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Research Paper

Investigation of particle segregation in a vertically vibrated binary mixture: Segregation process and mechanism

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ABSTRACT

The fabric structure and dynamic behaviour of granular materials have been extensively studied in geotechnical engineering due to their considerable impact on permeability and mechanical properties. However, particle segregation, causing significant structural changes, remains inadequately understood, especially concerning its dynamic evolution in both global and local segregation processes. This study aims to investigate the motion of particles and evolution of internal microstructure in binary mixtures under vibrational conditions. The emphasis lies in comprehending both global and local time segregation processes, along with elucidating the potential underlying mechanisms. Through DEM simulations, it is observed that large particles tend to rise to the surface of the container while small particles aggregate at the bottom, resulting in the well-known Brazil Nut Effect. As the vibration intensity increases, the degree of segregation becomes more pronounced. Vertical segregation precedes radial segregation and eventually leads to stable separation of the binary mixture. To comprehensively analyse the segregation behaviour, we introduce a segregation index and reveal a correlation between vertical and radial segregation. Additionally, the ascending process exhibits characteristics similar to compressed solid blocks, while the descending process resembles fluid-like behaviour, suggesting a phase transition phenomenon during particle segregation. The study further highlights the role of pore filling and convective rolling as driving mechanisms for particle segregation. These findings emphasize the potential impact of external disturbances on the microstructure of granular mixtures, with implications for scenarios such as earthquakes, debris flows, and traffic loads.

1. Introduction

The study of granular materials holds great significance, as they possess distinct solid characteristics, yet at the same time exhibit fluid-like behaviour under certain conditions (Baker et al., 2016; Brandao et al., 2020; Gao et al., 2022; Indraratna et al., 2011). Understanding the mechanical properties of quasi-solids and quasi-fluids, as well as the transition between them, represents a substantial and highly challenging task within soil mechanics and granular material mechanics (Arifuzzaman et al., 2022; Breu et al., 2003; He et al., 2018a; Lambiotte et al., 2005; Qiao et al., 2021). Capturing the behaviour of granular materials poses great challenges due to their complex nature. The inherent disorder and lack of structural organization make it difficult to accurately characterize these materials. Consequently, comprehending crucial aspects such as deformation, damage, energy dissipation, and structure–property relationships becomes problematic (Gu et al., 2019; He et al., 2018b,2019; Hu, 2019; Liu et al., 2022; Mollon and Zhao, 2012). As a result, granular materials give rise to numerous unanswered questions that persist as ongoing challenges in the field of research and engineering. In recent years, the remarkably rich dynamics of granular materials have attracted the attention of scholars from various fields (Chang and Deng, 2020; Zhao and Guo, 2015; Zhao et al., 2019). Under external stimuli, granular materials exhibit a wide range of peculiar phenomena, including segregation (Bancroft and Johnson, 2021; Chassagne et al., 2020), convection (Rehman et al., 2016; Wibowo et al., 2016), mud pumping (Bian et al., 2022; Duong et al., 2014; Indraratna

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et al., 2015; Zhang et al., 2021), and liquefaction (Bao et al., 2019; Ghani and Kumari, 2021). Within these phenomena, energy is continuously injected into the system through oscillating boundaries and propagates throughout the entire system via inter-particle contact. The system reaches equilibrium when the energy input and dissipation achieve a balance. Given that both energy input and dissipation heavily depend on the configuration of the system, a multitude of intriguing steady and even oscillatory states can be created. One of the most captivating phenomena is the tendency for segregation (Alam et al., 2006; Hong et al., 2001; Xie et al., 2012), where different types of particles separate and redistribute themselves, ultimately resulting in a segregated state.

In the typical size segregation of granular materials, when subjected to vibrations, the initially disordered mixture surprisingly tends towards order: larger particles may rise or sink (Ludewig and Vandewalle, 2005; Metzger et al., 2011). These vibrations induce convection and greatly influence the movement of particles (Amirifar et al., 2021; Hong et al., 2001). The upward movement of larger particles, eventually reaching the top of the particle system, is known as the Brazil Nut Effect (BNE) (Nair et al., 2020; Qiao et al., 2021). This effect, known as segregation, is a common characteristic of many natural and industrial granular flows. Particle segregation has been widely observed in industrial production (Denies and Holeyman, 2017; Li et al., 2021). It spans across various disciplines, ranging from materials science (Liao and Huang, 2021; Zhou et al., 2020) and process engineering (Jarray et al., 2019; Xu et al., 2017) to pharmaceutical sciences (Khakhar et al., 2003). In geophysical events, particle segregation gives rise to a series of complex phenomena, such as layering patterns observed in avalanche deposits (Gray and Hutter, 1997; Hao et al., 2023), the upward displacement of larger stones in fields after freeze–thaw cycles (Hallet, 2013), the presence of larger boulders at the foot of a mountain and smaller boulders near the base following landslides (Guo et al., 2021; Tang et al., 2022; Yang et al., 2021), particle sorting on the windward side of sand dunes (Lancaster et al., 2002), grain size segregation in mountain streams driven by gravity (Rousseau et al., 2021), and the impact of sediment transport on the flow dynamics and overall morphology of river channels (Huai et al., 2021; Yuan et al., 2021). Segregation profoundly affects the physical properties of granular mixtures with varying sizes or shapes. However, particle segregation remains a relatively unknown phenomenon in geotechnical engineering and has not received sufficient attention. This occurrence is prevalent in various geotechnical engineering activities, and here are a few examples:

Subgrade Fluidization under Traffic Loads: In recent years, the increase in train speeds and axle loads has intensified both vibration and permanent settlement of ballast layers (Luo et al., 2023; Dai et al., 2023). Continuous railway operations provide sustained energy input to the subgrade. The ballast layer consists of gravels of varying sizes and represents a prototypical granular material. It plays a crucial role in dispersing train loads and facilitating water drainage from the track structure. Recent observations have identified challenges such as weak interlayers and mud pumping, posing a potential threat to railway safety (Gao et al., 2022). Roadbed soils are frequently subjected to vibrations, creating conditions similar to particle segregation. This underscores the importance of investigating segregation under these conditions to gain insights into the mechanisms underlying related issues and diseases.

Particle segregation under earthquake effects: Geological observations following the 1999 Chi-Chi earthquake revealed particle size segregation within the mud of the Chelungpu Fault (Boullier et al., 2009). Laboratory experiments have similarly demonstrated segregation in water-saturated clay fault gouge under conditions of high sliding velocities and substantial displacements (Ujiie and Tsutsumi, 2010). Numerical simulations have explored the repercussions of particle segregation during shear processes in earthquake faults (Itoh and Hatano, 2019). The development of strata due to size segregation induces notable differences in strength. Previous research on sand has emphasized that the stratified structure resulting from segregation significantly influences physical properties and liquefaction resistance (Yoshimine and Koike, 2005). These findings underscore the necessity of incorporating particle segregation considerations into geotechnical engineering practices.

It is widely known that the properties of ideal crystalline materials are determined by their structure. However, in granular materials, the inherent complexity of the structure arises from the random packing of particles (Chang and Deng, 2020; Wang et al., 2022). Furthermore, under the influence of a vibrating field, particle segregation occurs, leading to the reassembly of particles and continuous structural evolution (Dai et al., 2022,2020,2021). As a result, accurately grasping the physical and mechanical properties of granular materials becomes increasingly challenging. The redistribution of particles greatly influences the physical properties of granular mixtures involving various sizes or shapes. Many physical properties, such as permeability, shear strength, elastic modulus, thermal conductivity, and electrical resistivity, depend on the material's packing state (or porosity) (Pillitteri et al., 2020; Zuo et al., 2023). Geotechnical engineering typically deals with major events like high-frequency earthquakes, construction-induced vibrations, and traffic loads on road embankments. These disturbances can have a profound impact on various geotechnical structures, leading to potential hazards and challenges. Despite some research efforts in this field, the underlying physical mechanisms governing these processes are still poorly understood. Several researchers have approached these segregation stages in various ways and have attempted to uncover the physical mechanisms driving the patterns of segregation (Bancroft and Johnson, 2021; Huang et al., 2022). However, a comprehensive understanding of the entire process of segregation and its patterns is still required. Previous studies have predominantly focused on separation patterns and influencing factors in particle segregation, overlooking the occurrence processes, especially the local separation processes. More detailed investigations from both global and local perspectives are essential for a comprehensive understanding of particle segregation. Additionally, closer attention needs to be paid to contact mechanics within particle systems, as it constitutes the intrinsic reason for the overall strength of the particle system and the local relative motion of particles. It serves as a primary mechanism for the manifestation of solid, liquid, and solid–liquid transitions in particle materials - aspects that have been largely overlooked in past research on particle segregation.

In geotechnical materials, the particle size distribution typically conforms to either a unimodal or multimodal pattern, characterized by varying quantities of particles of different sizes. The mathematical description of such three-dimensional packing is highly complex. Therefore, to simplify the analysis and avoid the complexity arising from high dispersion, we will restrict ourselves to using mixtures with two particle sizes (binary mixtures). Considering the widespread application and significance of even binary mixtures of particle sizes (Glover and Luo, 2020; Uchida et al., 2020), research on them remains limited. As mentioned earlier, the applicability of this study is extensive. Binary mixtures provide an essential simplification for many such applications. However, extracting detailed information from granular flow experiments can be challenging, even with the use of advanced techniques such as magnetic resonance imaging (Teng et al., 2019), Particle image velocimetry (PIV) (Gollin et al., 2017), and micro-CT (Teng et al., 2022) for direct measurements of spatial structure. In the study of granular materials, numerical simulations, particularly the Discrete Element Method (DEM), serve as effective and feasible alternative approaches for modelling various processes (He et al., 2020; Lu et al., 2022; Nie et al., 2022; Tran et al., 2022; Xiong et al., 2021; Zhao et al., 2017). The primary advantage of DEM is its ability to provide detailed particle-scale information, such as particle trajectories and forces acting on the particles. By simulating the behaviour of individual particles and their interactions, DEM enables researchers to gain insights into the complex behaviour of granular materials.

In this work, DEM approach is used to investigate particle segregation in a cylindrical container. The main objective is to examine and analyse both the global and local processes of particle segregation. Additionally, the study aims to explore and understand the underlying mechanism behind the segregation phenomenon. The paper is organized as follows. Section 2 introduces the DEM model. Section 3 presents the overall observations from the test to enhance our understanding of particle segregation. Sections 4 and 5 delve into the detailed explanation of the global and local segregation processes, respectively. In Section 6, the mechanism behind particle segregation is discussed. Finally, Section 7 summarizes the key findings obtained from this study.

