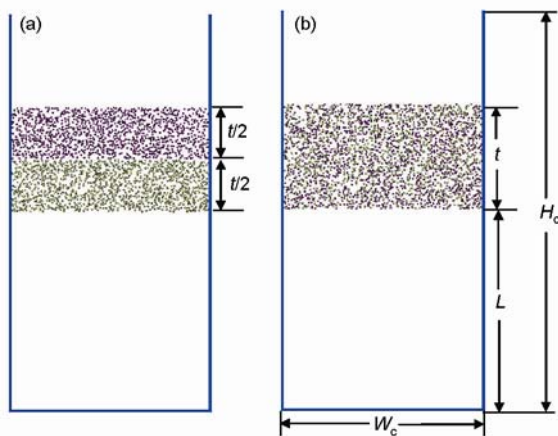
The coupled DEM/CFD method<sup>[15]</sup>, which has been approved to be a robust numerical model for simulating the flow of solid particles in the presence of air<sup>[13,14]</sup>, was

employed to analyze the deposition process of the dilute granular systems of elastic particles. In this method, the solid particles and air are modelled using DEM and CFD, respectively. A two-way coupling term has been incorporated to consider the particle-air interaction. The movement of individual particles is governed by Newton's second law, and a finite difference explicit integration scheme is used to solve the equations of motion to give the translational and rotational displacements of each particle in each time step. The particle-particle contact is governed by the classical contact mechanics, in which the Hertz theory<sup>[16]</sup> is used to model the normal interaction and the theory of Mindlin and Deresiewicz<sup>[17]</sup> is used for the tangential interaction. The air is treated as a continuous phase governed by the fluid continuity and momentum equations. The interaction forces between particles and air have been taken into account in the form of a combination of pressure gradient, viscous stress and drag force. These particle-air interaction forces were considered in solving the governing equations for both particle and gas phases, so that a two-way coupling is achieved to model the interactions between solid particles and air more realistically than standard DEMs<sup>[18–20]</sup> and the one-way coupling approach to consider the influence of the presence of air<sup>[18]</sup>. The detailed description of DEM/CFD used in this study can be found in ref. [15].

The initial configurations of the model systems considered are shown in Figure 1. The granular materials are deposited into a two dimensional container with a dimension of  $W_c \times H_c$ . For the simulations considered in this study, the width of the container  $W_c$  is fixed at 15 mm, while various heights are chosen in order to explore the influence of initial height on the mixing and segregation behaviour. In all the simulations, only monodisperse systems of particle diameter of 130  $\mu\text{m}$  are considered, while the particle densities are set to  $\rho_1 = 400 \text{ kg/m}^3$  and  $\rho_2 = 7800 \text{ kg/m}^3$ , respectively. Hence, from eqs. (1)–(3), the air sensitivities of these two types of particles are significantly different (i.e.  $\zeta_1 = 0.4233$  and  $\zeta_2 = 0.0535$ ). The particles are assumed to be elastic with a Young's modulus of 8.7 GPa and Poisson's ratio of 0.3, which corresponds to the material properties of microcrystalline cellulose. The walls of the container are elastic with a Young's modulus of 210 GPa, Poisson's ratio of 0.29 and density of 7900  $\text{kg/m}^3$ , which is representative of typical steel. The interparticle and particle-

wall friction coefficients are set to a value of 0.3.

Dilute granular mixtures of the two types of particles with a specified void fraction are initially generated as a granular bed of a thickness  $t=8$  mm, which are located at a distance of  $L$  from the base of the container (see Figure 1). Two initial configurations are considered: (i) bilayer mixture, for which the powder with a lower air sensitivity index ( $\zeta_2$ ) is generated as the top layer and the one with a higher air sensitivity index ( $\zeta_1$ ) as the bottom layer; (ii) random mixture, for which the same number of particles are randomly generated and mixed. The two types of particles are colour-coded so that the mixing and segregation behaviour can be directly visualised. After the sample generation, the granular mixtures flow under gravity until they settle at the bottom of the container with a negligible kinetic energy (i.e. the mean particle velocity is of the order of  $1 \times 10^{-6}$  m/s or less), at which the deposition process is assumed to be completed.



**Figure 1** The computational setup for the deposition of dilute particulate systems in a container. The light and heavy particles are shown in yellow and magenta, respectively. (a) Bilayer mixture; (b) random mixture.

