Numerical Investigation of the Effects of Particle Density and Dimensionless Acceleration on Segregation in 2D Vertically Vibrated Binary Granular Mixtures

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Abstract

The present work aims to investigate the influences of particle density and dimensionless acceleration on segregation phenomena in 2D binary granular mixtures by using contact dynamics method. The granular samples were prepared by randomly depositing two species of regular pentagonal particles inside a rectangular container. These two particle species are the same in size, but differ in terms of particle density. Different levels of vertical vibration were then applied to the mixtures. The simulation results were systematically analyzed by using segregation coefficient ($H$), segregation pattern, and velocity field related to convection mechanism. It was found that segregation phenomena are not observed in this study. This could be explained by the fact that a value of friction coefficient between interparticle and that value between wall and particle is set to be the same, that is why no segregation was found in the present study. Due to the friction, only convection rolls were observed for all the density ratios when dimensionless acceleration is greater than 2.

Keywords: Granular materials, Segregation, Density, Vertical vibrations, Contact dynamics method

1. Introduction

Granular materials are omnipresent around us in such a way that we can encounter in our daily life. For example, coffee beans, sugar, sands, rocks, etc. In this context, granular materials are defined as a collection of solid particles whose macroscopic mechanical behavior is governed by the contact forces between the particles. Due to a great diversity in grain properties, granular materials generally display complex behaviors, which cannot be easily categorized into ordinary solids, liquids, or gases [1]. These behaviors cause an occurrence of various phenomena that remains partially understood. One of the interesting phenomena is segregation, which is observed when a homogeneous bulk solid composed of various constituents or species evolves from an initially mixed state to a spatially non-uniform state due to the relative movement within the material [2]. The segregation is indeed an undesirable phenomenon observed in many industrial processes involving the processing and handling of granular mixtures such as pharmaceutical, powder metallurgy, agriculture, and food processing [2-4]. Such segregation often occurs during transportation and handling of granular mixtures due to shaken or vibrated systems [4-6].
It must be also noted that an occurrence of segregation phenomena is a major issue affecting low product yield and out-of-spec products. Consequently, this issue has motivated many researchers endeavoring to describe and understand the segregation phenomena in granular media for a long time. The particle size has been mainly employed to investigate such phenomena, compared to other particle properties such as density [2], shape [4, 6], or friction [7, 8]. It could be clearly seen that there is still a lack of knowledge and understanding in terms of the effects of other particle properties on the segregation phenomena.

Therefore, the influence of particle density on segregation phenomena is systematically investigated by changing densities of particles inside binary granular mixtures composed of regular pentagonal particles. These mixtures are subjected to various vertical vibrations characterized by dimensionless acceleration ($\Gamma$), in order to also understand the effect of driving parameters. The paper is organized as follows. Section 2 describes in brief about the fundamental of contact dynamics (CD) method, the details of numerical samples, and parameters used for segregation analysis. Section 3 is devoted to analyze and discuss the results obtained in the present work. Finally, the conclusions are then provided in Section 4.

2. Numerical Simulations
An open-source software so-called “LMGC90” [9, 10], which has been well-known and widely used for the simulations of granular materials, was employed in this study. It must be noted that LMGC90 is dedicated to the modelling of a large number of deformable or un-deformable interacting objects of any 2D or 3D shape with various mechanical behaviors. It also aims at considering interaction laws as complex as necessary, including multi-physics couplings such as thermal effects, fluids, etc.

2.1. Contact dynamics (CD) method
In this study, the simulations were performed by using the contact dynamics method or sometime called non-smooth contact dynamics (NSCD). This method is based on implicit numerical algorithms together with a non-smooth dynamic contact law and Coulomb’s law of friction to integrate equations of motion of rigid bodies. It must be noted that elastic repulsive interactions and smooth Coulomb’s law of friction are not required for the determination of contact forces. In the CD method, contact laws are employed to characterize the interactions between particles, instead of force laws. Only three parameters are required for the characterization of these interactions: the coefficient of friction when it is nonzero and the coefficients of normal and tangential restitution that control the dissipation rate. The unknown variables are only particle velocities and interaction forces. These variables are handled with an iterative method based on nonlinear Gauss-Seidel algorithm at each step for all potential contacts. A set of potential contacts is then identified or updated in each step. Note that the contact between two particles is detected by the overlaps of the space between them. In 2D simulations of the present study, the so-called “shadow overlap method” [11] was employed for the detection of contact between two convex polygonal bodies. For additional details in the implementation of the CD method, please see in refs. [12, 13].