2. Methodology

2.1. Governing equations

Particle systems in experiments often have limited observations, mainly confined to the surface. However, DEM serves as a powerful tool for studying particle flow and allows for obtaining more extensive information about each individual particle compared to experiments. Since its introduction by Cundall and Strack (1979), DEM has proven to be an effective technique for studying granular materials at the particle scale (Kildashti et al., 2023; Li et al., 2020). DEM simulations are commonly used to investigate various physical phenomena such as particle flow, segregation, packing, breakage, and collisions. In this research, the EDEM software (Qiao et al., 2021), a 3D particle flow code, is employed to simulate the Brazil Nut segregation of a binary mixture. According to Newton's laws of motion, the translational and rotational motions of particle "i" are determined by the following equations:

For translational motion:

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_j (\mathbf{F}_{ij}^n + \mathbf{F}_{ij}^t) + \mathbf{F}_g \tag{1}$$

For rotational motion:

$$I_i \frac{d\omega_i}{dt} = \sum_j \mathbf{T} \tag{2}$$

where m_i and I_i are the mass and the moment of inertia of particle i, respectively; $\mathbf{v}_i$ and ω_i are the translational and angular velocities of particle i, respectively; $\mathbf{F}_g$ represents the gravity acting on particle; $\mathbf{F}_{ij}^n$ and $\mathbf{F}_{ij}^t$ denote the normal and tangential contact forces, respectively; $\mathbf{T}$ represents the torque acting on particle, including the rolling friction torque and tangential friction torque. Considering the computational efficiency and successful experience in previous literature, the typical Hertz-Mindlin contact model is adopted to calculate these forces.

Fig. 1 illustrates the fundamental principles of the Hertz-Mindlin contact model. The normal force component is derived from Hertzian contact theory (Hertz, 1882). While the tangential force model is based on the pioneering work of Mindlin and Deresiewicz (Mindlin, 1949; Mindlin and Deresiewicz, 1953). Both the normal and tangential forces incorporate damping components where the damping coefficient is associated with the coefficient of restitution, as described in the study by Tsuji et al. (1992). The tangential friction force follows the Coulomb law of friction model, as exemplified by the research conducted by Cundall and Strack (1979). Additionally, the model incorporates rolling friction using a contact-independent directional constant torque model, as demonstrated in the work of Sakaguchi et al. (1993).

The normal force, $\boldsymbol{F}_n$, can be determined by the normal overlap, δ_n, and is expressed as follows:

$$\boldsymbol{F}_n = \frac{4}{3} E^* \sqrt{R^*} \delta_n^{\frac{3}{2}} \tag{3}$$

The equivalent Young's Modulus E^*, and the equivalent radius R^* are defined as:

$$E^* = \frac{E_i E_j}{E_j(1-\boldsymbol{v}_i^2) + E_i(1-\boldsymbol{v}_j^2)} \tag{4}$$

$$R^* = \frac{R_i R_j}{R_i + R_j} \tag{5}$$

where E_i, $\boldsymbol{v}_i$, R_i, and E_j, $\boldsymbol{v}_j$, R_j, being the Young's modulus, Poisson ratio and radius of each sphere in contact. Additionally, there is a damping force, $\boldsymbol{F}_n^d$, given by:

$$\boldsymbol{F}_n^d = -2\sqrt{\frac{5}{6}} \beta \sqrt{S_n m^*} \overrightarrow{\boldsymbol{v}_n^{rel}} \tag{6}$$

Here $m^* = m_j m_i / m_i + m_i$ is the equivalent mass, $\boldsymbol{v}_n^{rel}$ is the normal component of the relative velocity, and β and S_n (the normal stiffness) are given by:

$$\beta = \frac{-\ln e}{\sqrt{\ln^2 e + \pi^2}} \tag{7}$$

$$S_n = 2E^* \sqrt{R^* \delta_n} \tag{8}$$

Where e is the coefficient of restitution. The tangential force, $\boldsymbol{F}_t$, depends on the tangential overlap δ_t and the tangential stiffness S_t.

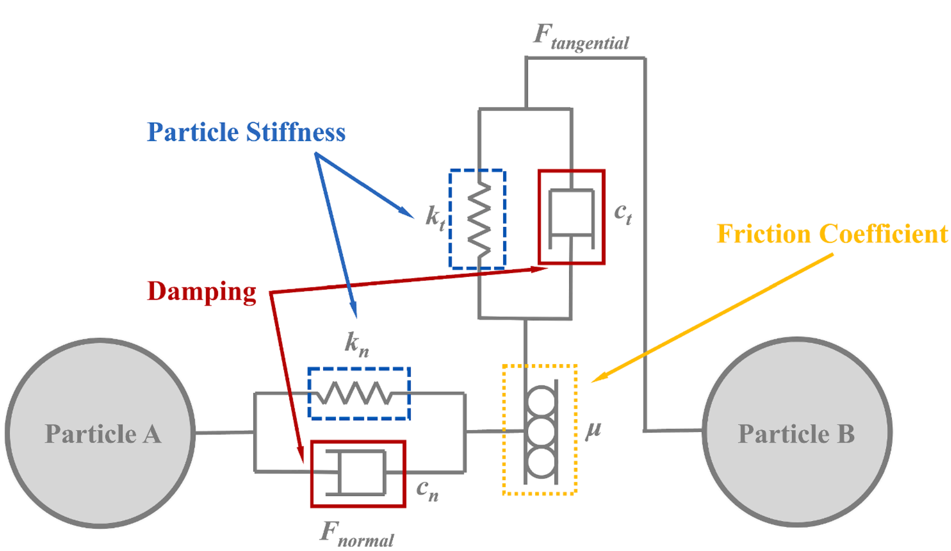

Fig. 1. Basic principles of Hertz-Mindlin contact model.

$$F_t = -S_t\delta_t \tag{9}$$

Where $S_t = 8G^*\sqrt{R^*\delta_n}$, and G^* is the equivalent shear modulus. Additionally, there is tangential damping given by:

$$F_t^d = -2\sqrt{\frac{5}{6}}\beta\sqrt{S_t m^*}\,\overrightarrow{v_t^{rel}} \tag{10}$$

Where v_t^{rel} represents the relative tangential velocity. The tangential force is limited by Coulomb friction, $\mu_s F_n$, where μ_s is the coefficient of static friction.

2.2. Simulation configuration

To minimize errors caused by container corners, a 3D cylindrical container with an inner diameter (D_{cyl}) of 150 mm is utilized for simulation, as shown in Fig. 2. In this study, an initial binary mixture is created by mixing large particles with a diameter of 10 mm (D) and small particles with a diameter of 5 mm (d) in equal volume proportions. The total bed height $H\approx 20d$, and the container diameter $D_{cyl}\approx 30d$ or $15D$. Referring to previous research results (Feng et al., 2020; Qiao et al., 2021), we determined the basic parameters for the DEM simulation, as outlined in Table 1. These specified parameters are aptly chosen for simulating the strength characteristics of fine-grained sand (Feng et al., 2020). To gain a comprehensive understanding of the entire segregation process and its patterns, a crucial approach is to investigate and compare the influence of vibration and system parameters on the final segregation outcomes. Several particle material properties and vibration parameters, such as the density ratio of binary particles, diameter ratio, coefficient of friction, frequency (f), and dimensionless intensity ($\Gamma = 4\pi^2 A f^2/g$), are considered as the main influencing factors (Metzger et al., 2011; Pillitteri et al., 2020). Numerous experiments have been conducted to study the impact of these factors. In this investigation, a fixed vibration frequency and a wide range of amplitudes are considered to control the desired dimensionless vibration intensity ($\Gamma = 1, 2, 3$, and 4). Specifically, we fix the vibration frequency (f) to be 20 Hz while adjusting the amplitude (A) to achieve a controllable vibration intensity. Consistent with previous research (Qiao et al., 2021), the container is subjected to continuous sinusoidal vibration in the z-direction, given by $Z = A\sin(2\pi ft)$. This harmonic motion is defined by the amplitude A, vibration frequency f, and time t. In our study, each case undergoes a total of 1200 cycles of vibration. Unlike in industrial production, where granular materials can exhibit pronounced density variations, the density of granular materials in geotechnical engineering is generally confined to a narrow range. Therefore, a binary mixture with the same density is considered. The simulation time step is set to 1×10^{-6} s, which corresponds to 5.2 % of the Rayleigh time step.

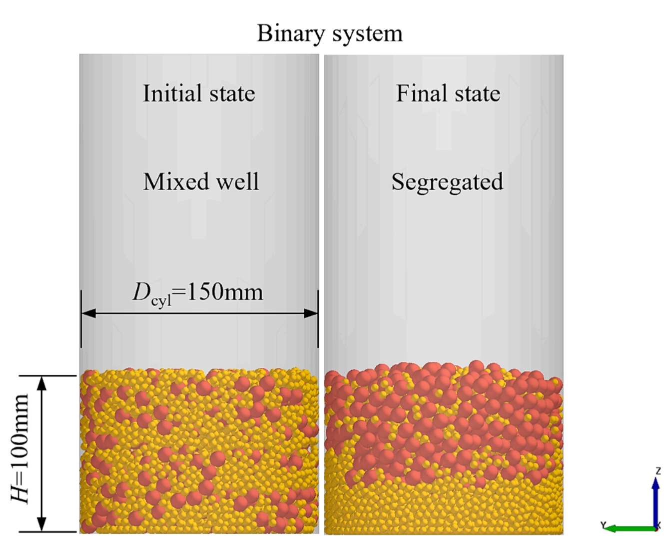

Fig. 2. Simulated segregation of a binary granular system.

Table 1
Parameters used in the simulations.

Variable	Symbol	Value
Diameter of large particles	D	10 mm
Diameter of small particles	d	5 mm
Poisson's ratio	ν	0.25
Young's Modulus	E	1.0 GPa
Coefficient of restitution	e	0.1
Coefficient of static friction	μ_s	0.7
Coefficient of rolling friction	μ_r	0.01
Number of large particles	N_L	982
Number of small particles	N_S	8391
density of large particle	ρ_L	2000 g/cm^3
density of small particle	ρ_S	2000 g/cm^3
Time step	Δt	1×10^{-6} s

3. Overall observations

To aid in our understanding of the segregation behavior under cyclic vibration, overall observations of the binary mixture are presented in Fig. 3. The figure illustrates the spatial distribution of the binary mixture after a certain number of vibration cycles, with the color of the particles indicating their initial bed height. The particle system is complex and dynamic, with multiple processes occurring simultaneously. Initially, the binary mixture exists predominantly in a delicate state of gravitational equilibrium, and various factors can lead to its instability and subsequent particle movement. The internal factors triggering particle segregation are mainly related to the flow processes within the binary mixture, which intensify as the vibration intensity increases.