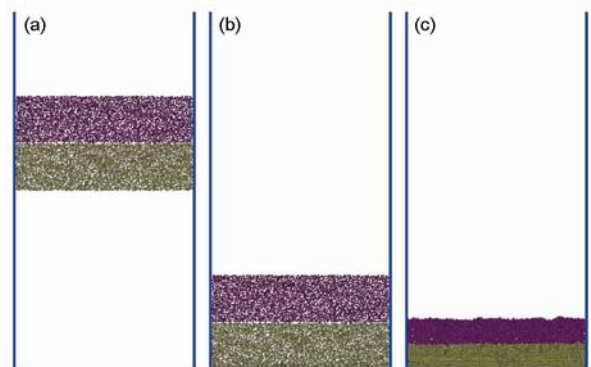
For the deposition in air, the air is initially distributed inside the container with a uniformly initial pressure of the standard atmospheric pressure ( $1.01325 \times 10^5$  Pa). It is assumed that the air has a temperature of 293 K and a viscosity of  $1.8 \times 10^{-5}$  kg/(m · s). The air is initially static, once the deposition process starts, it begins to flow as the particles flow downwards. The domain inside the container is discretised with the interior fluid cells to model the air flow using CFD. The walls of the container are treated as the impermeable and no-slip boundaries for the airflow, and the top of the container is assumed to be free (open) and is set as the continuous

gas outflow boundary with free-slip.

In this study, dilute granular mixtures with various void fractions in the range of 70%–90% are considered to investigate the effect of void fraction on the mixing and segregation behaviours. The samples with various solid fractions are generated by keeping the height of the initial granular bed constant (see Figure 1) and varying the number of particles to be used. By changing the distance  $L$  between the bottom of the initial granular bed and the base of the container, the dependence of the mixing and segregation behaviour on the deposition height is also investigated.

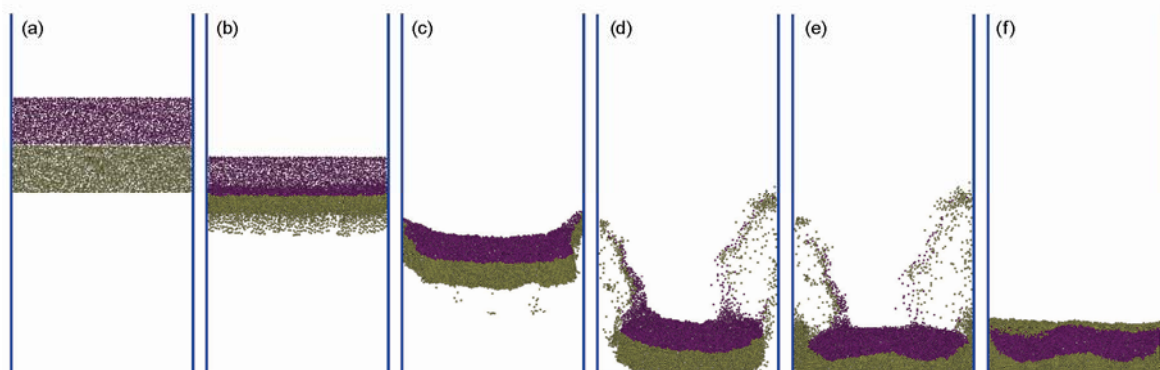
## 2 Deposition of bilayer granular systems

Bilayer mixtures consisting of particles with different air sensitivities were considered to explore the mixing behaviour during deposition, for which mixtures of various initial void fractions (i.e. 70%–90%) were examined. When no air is present in the container (i.e. in a vacuum), as shown in Figure 2, the two granular layers flow together at the same speed until the particles start to get in contact with the base of the container (Figure 2(b)). Thereafter, the packing of the granular system occurs under gravity. Two distinctive layers are formed at the end of the deposition process (see Figure 2(c)). The same phenomena were observed for the systems of different initial void fractions.



**Figure 2** Flow behaviour of the bilayer mixture with an initial void fraction of 70% during the deposition in a vacuum ( $L=15$  mm). (a)  $t = 1.91 \times 10^{-3}$  s; (b)  $t = 5.53 \times 10^{-2}$  s; (c)  $t = 1.89$  s.