Figure 1. Example of preparation of granular samples in the present work. Dense particles are represented by “blue” color, while loose particles are in “red” color.
2.2. Numerical preparations
Figure 1 shows an example of sample preparation in this study. Granular samples were prepared by two species of regular pentagonal particles with the same size, but different in terms of density. Five different density ratios consisting of 1.0, 1.7, 4.0, 8.0, and 12.0 were used in this study. Note that this density ratio is specified by the density between dense particle and loose particle ($\rho_d/\rho_l$). However, in order to prevent the effect of monodisperse granular materials, the particle sizes were necessary to be slightly different. Therefore, the particle sizes were generated by using a normal distribution between two values of the length measured from a centroid to a peak of the regular pentagon ($s$), i.e. $s_{\min} = 5.63$ mm and $s_{\max} = 5.86$ mm (see in Figure 1). Each particle species has the same number of particles, i.e. 2000 particles, which were randomly placed inside a rectangular container. It means that the total number of particles inside the granular sample is equal to 4000 particles. The aspect ratio between width and height of the container ($w/h$) was fixed at 2, see in Figure 1. The coefficient of friction between particles and that between the container wall and particle were set to be the same value of 0.3. Under the gravitational force, vertical vibrations in the manners of the sinusoidal wave were then applied to the granular samples. It must be also noted that the level of vibration was controlled by the dimensionless acceleration ($\Gamma$), which is defined by

\[
\Gamma = \frac{A\omega^2}{g} = \frac{A(2\pi f)^2}{g}
\]

where $A$ is the vibrational amplitude, $f$ is the vibrational frequency, and $g$ is the gravity. In this study, the vibrational amplitude was fixed at 5.0 mm, while the vibrational frequency was progressively varied to reach the values of $\Gamma = 1 - 5$. During the simulations, the kinematical data were saved every 10 seconds until the simulation finished at 300 seconds.

2.3. Segregation analysis
After the simulations were completed, the kinematical data obtained during the simulations were used to methodically analyze the segregation. Segregation coefficient ($H$), segregation pattern, and velocity fields were employed for this purpose.

2.3.1. Segregation coefficient ($H$)
This parameter is applied to quantify the degree of segregation of the binary mixtures in a static state [14], which is defined as

\[
H = 2\frac{h_d - h_l}{h_d + h_l}
\]

where $h_d$ is the average height of dense particles and $h_l$ is the average height of loose particles. The height of each particle was measured at their centroid with respect to the container base. Factor 2 is a multiplication factor arising from the equal solid fraction of each particle species which limits the average height of particles in such species to $0.25 < h_0 < 0.75$ and thus $-1 < H < 1$. In this case, the dense particles initially rise to the top of the container when $H > 0$, while the dense particles start to migrate to the bottom of the container when $H < 0$. Note that the segregation coefficient at the initial configuration of each granular sample is equal or approach to zero.

2.3.2. Segregation pattern
Previously, no segregation indices or coefficients can be used to characterize the segregation pattern. Until in 2016, Coletto et al. [15] developed and proposed a new segregation index named “Three Thirds Segregation Indices Set (TTSIS)”. This index cannot only describe the degree of segregation of the mixtures, but also the segregation pattern of interesting species. Hence, the TTSIS was applied for the analysis of the segregation pattern by modifying some conditions for the segregation patterns classification to consist of the conditions used in this study. In a classification of the segregation patterns,
a total number of particle centroids of interested species along every three ranges inside the container were necessary to be quantified by three corresponding indicators (see in Table 1): a bottom indicator ($p_B$), Middle indicator ($p_M$), and top indicator ($p_T$). It must be noted that the species of interest in this study was taken into account only dense particles.

**Table 1.** Conditions used in this study for classification of segregation patterns

| $p_B$  | $p_M$  | $p_T$  | and Segregation pattern |
|--------|--------|--------|-------------------------|
| ≥ 0.33 | ≥ 0.33 | ≥ 0.33 | PU Pure uniform         |
| Else if $0.3 \leq p_B \leq 0.4$ | $0.3 \leq p_M \leq 0.4$ | $0.3 \leq p_T \leq 0.4$ | U Uniform               |
| Else if $0.55 \leq p_B < 0.98$ | - | $|p_T - p_M| < 0.14$ | B Bottom                |
| Else if $- | 0.55 \leq p_M < 0.98$ | - | $|p_T - p_M| < 0.14$ | C Central               |
| Else if $- | - | 0.55 \leq p_T < 0.98$ | $|p_T - p_M| < 0.14$ | T Top                   |
| Else if $0.47 \leq p_B < 0.54$ | - | $0.47 \leq p_T < 0.54$ | V Pure V                |
| Else if $> p_M$ | - | $> p_M$ and $> p_B$ | VT V-top                |
| Else if $> p_M$ and $> p_T$ | - | $> p_M$ and $> p_B$ | VB V-bottom             |
| Else if $- | p_B < p_M < p_T$ | - | $p_M - p_B \geq 0.14$ | TC Top central          |
| Else if $- | p_B > p_M > p_T$ | - | $p_M - p_T \geq 0.14$ | BC Bottom central       |
| Else if $- | p_M > p_T > p_B$ | $|p_T - p_B| \geq 0.14$ | CT Central top          |
| Else if $p_M > p_B > p_T$ | - | - | $p_B - p_T \geq 0.14$ | CB Central bottom       |
| Else | - | - | - | TS Transition          |