The flow process of particle system in a vibrational field is relatively straightforward to comprehend. From the simulations, it can be observed that the binary mixture can form an "eruption" pattern. Initially, particles in the upper region move upward in a convex manner and, upon reaching the top, shift towards the sides. As time progresses, the vibrational effects extend to the lower layer of particles, causing the particles near the sidewalls to move towards the central region and erupt upwards. With increasing vibration intensity and continued vibrational action, the binary mixture undergoes segregation, and its particles eventually become disordered, independent of their initial positions. Based on our observations, the particle system generally forms a columnar upwelling channel in the central region. As the particles ascend and reach the top, a subsequent process of interlayer particle mixing takes place on both sides.

4. Global segregation process

4.1. Particle segregation

To gain a comprehensive understanding of the separation kinetics of particle systems, especially in the context of particle segregation in binary mixtures, researchers have extensively analysed the formation conditions and classification related to the Brazil Nut Effect. However, there is a lack of available information regarding the evolution of particle distribution throughout the process. To address this gap, a statistical analysis is conducted on the particle number distribution. This analysis involves projecting the positions of all particles within the container onto a two-dimensional plane using parallel projection with equal-area grids. Initially, the particle system exhibits a naturally random packing in both the horizontal direction (XY plane) and the vertical direction (YZ plane), as depicted in Fig. 4. Due to the non-uniform spatial projection of the cylindrical container onto the YZ plane, the particle distribution is concentrated in the central region along the Y-axis, while the initial particle number becomes

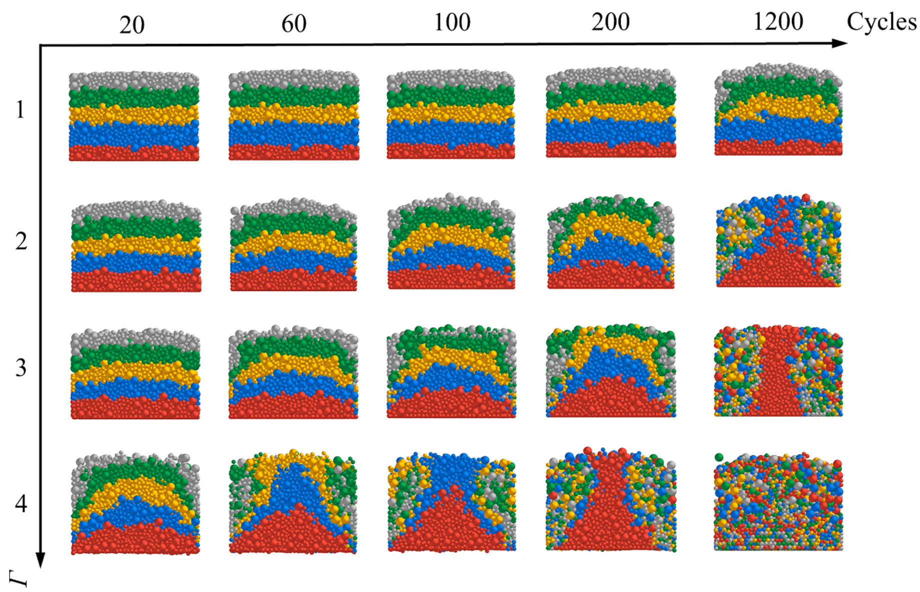

Fig. 3. Segregation patterns in a vibrated binary mixture.

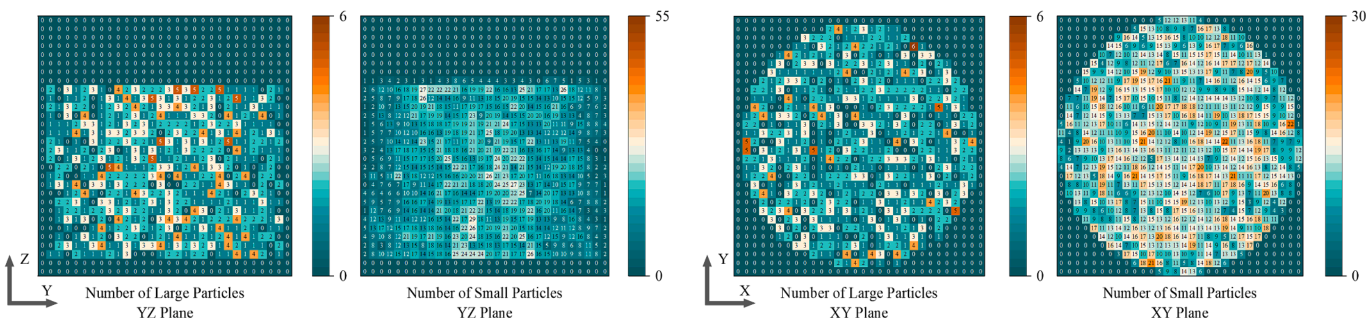

Fig. 4. Distribution of the initial particle system in the YZ and XY planes.

approximately uniform along the Z-axis. The projection from the XY plane also reveals that, although particles exhibit localized clustering, the overall distribution remains uniform.

4.1.1. YZ plane

Fig. 5 displays the distribution of the particle system after 1200 cycles under different vibration intensities. Evidently, as the vibration intensity increases, both the overall motion of the particle system and the local motion between particles become more pronounced. This increased motion allows small particles have a greater opportunity to enter the voids formed by large particles. As a result, small particles can reach the bottom of the container while large particles remain at the top, leading to vertical segregation. This phenomenon is referred to as the voids-filling mechanism mentioned in the reference (Breu et al., 2003; Xie et al., 2012). According to the DEM simulations, when the vibration intensity is $\Gamma = 1$, the particle system remains relatively consistent with its initial state. Small particles are uniformly distributed alongside large particles within the cylindrical container, indicating minimal particle segregation. However, at $\Gamma = 2$, segregation becomes noticeable. There is a decrease in the presence of large particles at the lower sides of the specimen, and their distribution exhibits a radial contraction. Large particles show a mushroom-like distribution in the vertical direction, while small particles permeate to the lower part. Similarly, in the upper regions, there is a reduction in small particles near the walls, and they tend to concentrate in the central region. As the vibration intensity Γ exceeds 3, the binary mixture generally reaches a stable state of high separation. Large particles tend to rise to the surface, while small particles accumulate in the lower part. A clear separation pattern emerges, although a few small particles remain in the upper region due to the compact stacking of large particles, preventing complete separation.

4.1.2. XY plane

Fig. 6 presents a visualization of the spatial distribution of particle quantities in the XY plane after 1200 cycles. It is evident that particle segregation occurs not only in the vertical direction but also in the radial direction. Specifically, large particles tend to concentrate near the walls along the radial direction, while small particles have a tendency to aggregate towards the centre. This radial segregation becomes more pronounced at higher vibration intensities, particularly at $\Gamma = 3$ and 4, where only a few large particles are present in the intermediate radial region of the container. In contrast, at a vibration intensity of $\Gamma = 1$, the distribution of large particles appears relatively uniform, indicating a lower degree of radial segregation. During the process of particle segregation, two primary modes of motion can be identified. The first mode involves the upward movement of large particles and the downward movement of small particles, leading to vertical segregation. The second mode entails the horizontal centripetal movement of small particles towards the centre and the horizontal centrifugal movement of large particles in the upper region, contributing to radial segregation. These aspects will be further explored in the following section through segregation index analysis.

Our focus now shifts to quantifying the trends in particle distribution after confirming that the DEM simulation reproduces the observed

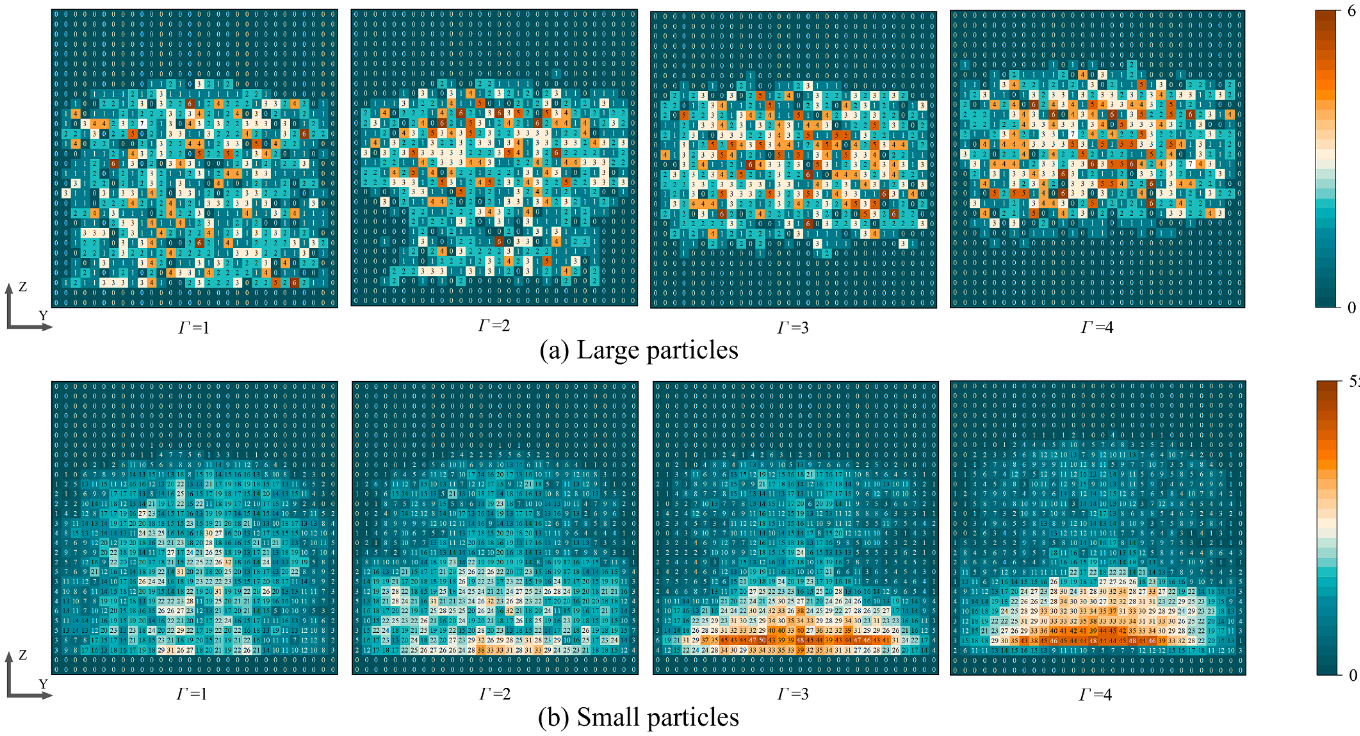

Fig. 5. Distribution of the particle system after 1200 cycles in the YZ plane.