However, when air is present during the deposition process, different flow and packing patterns are observed. Figure 3 shows the deposition process of the bilayer mixture with an initial void fraction of 70%. It can be seen that, as the particles start to fall, the air inside the container inhibits the flow of the more air-sen-



**Figure 3** Flow behaviour of the bilayer mixture with an initial void fraction of 70% during the deposition in air ( $L=15$  mm). (a)  $t = 1.91 \times 10^{-3}$  s; (b)  $t = 3.24 \times 10^{-2}$  s; (c)  $t = 6.29 \times 10^{-2}$  s; (d)  $t = 9.15 \times 10^{-2}$  s; (e)  $t = 9.73 \times 10^{-2}$  s; (f)  $t = 3.41 \times 10^{-1}$  s.

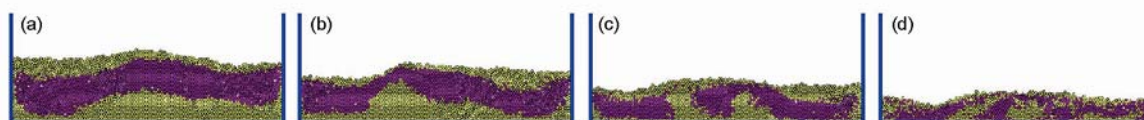
sitive particles in the bottom layer, while the flow of the less air-sensitive particles in the top layer is less affected. Consequently, the light particles that are more sensitive to the air fall more slowly than the heavy ones, due to the effect of air drag. Therefore, some of the heavy particles can sink into the top of the light particle layer and a mixing state is observed at the interface (Figure 3(b)). During the deposition, the air is entrapped inside the container and the downward movement of the particle system is prevented, so that the dilute granular system is densified along the interface between two layers under the combined effects of entrapped air and gravity, as shown in Figure 3(b).

As the densified particle system flows further, the friction along the powder-wall interfaces causes shearing that induces the dilation of the particle system close to the walls (Figure 3(c)). The dilation facilitates the escape of the entrapped air, so that at the late stage of the deposition, the entrapped air escapes from the sides close to the walls and expels a number of light particles (Figure 3(d)). These expelled particles are then fluidised (Figure 3(e)) and eventually settle on the top of the heavy powder bed (Figure 3(f)). It is hence demonstrated that the entrapped air plays an important role in the mixing of the bilayer mixture, in particular, the migration of the light particles from the bottom to the top

of the granular systems.

The mixing behaviour of bilayer systems during deposition in air depends upon the initial void fraction. Five initial void fractions in the range of 70%–90% air examined by adjusting the number of particles in the same region are as shown in Figure 1(a). Figure 4 shows the final states of the bilayer mixtures with various initial void fractions. When the initial void fraction is less than 80%, a thin layer of light particles is migrated to the top of the heavy particles due to the fact that the light particles are expelled to the top when the entrapped air escapes. Consequently, the layer of heavy particles is sandwiched by two thin layers of light particles (Figures 4(a) and (b)). For the mixtures with even higher void fractions (i.e. 85% and 90%), there is more void space inside two layers, so that the light particles, which are entrained by the flow of air, can penetrate into the layer of heavy particles, while the heavy particles filtrate into the thin layer under gravity. Consequently, the initially separated layers mix together in a complicated manner (Figures 4(c) and (d)).

The mixing behaviour can be better characterised by examining the distributions of the relative concentration of light particles (i.e. the ratio of the solid fraction of light particle to the total solid fraction). The vertical concentration of light particles in the final states for

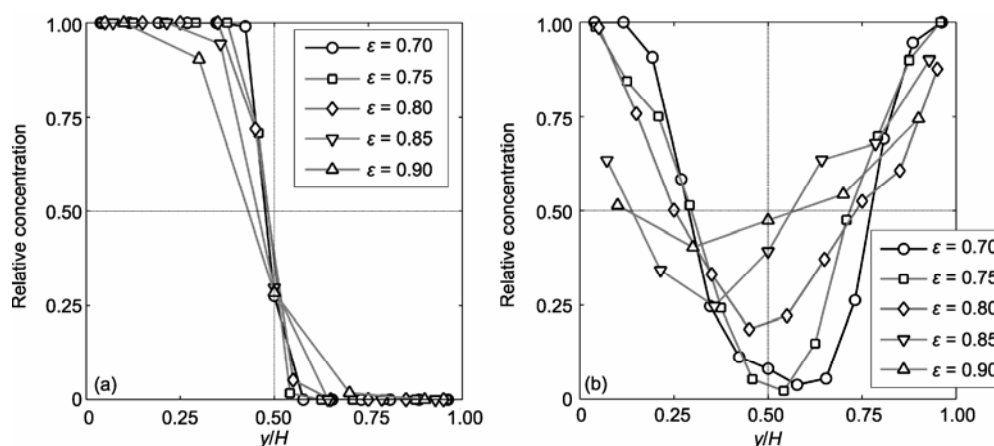


**Figure 4** Final packing patterns for the deposition of bilayer mixtures with various initial void fractions in air. (a)  $\varepsilon = 75\%$ ; (b)  $\varepsilon = 80\%$ ; (c)  $\varepsilon = 85\%$ ; (d)  $\varepsilon = 90\%$ .

various systems considered is plotted against the relative position  $y/H$  (where  $y$  is the distance from the bottom of the container and  $H$  is the height of the final packed powder bed) in Figure 5. It is clear that for the deposition in a vacuum (see Figure 5(a)), the light and heavy particles are separated as two distinctive layers with light particles at the bottom (i.e. the relative concentration of light particles equals to unity) and heavy particles at the top (i.e. the relative concentration of light particles is zero). A certain degree of mixing takes place along the boundary between two layers due to the collisions between particles of different inertia at the end of the deposition. The relative thickness of the mixing layer (to the thickness of the packed powder bed) increases as the initial void fraction increases. For the deposition in air (see Figure 5(b)), when the initial void fraction is less than 0.8, the relative concentration of light particles at the top ( $y/H=1$ ) and bottom ( $y/H=0$ ) of the container is close to unity, indicating that in these regions there are only light particles, while at the middle height ( $y/H=0.5$ ), the relative concentration is close to zero, implying that this region is primarily occupied by heavy particles. As the initial void fraction increases (say  $>85\%$ ), the relative concentration of light particles at the top and bottom of the powder bed decreases while the relative solid fraction of light particles at the middle height increases. This indicates that the two types of particles that are initially separated mingle together during deposition due to the effect of air. In particular, the relative concentration of light particles at the bottom decreases sharply when the initial powder bed has a relatively high initial void fraction, indicating that due to the effect of air drag, the

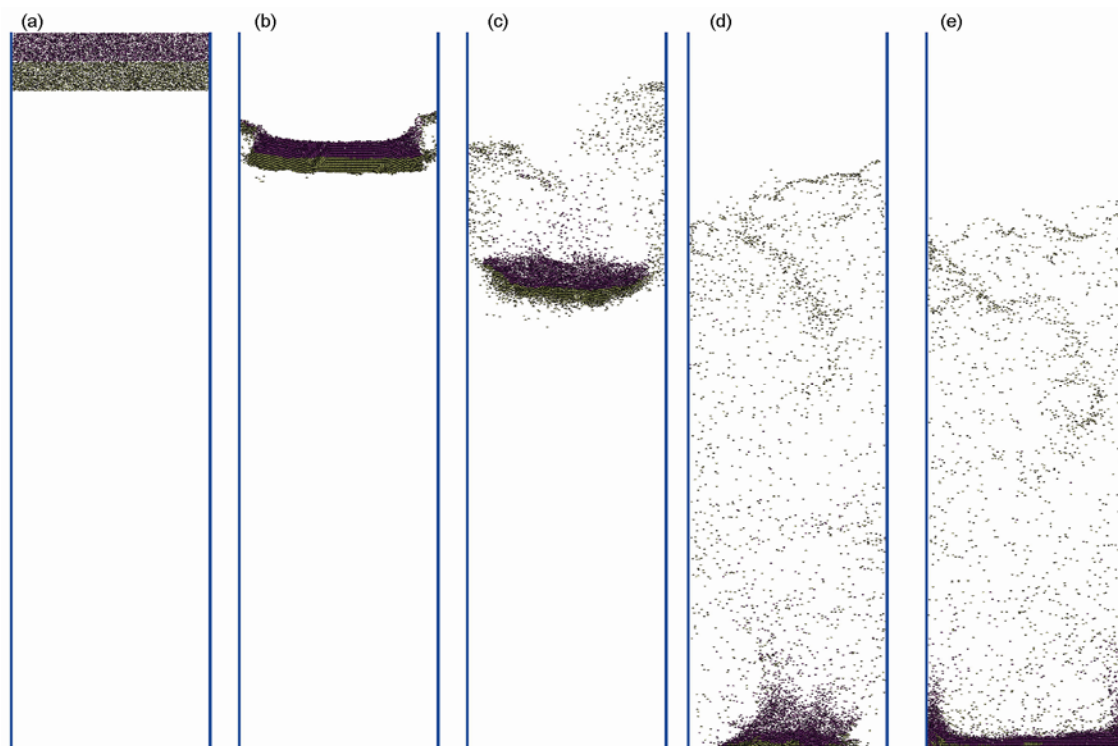
light and heavy particle layers can penetrate into each other and a good mixing is achieved at the bottom of the packed powder bed. It is hence clear that mixing can be induced as a result of the difference in particle inertia and the effect of air flow. The former can result in a small degree of mixing at the interface between two layers during the deposition in a vacuum, when airflow can lead to significant mixing between particles of different air sensitivities.