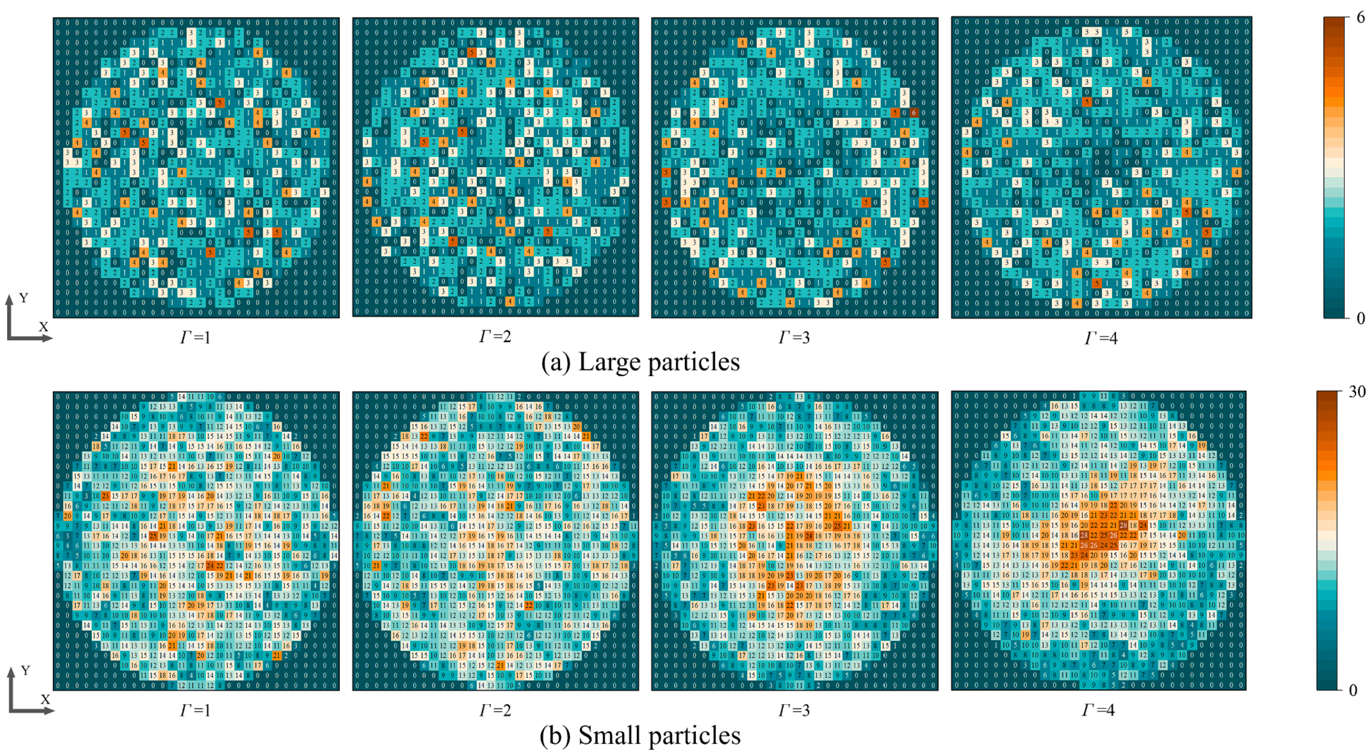

Fig. 6. Distribution of the particle system after 1200 cycles in the XY plane.

segregation patterns and characterizes vertical and radial segregation. By traversing the particle positions at different time steps, we statistically analyse the probability density distribution of particle positions for $\Gamma = 4$, as shown in Fig. 7. This provides a description of the probability density of particle occurrences in both the vertical and radial directions. The initial particle distribution in the simulation is observed to be nearly uniform. However, the changes in probability density over time reveal distinct segregation trends. In terms of temporal progression, vertical segregation of the particle system occurs within the first 200 cycles. Large particles move upward, while small particles deposit downward simultaneously. On the other hand, radial segregation primarily occurs between 400 and 600 cycles. During this stage, large particles move

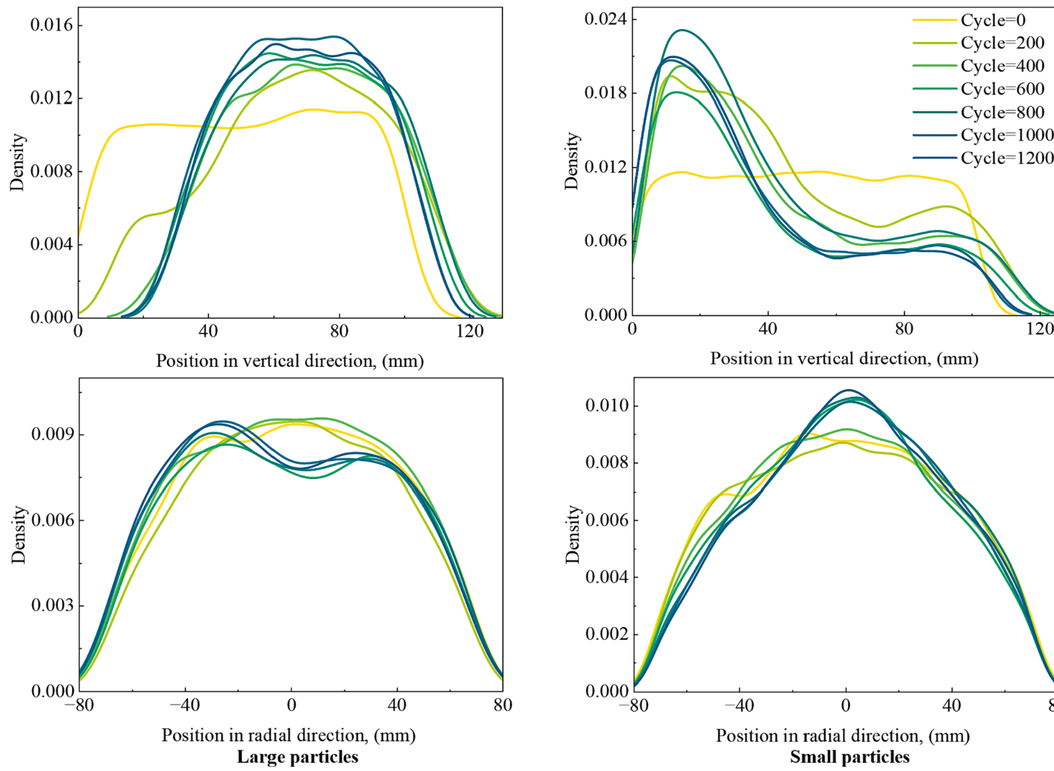

Fig. 7. Probability density distribution of particle positions for $\Gamma = 4$.

from the centre towards the boundaries, while small particles move towards the centre within a certain range of the specimen. In subsequent stages, the curves obtained at different time intervals tend to collapse onto each other, indicating that the segregation of the binary mixture eventually reaches a stable state. Overall, the DEM simulation results presented in this section suggest that vertical segregation tends to occur before radial segregation, with a broader range and greater extent. Further investigations are required to capture the subtle segregation behaviour in granular materials.

4.2. Evaluation index

A mixing metric, capable of quantifying the degree of vertical segregation in the binary mixture system, is employed to quantitatively examine the systems and compare the impact of vibrational intensity. The degree of particle segregation in the vertical direction (D_{sv}) can be calculated using the following formula:

$$D_{sv} = 2\frac{h_l - h_s}{h_l + h_s} \tag{11}$$

Where h_p represents the average height of particles of species $p = l; s$ ($h_p = (1/N_p)\sum_{i=1}^{N_p} z_i$), here z_i is the height of particle i with respect to the container base. In this study, we initialize the system in a random state, characterized by $D_{sv} \approx 0$. According to this definition, the binary system is uniformly mixed.

When subjected to vibrations, the state of mixture evolves, and the segregation degree undergoes changes until it reaches a stable state. D_{sv} serves as a valuable metric in characterizing this process. A value of $D_{sv} = 1$ represents the system in a Brazil Nut state, where large particles completely ascend to the top and segregated from the small particles. Conversely, as D_{sv} approaches -1, large particles settle at the bottom, indicating a Reversed Brazil Nut state. The D_{sv} values range between -1 and 1, providing a measure of mixing and segregation in granular mixtures. Due to computational constraints, all simulations are only run for 1200 cycles. Nonetheless, in this study, our focus lies more on the segregation process rather than the steady state, emphasizing the time during which segregation is still ongoing.

Fig. 8(a) illustrates the temporal evolution of the segregation index, quantifying the segregation behaviour of the binary mixture due to particle size. In this study, the initial state exhibits a relatively homogeneous mixture with a segregation index of 0.028. From the graph, it is evident that the segregation index gradually increases over time. Consistent with previous overall observations, at vibration intensity of $\Gamma = 1$, the degree of particle segregation is minimal. However, as the vibration intensity increases, the attained segregation becomes more pronounced, with large particles aggregating at the upper region of the system while small particles deposit at the lower region. At $\Gamma = 4$, the final segregation index reaches approximately 0.6. This can be attributed to the insufficient pore channels formed by the accumulation of large particles, which restrict the free passage of small particles. As a result, some small particles remain entrapped within the large particles, making complete segregation challenging to achieve. Moreover, it is apparent that the vertical segregation of the particle system develops rapidly during the initial stage and eventually reaches a relatively stable limit of segregation. The temporal evolution of the segregation index can also be well described by first-order kinetics, expressed as:

$$D_{sv} = D_{svF} + (D_{svI} - D_{svF})e^{-kt} \tag{12}$$

where D_{sv} represents the segregation index, D_{svI} and D_{svF} represent the initial and final steady-state segregation indices, k is the segregation rate constant, and t is the segregation time.

The influence of vibration intensity on the segregation rate constant (k) and the final segregation index (D_{svF}) can be further examined from Fig. 8(b). In this study, the segregation rate constant generally increases with vibration intensity. This can be attributed to the higher kinetic energy of particles resulting from increased vibration velocity, which continuously supplies more external energy to the particle system. With the increase in vibration intensity, particle motion becomes more active, and the corresponding packing in the flowing zone becomes less dense. Therefore, due to enhanced percolation effects, small particles tend to

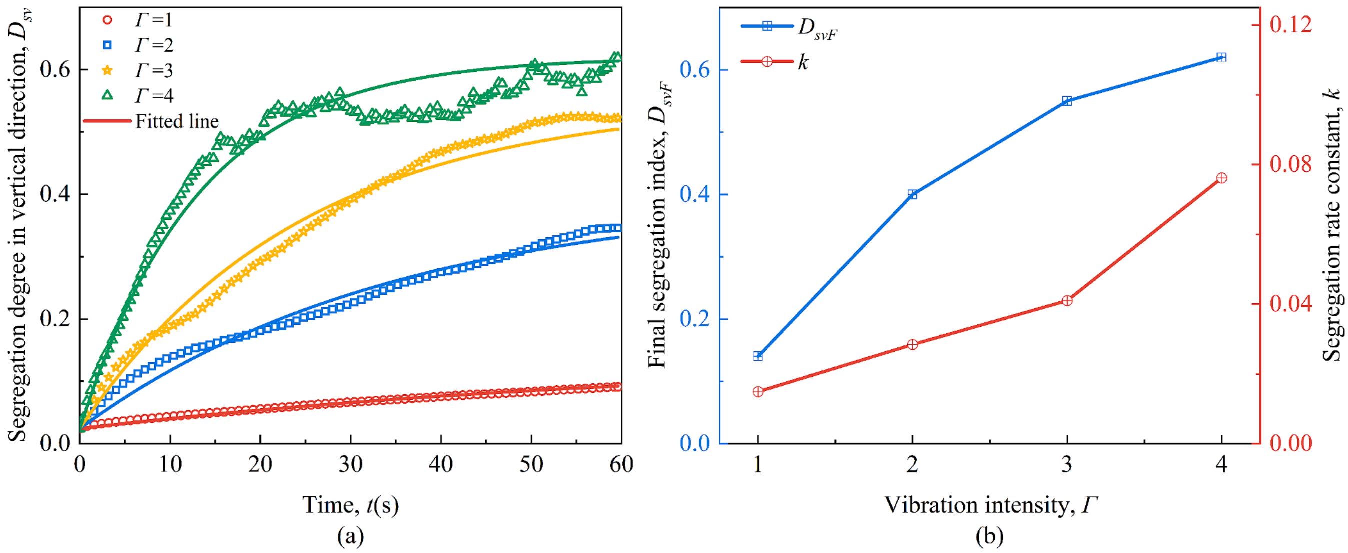

Fig. 8. Evolution of the segregation index in the vertical direction.

settle more easily during the relative motion of particles, leading to faster segregation. Furthermore, the value of D_{svF}, representing the final segregation index, also exhibits a monotonic increase with vibration intensity. However, the rate of increase gradually diminishes. This can be understood considering the particle size ratio in the system, which in this study is 2. Even with further increases in vibration intensity, the final segregation index will eventually approach a limit, making it challenging to achieve further segregation. It should be noted that various factors, such as particle friction and shape, can influence this phenomenon. In geotechnical engineering, different materials often display variations in properties related to friction and shape. Therefore, further research is necessary to investigate these factors and their impact on segregation behaviour.

The particle distribution in the XY plane indicates that segregation occurs not only in the vertical direction but also in the radial direction. Similar to the definition of D_{sv}, we have established a radial segregation index to describe the relative motion of particle system. The degree of particle segregation in radial direction (D_{sr}) is calculated using the

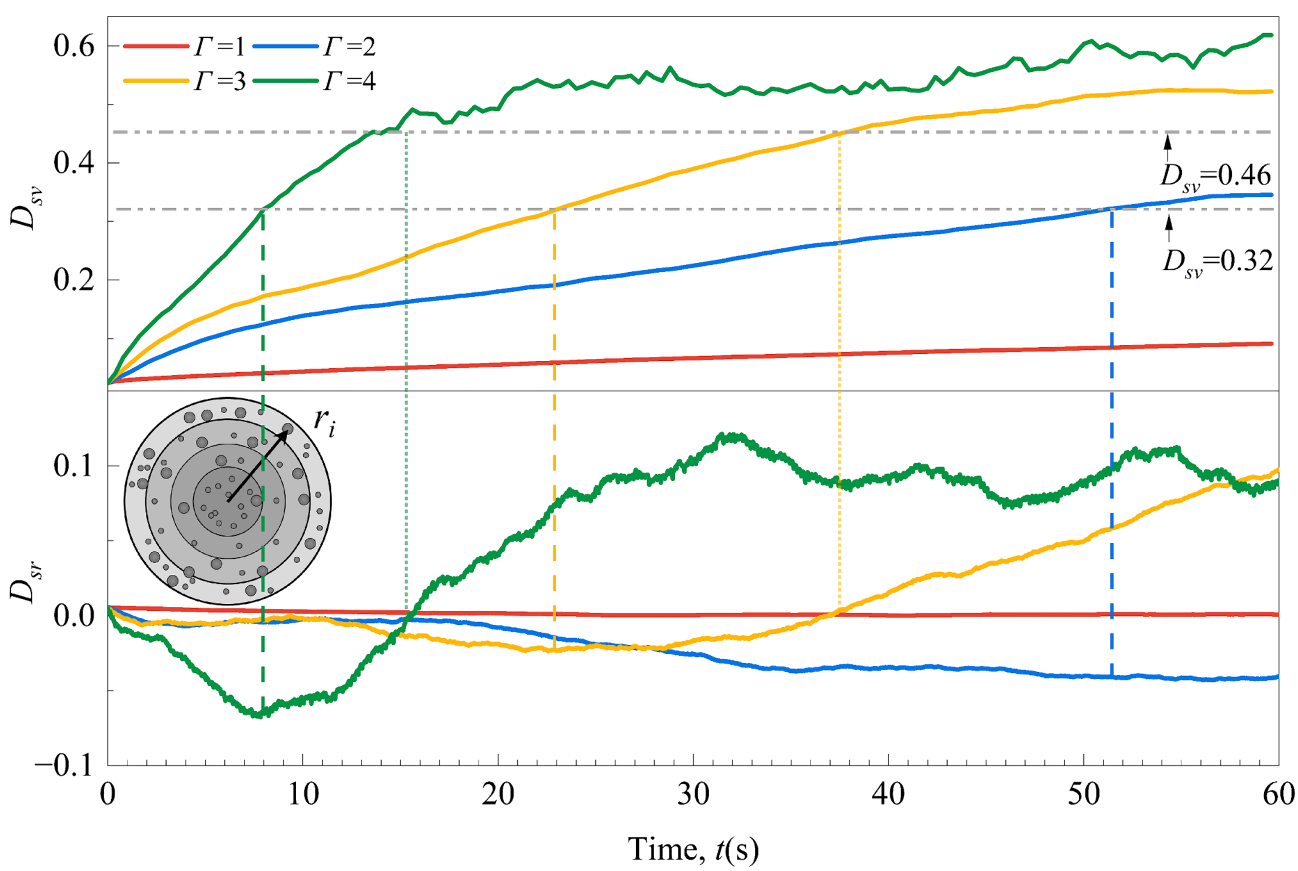

Fig. 9. Evolution of the segregation index in the radial direction.

following formula:

$$D_{sr} = 2\frac{r_l - r_s}{r_l + r_s} \tag{13}$$

Where r_p is the average radius distance of species $p = l$; s relative to the centre of the container ($r_p = (1/N_p)\sum_{i=1}^{N_p} r_i$), here r_i represents the radial distance of particle i relative to the centre of container. In this work, the initial state exhibits relatively good mixing with a segregation index of 0.03.

Fig. 9 illustrates the evolution of particle radial segregation, and interestingly, there seems to be a potential connection between radial and vertical segregation. In our study, when $D_{sv} < 0.32$, the radial segregation decreases over time and reaches a minimum, during which D_{sr} is consistently less than 0. Then, as D_{sv} increases from 0.32 to 0.46, the radial segregation index gradually increases to 0. Although specific numerical values require further research for confirmation, we can still observe that vertical and radial segregation develop simultaneously, demonstrating an intrinsic connection. The trend of radial segregation development follows a consistent pattern, similar to the case of $\Gamma = 4$, where it initially decreases with time and then increases towards a relatively stable state. The radial segregation observed at $\Gamma = 1$ or 2 corresponds to the initial decreasing stage of the segregation pattern. Overall, for the same particle system, the variation in vibration intensity governs both the rate of development and the final state of radial segregation.

4.3. Evolution of contact

Granular materials, particularly those comprising particles of varied sizes, exhibit notable heterogeneity in the transmission of contact forces. This nonuniformity plays a crucial role in governing the soil's strength and serves as a primary driver for relative particle motion. The transmission characteristics of loads in discrete element analysis are represented by interconnected contact force chains among particles. Fig. 10 compares the distribution of force chain in the initial sample and after segregation. Cylindrical links are used to connect the centres of contacting particles, with the colour and thickness of these links representing the magnitude of the corresponding contact forces. In granular systems, a few contact forces are clearly larger than others, leading to the distinction between strong force networks and weak force networks. Consequently, the contact force chains can be classified as either strong or weak. Strong force chains play a crucial role in maintaining the overall structure and stability of the particle system. They achieve this through establishing tight contact between particles, contributing significantly to processes such as energy transfer, structural stability, and stress transmission. Weak force chains serve the purpose of connecting and contributing to the shear stability of the strong force chains. Additionally, they play a role in redistributing forces following the rupture of strong force chains. Analysis of the force chain distribution patterns reveals that during the initial stages, the particle system undergoes packing in response to gravitational forces, resulting in an increase in the size of the force chains with depth. In cases with $\Gamma = 1$, the