The mixing behaviour of the bilayer granular system also depends upon the deposition distance. As shown in Figure 6, in which the deposition distance is  $L=90$  mm (i.e. six times longer those shown in Figures 2–5), the initial flow patterns (Figures 6(a) and (b)) are similar to those presented in Figure 3. However, once the entrapped air starts to escape from the gaps between the consolidated powder bed and the walls, more and more light (air-sensitive) particles in the bottom layer are entrained in the upward flowing air streams (Figures 6(c) and (d)). These light particles can be suspended in the tube for a prolonged period (Figure 6(e)) and eventually settled on the top of the powder bed. It is also observed that as the initial deposition height increases, more light particles originally located in the bottom layer are migrated to the top of powder bed. The suspension of air-sensitive particles induced by the presence of air induces can cause dusting problems encountered in many industrial practice. It can also be seen in Figure 6 that, when the cluster of heavy particles reaches the bottom of the container, it collides with the container base. Consequently, this cluster of heavy particles spreads along the base and some heavy particles bounce upwards



**Figure 5** Relative concentration profiles of fine particles in the packed powder bed for the deposition of bilayer mixtures with various initial void fractions. (a) In a vacuum; (b) in air.





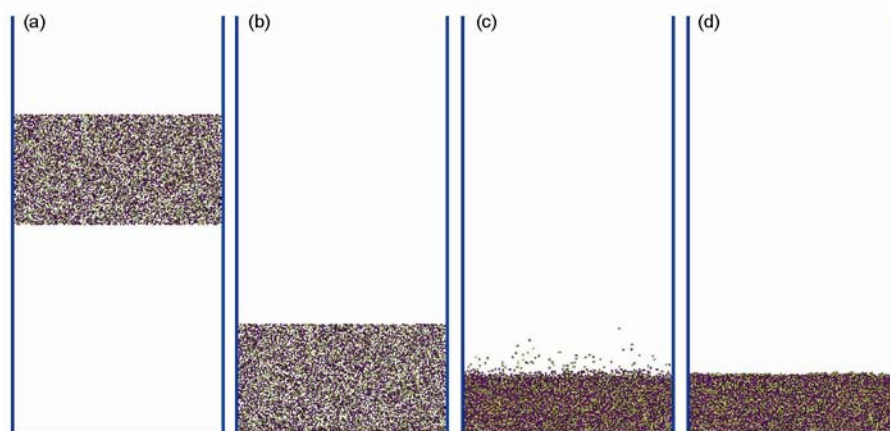
**Figure 6** Flow behaviour of the bilayer mixture with an initial void fraction of 70% during the deposition from a height of  $L=90$  mm in air. (a)  $t = 1.91 \times 10^{-3}$  s; (b)  $t = 6.67 \times 10^{-2}$  s; (c)  $t = 1.09 \times 10^{-1}$  s; (d)  $t = 1.81 \times 10^{-1}$  s; (e)  $t = 1.93 \times 10^{-1}$  s.

along the container walls (see Figures 6(d) and (e)).

### 3 Deposition of random granular mixtures

The deposition of a random granular mixture consisting of the two types of particles with various initial void fractions is also simulated. The typical flow behaviour during deposition in vacuum is shown in Figure 7. It is clear that the granular mixture flows as a whole (i.e. all the particles flow at the same speed) until it reaches the

bottom of the container (Figures 7(a) and (b)), and thereafter the powder bed is densified under gravity. At the end of deposition, some light particles bounce upwards (Figure 7(c)), which is due to the difference in inertia so that, compared with the heavy particles, the light ones gain a high rebound velocity when they collide with each other with the same initial kinetic energy. These light particles eventually settle on the top of the powder bed and form a thin layer (Figure 7(d)).