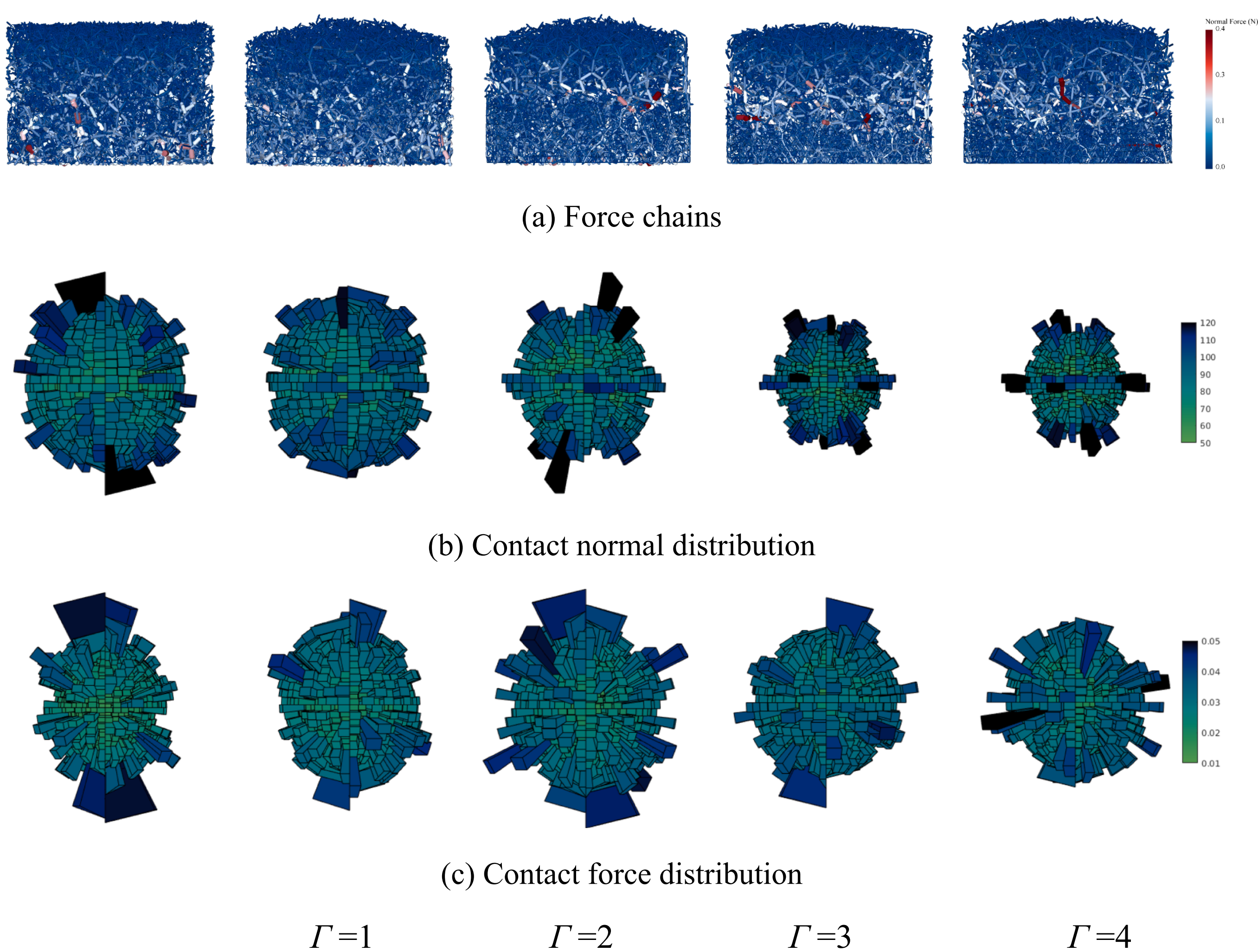

Fig. 10. Contact information before and after segregation.

application of vibration promotes particle redistribution. This vibration acts as a loosening mechanism on the initially gravity-formed particle system, leading to a more uniform distribution of force chains. However, as the vibration intensity increases, Brazil Nut segregation becomes apparent. This results in the upward movement of large particles and the downward movement of small particles, leading to an overall non-uniform stratification of the particle system. Strong force chains begin to concentrate at the interface between large and small particles, while weak force chains primarily maintain the structural integrity within regions of large and small particles. This phenomenon ultimately leads to a uniform distribution of force chains within their respective regions.

Granular materials generally exhibit initial anisotropy due to the inherent non-uniformity of particle distribution and the influence of gravity. As particle segregation occurs, the microstructure of the material undergoes changes, and discrete element analysis enables quantitative observation of the evolution of microscopic anisotropy. Fig. 10(b) and 10(c) illustrate the rose diagrams representing the contact normal directions and contact normal forces before and after segregation, respectively. Initially, the contact normal directions exhibit a relatively even distribution, with a slight concentration in the vertical direction. The contact normal forces are primarily concentrated in the vertical direction, with smaller forces in the horizontal direction. As mentioned previously, in the case of $\Gamma = 1$, where the particle system exhibits release-like behaviour, segregation results in a nearly isotropic distribution of contact directions and a more uniform distribution of contact normal forces. However, as the vibration intensity increases, particle segregation occurs, leading to a concentration of contact directions in both the vertical and horizontal directions.

In the simulation presented in this study, three types of contacts are defined based on the characteristics of particle sizes: C-F (coarse–fine) contacts, C-C (coarse-coarse) contacts, and F-F (fine-fine) contacts. These contacts represent the interactions between particles of different size combinations: coarse–fine particles, coarse-coarse particles, and fine-fine particles, respectively. Fig. 11 depicts the changes in the number of contacts within the sample, which offer valuable insights into the trend of particle contacts development toward an uneven distribution. With an increase in vibration intensity, there is an observed increase in the proportions of C-C contacts and F-F contacts, while the proportion of C-F contacts decreases. These findings indicate that the particle system undergoes a process of reorganization, resulting in an uneven distribution of particle contacts. Notably, starting from an initially well-mixed condition in the simulation, the small particles self-organize into a densely packed layer at the bottom, with limited penetration of large particles. This results in the formation of a densely packed particle bed at the bottom of the sample, as illustrated in Fig. 12. This region has been previously referred to as the crystallization zone at the bottom (Metzger et al., 2011). The force chain structure within this region reveals the formation of a stable state characterized by parallel force arches, which collectively create a strong skeleton.

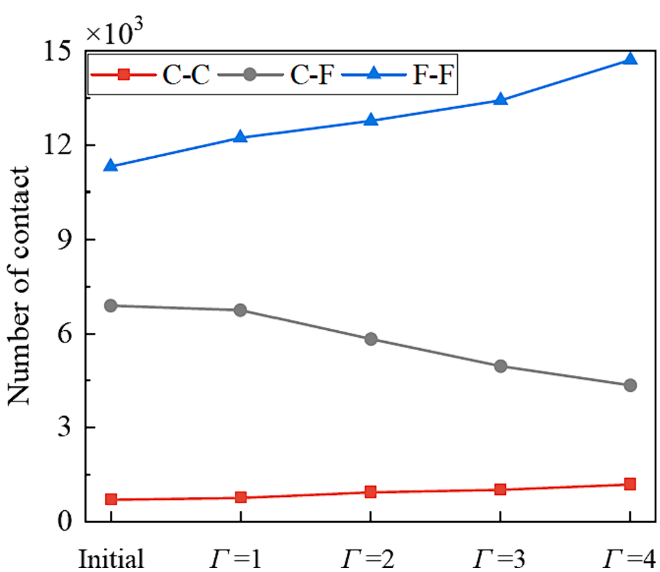

Fig. 11. Changes in the contact number before and after segregation.

4.4. Particle trajectories

The binary mixture undergoes relative motion within the vibrational field, eventually resulting in distinct segregation. To further investigate the evolution of segregation, we analyse the dynamics of representative particles and track their trajectories. Specifically, we randomly select particles from the top, middle, and bottom regions of the model (in the case of $\Gamma = 4$) to explore the general patterns of their motion. Fig. 13 illustrates the initial selection of particles at different heights before the Brazil Nut effect occurs. Following the segregation process, large particles become concentrated at the top, while small particles accumulate at the bottom. In this Figure, the trajectories of the selected particles are projected onto the YZ plane, with the colour indicating the magnitude of particle velocity. It is evident that convection zones form on both sides of the upper region, where particles exhibit concentrated relative motion. Additionally, an upward flow region emerges in the central region, creating channels for particle ascending. Furthermore, particles at the bottom initially demonstrate a slower upward velocity, consistent with the "waiting period" previously reported in the literature (Qiao et al., 2021). This period is characterized by a lower intensity of convection in the particle motion.

Convection plays an essential role in particle segregation. By tracking particle trajectories, we can gain insights into the overall convection patterns of representative particles. Notably, there are subtle distinctions in convection behaviour between the two particle types. The convection of large particles is primarily concentrated in the upper region, whereas small particles exhibit convection throughout the entire height of the system. The driving force behind convection arises from particles ascending in the centre region and moving downward in thin sheets along the shear walls. In the binary mixture, we observe various forms of particle convection, each characterized by distinct features during the oscillatory phase. The convection flow of small particles is intense and resembles a fountain-like motion, with particles rising from the bottom to the top and subsequently dispersing. In contrast, the motion of large particles is slower. Through friction and collision interactions, a dynamic equilibrium is established between the large and small particles within the stable phase. It is evident that particles are predominantly confined within their respective convection rolls, with small particles penetrating deeper into the system, while large particles remain on the surface. The absolute size of the large particles prevents

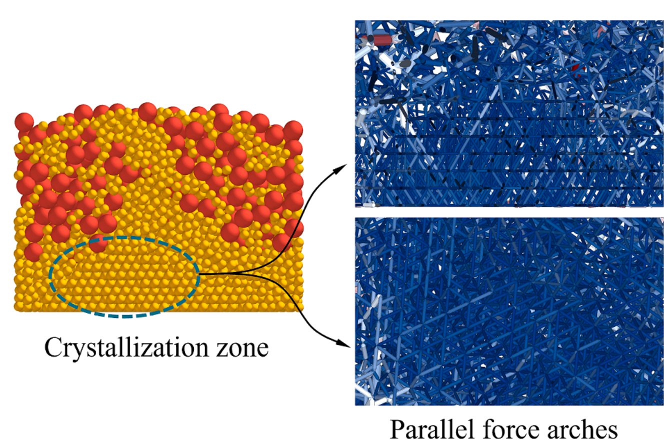

Fig. 12. Crystallization zone at the bottom.

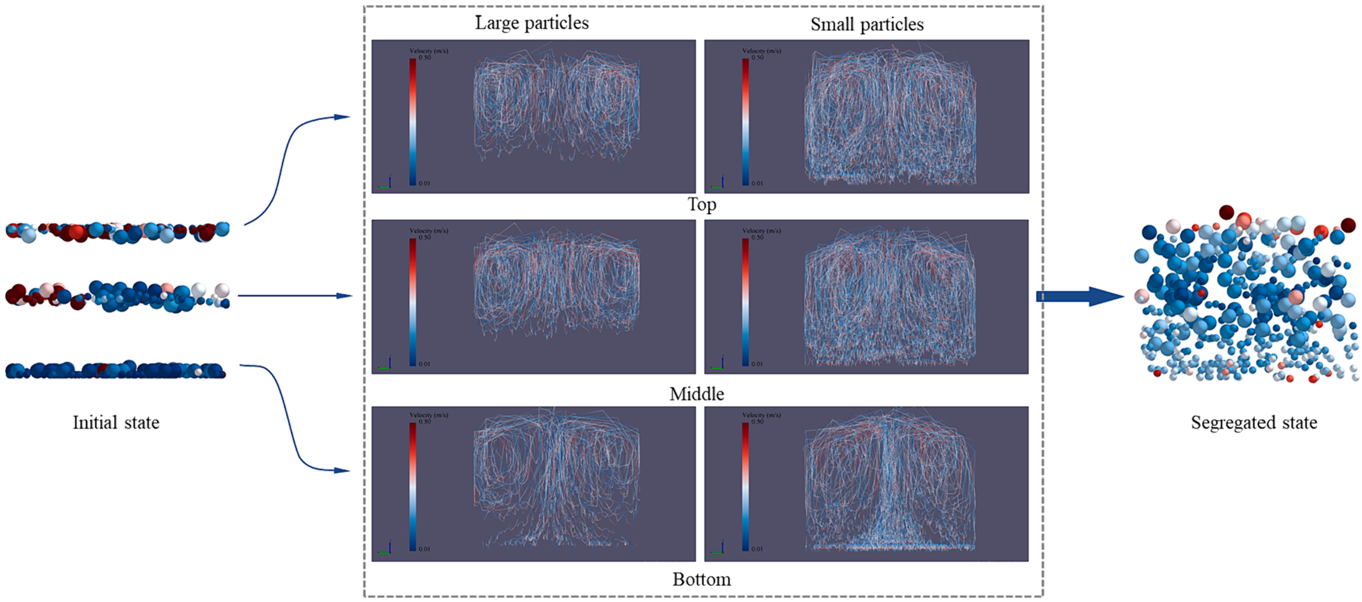

Fig. 13. Trajectories of representative particles at $\Gamma = 4$.

them from entering the downward convection rolls, contributing to their confinement near the surface.