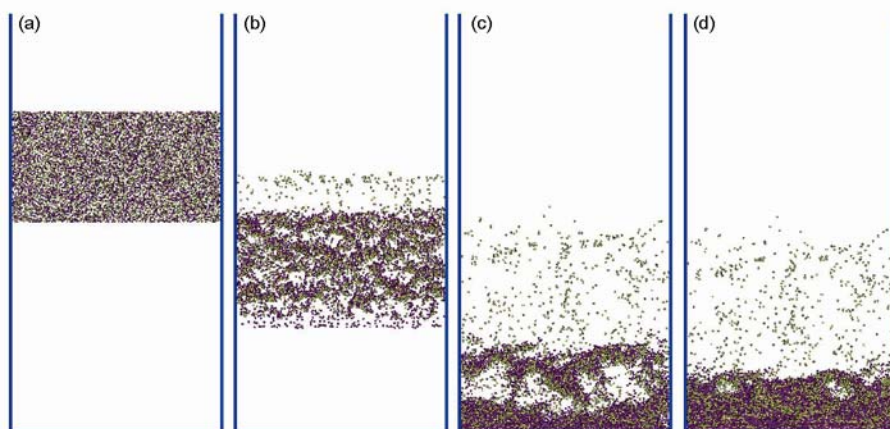


**Figure 7** Flow behaviour of the random mixture with an initial void fraction of 70% during the deposition in a vacuum. (a)  $t = 1.91 \times 10^{-3}$  s; (b)  $t = 5.53 \times 10^{-2}$  s; (c)  $t = 6.48 \times 10^{-2}$  s; (d)  $t = 3.43 \times 10^{-1}$  s.

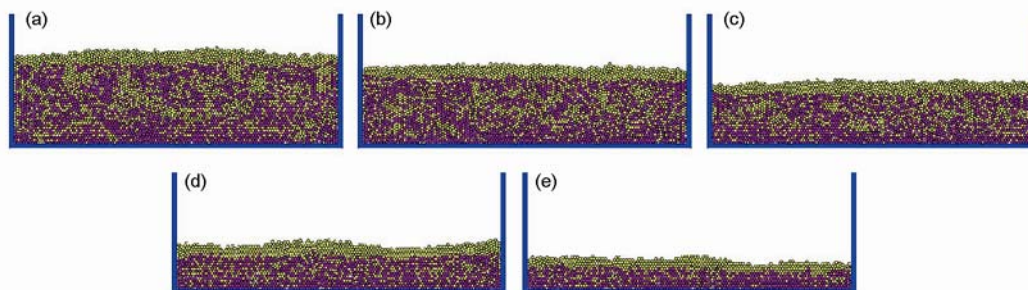
For the deposition in air, as shown in Figure 8, once the deposition starts, the light particles become entrained with the up-flowing air. For those situated near the top surface of the powder mixture, they can sift through the gap between heavy particles and float above the down-flowing powder mixtures (Figure 8(b)). However, the light particles inside the powder mixture are subjected to two forces that act in opposite directions: (1) the air drag force that tends to lift the light particles upwards, and (2) the contact forces from the down-flowing heavy particles. The down-flowing heavy particles tend to suppress the lifting of light particles caused by airflow. Consequently, clusters are developed inside the powder mixture (Figure 8(b)). These clusters generally consist of light particles at the bottom and heavy particles at the top, and situate on the top of small air bubbles (Figures 8(b) and (c)). These small air bubbles gradually merge into several large air bubbles that subsequently burst and expel some light particles from the powder bed (Figure 8(c)). These entrained light particles suspend in the con-

tainer for a certain period and gradually settle onto the top of the powder bed. Therefore, a layer of light particles rises to the top of the powder bed and a segregated system is formed.