5. Local time segregation process

Compared to the global particle segregation process, more detailed information can be obtained from local processes. The data is saved at a time step of 0.0005 s, which corresponds to 0.01 of a cycle. As a result, at least 100 data points can be collected within each cycle. Fig. 14 presents the coordination number data collected over four consecutive cycles at $t = 5$. The coordination number (*NumCoor*) is defined as the average number of contacts per particle:

$$NumCoor = 2N_c/N_p \tag{14}$$

where N_c and N_p are the numbers of contacts and particles, respectively.

The figure also includes rose diagrams depicting the particle contact numbers. These diagrams serve as a descriptive measure of the contact information during the local segregation process. By analysing the rose diagram, we can observe the changes in particle contact and their orientation throughout the segregation process. It allows us to understand how the contact patterns evolve over time and how particles reorganize themselves during the segregation process. Furthermore, the evolution of the rose diagram can be effectively characterized by changes in *NumCoor*. This information is valuable in understanding the

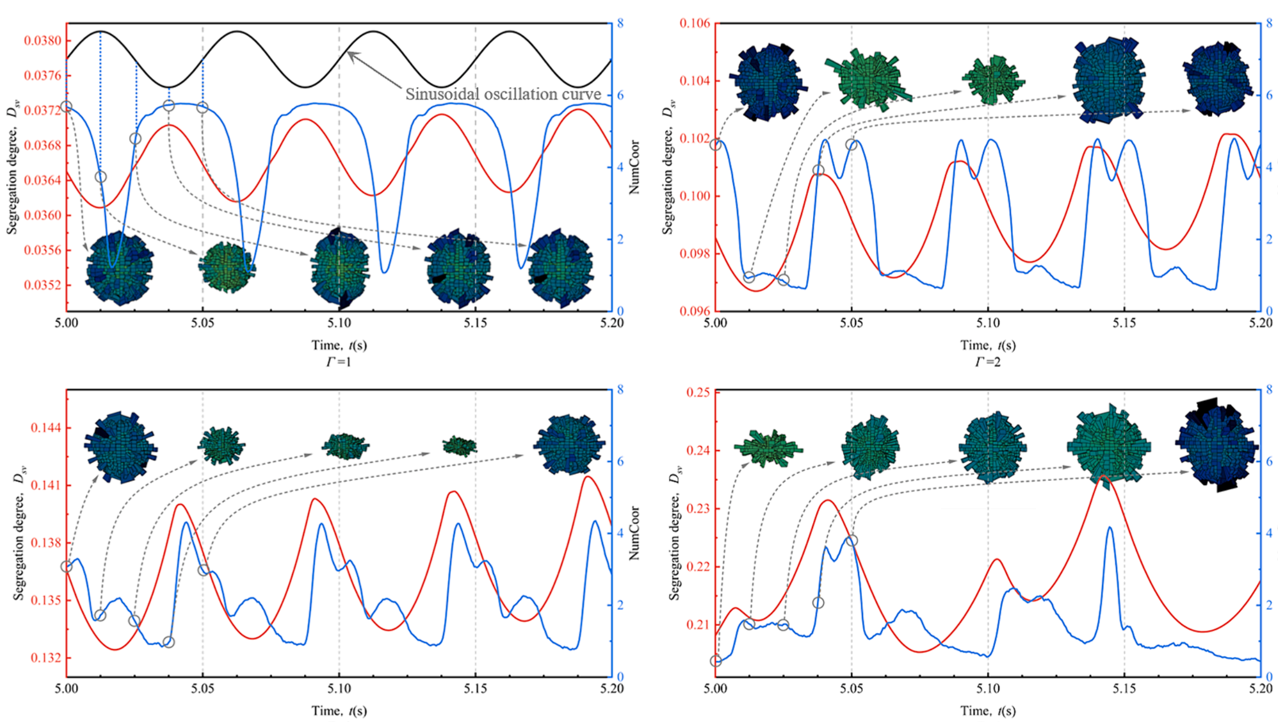

Fig. 14. Correlation between particle segregation and contact in local processes.

dynamics and behaviour of particles during local segregation events. During the upward phase of the particle system, the *NumCoor* is higher compared to the downward phase. Moreover, as the vibration intensity increases, the *NumCoor* within the particle system noticeably decreases. For $\Gamma = 1$, *NumCoor* decreases only in the initial stage of the downward phase and remains relatively high and stable for most of the time. An increase in *NumCoor* indicates a tighter particle contact and a gradual strengthening of particle interactions. When the particle system becomes sufficiently compact, a high *NumCoor* leads to interlocking between particles, resulting in a stable structure that inhibits particle motion. Conversely, when the particle system is loose, contact collisions between particles provide impetus for relative particle motion. Throughout the Brazil Nut segregation process, the microstructure of the sample undergoes continuous evolution. This internal structural evolution stems from particle rotation and displacement, as well as corresponding adjustments in contact characteristics such as coordination numbers, contact forces, and contact directions.

Fig. 14 presents four consecutive cycles, effectively illustrating the variability and stability of the parameters during the segregation process. A noteworthy observation is the consistent relationship between the vertical segregation degree and *NumCoor*. As the degree of segregation increases, so does *NumCoor*, exhibiting synchronous variations. This correlation is particularly evident at lower vibration intensities, where consecutive cycles demonstrate a higher degree of similarity in both *NumCoor* and the segregation degree. The pattern observed in one cycle closely resembles that of the next. However, as the vibration intensity increases, contact collisions between particles introduce destabilizing factors. Consequently, the variation in *NumCoor* becomes more chaotic, and the degree of fluctuation across consecutive cycles becomes more pronounced. Notably, a clear disparity emerges between the current cycle and the subsequent one (Fig. 14 $\Gamma = 4$).

Further analysis of local processes at different stages reveals interesting dynamics within the particle system. As shown in Fig. 15(a), particles in the lower region rise after colliding with the bottom, while those in the upper region continuously fall downward. The particle flow splits into two paths and then re-converges at a specific point. Subsequently, particles from above change direction upon colliding with those below, leading to compaction of the system. As depicted in Fig. 15(b), when all particles move upward, their velocities tend to equalize under the influence of gravity and friction against the container walls. Thus, particle segregation is suppressed during the rising process. Conversely, the decent process initiates from the lower region of the system. Particles in this region, particularly those near the sidewalls, are the first to descend, while others persist in moving upward, as shown in Fig. 15(c). Consequently, the particle system relaxes in the vertical direction, and as more particles descend, the gaps between them expand. Fig. 15(d) illustrates that when all particles are descending, those near the sidewalls experience faster movement due to wall friction until the gaps are filled. Throughout the transition from a compacted to a relaxed state, the gap size between particles increases. Therefore, the process of particle segregation can be considered a repetitive cycle involving compaction and relaxation. During the rising process, particles resemble a compressed solid block, while in the relaxed state, they exhibit fluid-like behaviour. This observation suggests that particle segregation can be viewed as a phase transition process, where the system undergoes transformations between quasi-solid state and quasi-liquid state.

The collective behaviour of granular mixtures can be categorized into two distinct states: a quasi-liquid state and a quasi-solid state. In the quasi-solid state, the granular system behaves like a solid, with minimal movement and limited changes in particle positions and spacing. In contrast, the quasi-liquid state is characterized by fluid-like properties, with apparent variations in particle positions and flow patterns. It is important to note the coexistence of these two states within the granular system, where a distinct interface delineates the transition between the quasi-liquid and quasi-solid regions. During the segregation of a particle system, when large particles experience upward leaping phenomena, the small particles located above them exhibit quasi-fluid motion, which is characterized by substantial variations in interparticle spacing. This dynamic behaviour creates spatial opportunities that enable the large particles to leap upward. Conversely, the small particles positioned beneath the large ones adopt a quasi-solid motion state, where there are minimal changes in interparticle spacing. This arrangement provides the necessary support for the large particles at the bottom, preventing their descent and thereby facilitating the successful completion of the leaping process.

6. Discussion

The phenomenon of convection motion in a binary mixture subjected to vertical vibration in a cylindrical container has been documented by Denies and Holeyman (2017). Due to the frictional forces exerted by the container walls, particles experience varying velocities, resulting in the formation of particle convection. During the overall upward motion of particles, those near the sidewalls exhibit slower velocities compared to

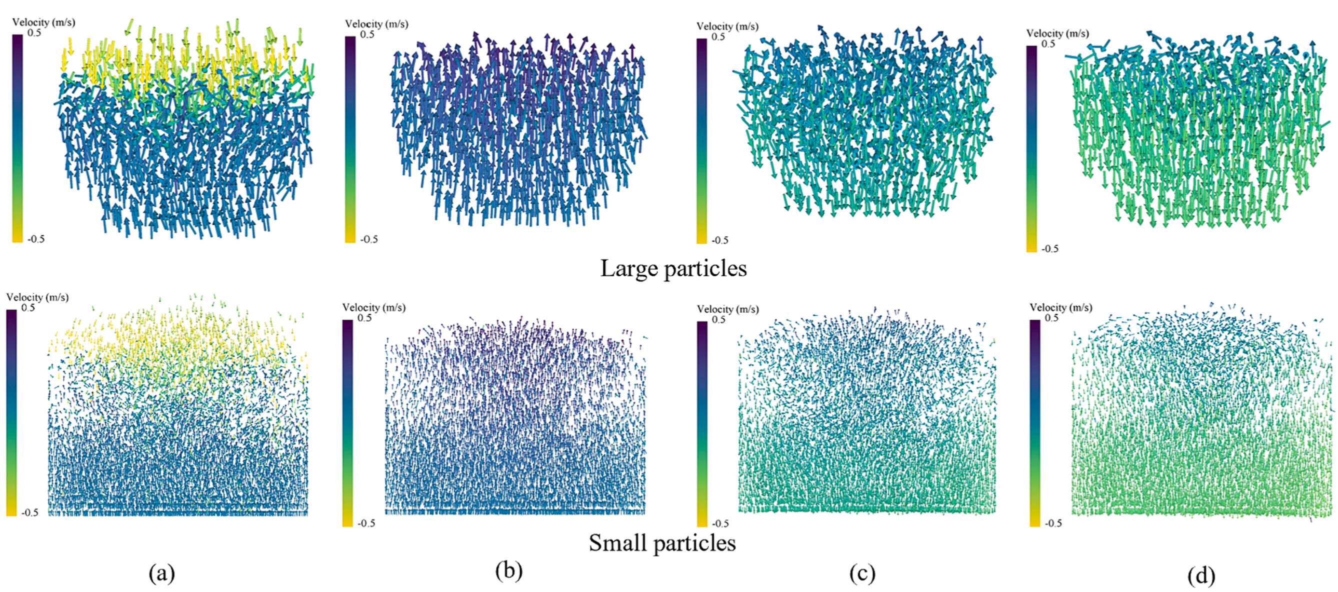

Fig. 15. Dynamics of the particle system during local processes.

those in the central region. This leads to the development of an upward convection, with a particle flow developing in the centre of the container and a downward flow along thin layers near the sidewalls (see Fig. 16). Grossman (1997) attributed this phenomenon to the non-elastic frictional interactions between the particles and the container walls. Indeed, the intensity of particle convection is influenced by the vibration intensity. In the case of lower vibration intensity, such as $\Gamma = 1$, the particle system exhibits minimal relative motion between particles, resembling a straight up and down motion. However, as the vibration intensity increases, as seen in the case of $\Gamma = 4$, the convection flow of particles becomes more pronounced and vigorous, resembling a fountain-like motion, where particles ascend from the bottom to the top before dispersing. This increased convection is a result of stronger frictional and collision interactions among particles. Despite the dynamic motion, both large and small particles reach a dynamic equilibrium within the stable phase, maintaining a balance between upward and downward motion.

If convection is the sole mechanism governing the final state of the system, it would be expected that all particles of different sizes would partake in a global convection process, leading to a more uniform distribution of particles. However, empirical observations reveal particle segregation on the surface, suggesting the involvement of an additional mechanism influencing the segregation process. The process of pore filling through penetration has been demonstrated as the mechanism responsible for this redistribution.

The particle system consists of individual particles with gaps between them, allowing for unrestricted movement. Under vibrating conditions, both large and small particles undergo reciprocating motion that synchronizes with the container's vibrations. As large particles move upward, voids are created in the lower region, subsequently filled by small particles. However, when large particles move downward, there is insufficient space in the lower region for them to reach the bottom. As a result, large particles accumulate at the top while small particles settle at the bottom. Nonetheless, under strong interaction conditions (increased vibration intensity), the gaps between particles become more pronounced, providing an opportunity for both large and small particles to potentially occupy these voids. The moving particles act as a randomly fluctuating sieve, with small particles having a greater likelihood and ability to penetrate through the gaps due to gravity. The downward motion of the particle system is counterbalanced by the upward pressure during compression, which affects both small and large particles. Large particles experience more pronounced resistance, while small particles can pass through the voids, ultimately leading to an overall downward motion of small particles relative to large particles. Hence, an important mechanism driving particle segregation is the ability of small particles to fill the voids created during particle motion. As depicted in Fig. 17, the distribution diagram of the particle system for $\Gamma = 4$ illustrates the occurrence of particle segregation, with small particles ultimately occupying the entire bottom region. The accumulation of small particles at the bottom restricts the width of the downward channel formed by the particles, impeding the descent of large particles to the bottom. Consequently, the larger components remain at the free surface, giving rise to the Brazil Nut Effect.

Particle segregation caused by size effects can be attributed to the interplay of two competing mechanisms. The first mechanism is the "pore filling through penetration" effect, where small particles find it easier to permeate through the gaps between large particles and reaching the bottom of the container. This effect becomes more pronounced as the size ratio between the particles increases. The second mechanism at play is convection, which involves global motion in the system that drives particle movement. While the permeation effect alone is not sufficient to cause visible particle segregation, convection rolls play a crucial role in transporting particles from the bed to the surface and downward along the walls, thereby enhancing the chances of small particles being pushed to the bottom through the gaps. The intensity of vibration influences the degree of particle segregation, as it affects the strength and dynamics of the convection rolls. Therefore, the final state of the system is determined by the delicate balance between the filtration of small particles through gaps and the convection rolls that facilitate the movement of particles between the bed and the surface. Both mechanisms play a crucial role in particle segregation, and their interplay determines the overall particle distribution within the system.

7. Conclusions

In this study, we investigated the phenomenon of particle segregation in a binary mixture subjected to vertical vibration in a cylindrical container. Our findings shed light on the underlying mechanisms driving the segregation process and provided insights into the dynamics and microstructural evolution of particles. The following conclusions can be drawn from this study.

The results demonstrated that under the influence of vibration, large particles tended to rise to the surface while small particles accumulated in the lower region of the system. These segregation patterns became more pronounced at higher vibration intensities. Additionally, the particle system exhibited a slight tendency for radial segregation. Statistical analysis of particle positions further confirmed the occurrence of both vertical and radial segregation. Vertical segregation occurred prior to radial segregation, and subsequently, the binary mixture reached a stable state of segregation. The segregation index provided a comprehensive analysis of the segregation behaviour, revealing an intriguing correlation between radial and vertical segregation.

Our results demonstrated the variability and stability of relevant parameters during the segregation cycle, revealing the repetitiveness of

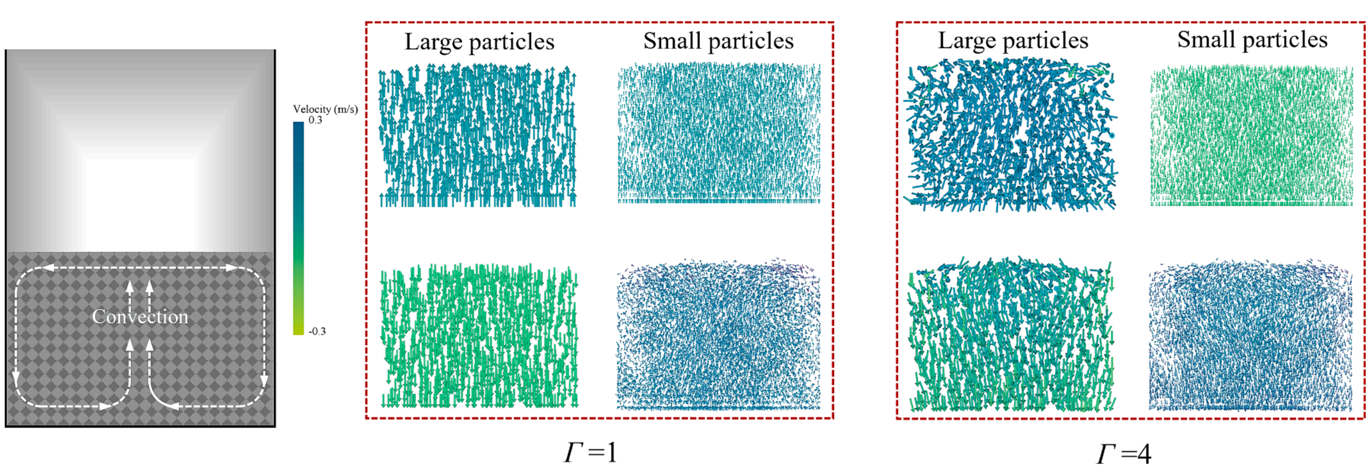

Fig. 16. Convective motion in segregation process.

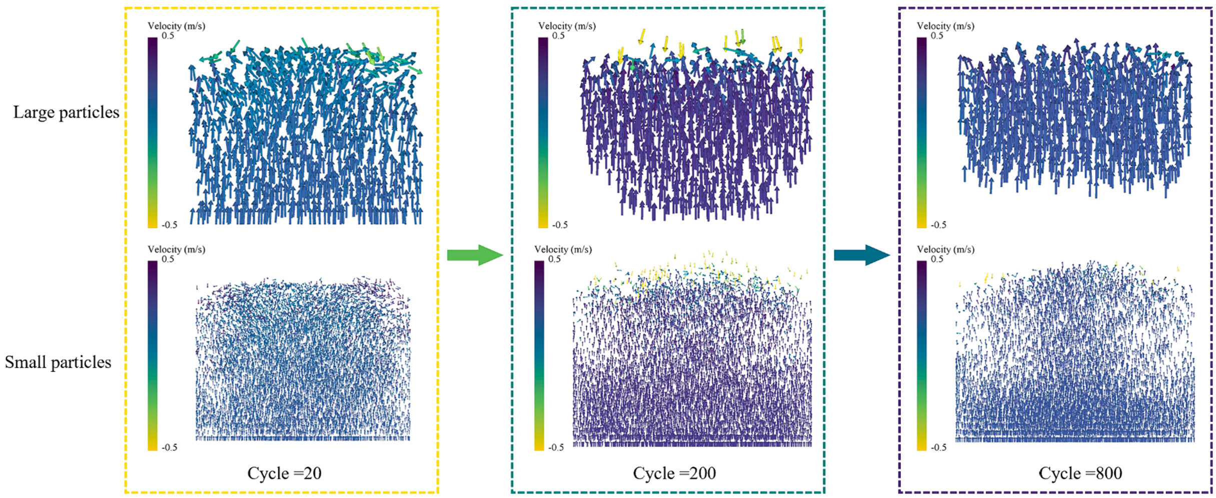

Fig. 17. Pore filling in segregation process.

compaction and relaxation processes. The rising process resembled the behaviour of a compressed solid block, while the relaxed state exhibited fluid-like behaviour. This repetitive compaction and relaxation process can be considered as a phase transition in particle segregation. We also observed that as the particle system became more compact, interlocking between particles occurred, resulting in the formation of a stable crystalline structure.

Through the analysis of particle trajectories and overall observations, we identified different motion patterns and convection behaviour between large and small particles. The study revealed that particle segregation was driven by the interaction between pore filling and convection rolls. The final state of the system was determined by the balance between the filtration of small particles through gaps and the convection rolls that facilitated particle movement.

The conclusions presented in this study contribute to an enhanced understanding of granular materials and provide a foundation for future research in the fields of granular dynamics and particle segregation. Moreover, they have implications for various applications such as landslides, debris flows, earthquake liquefaction, material transport, and mud pumping. Further research is required to explore the subtle segregation behaviour and its implications in these applications.

CRediT authorship contribution statement

Shaoheng Dai: Writing – original draft, Visualization, Software, Conceptualization. **Sheng Zhang:** Writing – review & editing, Supervision, Funding acquisition, Conceptualization. **Feng Gao:** Validation, Funding acquisition. **Xuzhen He:** Writing – review & editing, Validation, Supervision, Project administration, Funding acquisition. **Daichao Sheng:** Supervision, Project administration, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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