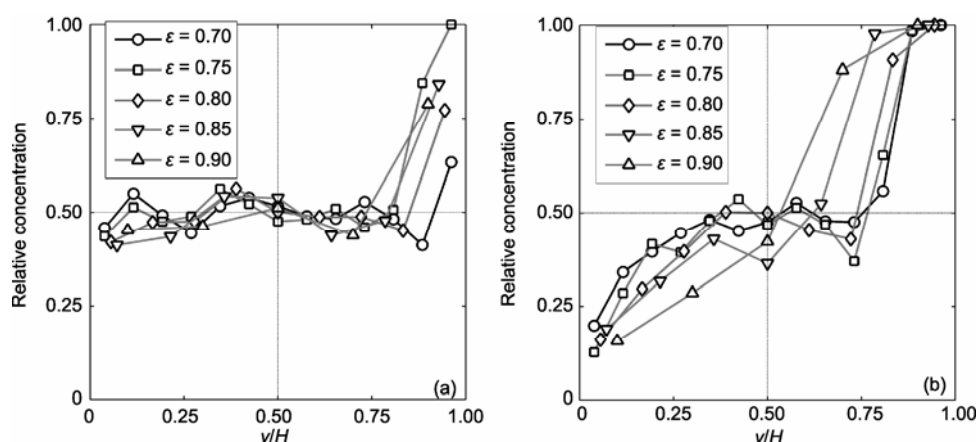
The rise of light particles can be clearly illustrated from the final packing patterns, as shown in Figure 9 for the deposition of random mixtures with various initial void fractions. It is clear that the overall patterns are similar. The segregation of original random mixtures is evident as light particles congregate at the top while heavy ones are at the bottom. More significant segregation is induced for the systems of high initial void fractions, for which the particles in the random mixture are separated to two layers (Figures 9(d) and (e)). Quantitative analysis of the final packing patterns are shown in Figure 10, which shows a relative concentration of the light particles in the vertical direction for the deposition in a vacuum and in air. It is clear that, for the deposition in vacuum (Figure 10(a)), the relative concentrations of the light and heavy particles inside the packed powder



**Figure 8** Flow behaviour of the random mixture with an initial void fraction of 70% during the deposition in air ( $L=15$  mm). (a)  $t = 1.91 \times 10^{-3}$  s; (b)  $t = 4.00 \times 10^{-2}$  s; (c)  $t = 7.06 \times 10^{-2}$  s; (d)  $t = 7.43 \times 10^{-2}$  s.



**Figure 9** Final packing patterns for the deposition of random mixtures with various initial void fractions in air. (a)  $\varepsilon = 70\%$ ; (b)  $\varepsilon = 75\%$ ; (c)  $\varepsilon = 80\%$ ; (d)  $\varepsilon = 85\%$ ; (e)  $\varepsilon = 90\%$ .



**Figure 10** Relative concentrations of fine particles in the packed powder bed for the deposition of random mixtures with various initial void fractions. (a) In a vacuum; (b) in air.

bed are essentially equal, except in the regions close to the top of the powder bed ( $y/H \sim 1$ ). In this region, the relative concentration of light particles is much higher than that of heavy particles. This is due to the fact that when the particles begin to settle in the container, collisions between particles occur. During the collisions, the light particles gain a higher rebound velocity than the heavy ones. Consequently, some light particles bounce upwards and then settle on the top of the packed powder bed (see also Figure 7(c)). For the deposition in air (Figure 10(b)), the top of the packed powder bed ( $y/H \sim 1$ ) is primarily occupied by light particles, as they are entrained in the up-flowing air stream. Hence, the bottom of the packed powder bed is dominated by heavy particles. Therefore, comparing Figures 10(a) and (b), it is clear that the presence of air during the deposition can cause significant segregation when the powder mixture consists of particles of different air sensitivities. Thus it can be concluded that the difference in inertia and the presence of air can cause segregation. In particular, the presence of air can induce significant segregation if the granular systems consist of particles of different air sensitivities. The difference in inertia is the main factor for causing segregation during the deposition in a vacuum, for which a layer of light particles is formed at the top of the powder bed.

## 4 Conclusions

The mixing and segregation behaviour of dilute bilayer and random granular mixtures of various initial void fractions were investigated using a coupled DEM/CFD method. It has been found that for the deposition in a vacuum, no obvious mixing occurs for the bilayer mixtures and no obvious segregation occurs for the random mixtures. During the deposition in air, the difference in air sensitivities of particles is observed to play a critical role in determining the mixing and segregation behaviour. For the deposition of bilayer mixture in air, some light particles (i.e. high air-sensitive particles) initially located at the bottom can be entrained in air and migrated to the top of the granular bed. The degree of mixing increases as the initial void fraction increases. For the deposition of random mixtures in air, a layer of light particles is also obtained at the top of granular system due to the effect of air drag, which causes segregation with a lower concentration of light particles at the bottom and a higher concentration at the top. The degree of segregation increases as the initial void fraction increases, since larger void space in the systems with higher initial void fractions facilitates the light particles to go through the matrix of the granular system and separate from the heavy ones.

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