2.3.3. **Velocity field**

According to the results obtained from previous researchers, it was found that convection is one of the important mechanisms influencing strongly on segregation phenomena in granular materials under vibrations [6, 16]. In general, two symmetric convection rolls were observed along two sidewalls of the vibrated container. The particles migrate downward along the side walls and move upward in the central part of the container. This phenomenon is known as “normal convection” [17]. This convection can be represented by a plot of the velocity of each particle inside the vibrated container. Therefore, the velocity fields will be employed in this study to analyze the occurrence of convection in the granular sample.

3. **Results and Discussions**

In this section, the effects of particle density and level of vibration on segregation phenomena analyzed by the three parameters for segregation analysis as mentioned in the previous section are presented and discussed as follows.

3.1. **Segregation coefficient ($H$)**

Figure 2 shows the relationship between the segregation coefficient ($H$) and time. It is clearly observed that the values of the segregation coefficient are uniform and close to zero ($H \approx 0$) along all the time of vibration for any density ratios and any dimensionless accelerations. In this case, it can be said in the beginning that segregation phenomena do not occur in the vertically vibrated granular system, even though both density ratios and dimensionless accelerations were changed in this study. In order to be undoubtedly ensure that no segregation arises in the present work, the segregation pattern which can characterize the distribution of a collection of interested particle species inside the container is then employed for this purpose.
3.2. Segregation pattern
The segregation pattern of the vertically vibrated granular mixtures at each time is presented in Figure 3. Note that only a collection of dense particles was used for the analysis of the segregation pattern. It can be seen that only three segregation patterns are observed: Pure Uniform (PU), Uniform (U), and Transition (TS). Distributions of these patterns have a similar characteristic, i.e. the number of the centroids of interested particles is distributed uniformly in each range of the container, excluding TS pattern that is attempting to change their distribution to other segregation patterns. As a result, it is clearly found that there is no occurrence of segregation phenomena in this study, corresponding to the results analyzed by the segregation coefficient.

Figure 2. Segregation coefficient ($H$) as a function of time in the cases of $\rho_d/\rho_l = 1.0, 1.7, 4.0, 8.0, \text{ and } 12.0$ under different dimensionless accelerations: a) $\Gamma = 1$, b) $\Gamma = 2$, c) $\Gamma = 3$, d) $\Gamma = 4$ and e) $\Gamma = 5$.

Figure 3. Segregation pattern as a function of time in the cases of $\rho_d/\rho_l = 1.0, 1.7, 4.0, 8.0, \text{ and } 12.0$ under different dimensionless accelerations: a) $\Gamma = 1$, b) $\Gamma = 2$, c) $\Gamma = 3$, d) $\Gamma = 4$ and e) $\Gamma = 5$. Note that the segregation highlight with green color is a uniform pattern.
3.3. Velocity field

Let us consider next the convection through a plot of velocity fields. As mentioned earlier, the convection is one of the main driving mechanisms for segregation phenomena. Therefore, the plotting of velocity fields enables us to clearly understand the role of the convection on the present work.

In the case of the dimensionless acceleration less or equal to 2, no convection rolls exist for any density ratios as shown in Figure 4a. It is evident that each particle inside the granular system just moves upward and downward alternately, according to a characteristic movement of the sinusoidal wave. In this manner, the granular system is more compacted by the vibration. In addition, it is interesting to note that some particles near the surface of the granular system are more excited in such a way that they move with high velocity and quite turbulence. In the case of the dimensionless acceleration greater than 2, the convection rolls are observed for all the density ratios used in this study as illustrated in Figure 4b. It is clearly seen that more than two convection rolls occurring in the granular system can be found in sometimes period. This observation corresponds to the experimental results reported in refs. [18, 19]. In addition, it is seemingly that a mixing occurrence of two types of convection is observed: normal and reverse convection.

![Figure 4. Examples of velocity fields of each particle in the granular mixtures with a) \( \rho_d/\rho_l = 12.0 \) at 140 seconds and b) \( \rho_d/\rho_l = 4.0 \) at 50 seconds under vertical vibrations](image)

![Figure 5. Examples of velocity fields of each particle in the granular mixtures with \( \rho_d/\rho_l = 8.0 \) under vertical vibrations with \( \Gamma = 3 \) at a) 190 seconds, b) 200 seconds, c) 210 seconds, and d) 220 seconds](image)

Apart from an occurrence of more than two convection rolls, it is interesting to also note that there are some movements of the convection rolls inside the container as shown in Figure 5. This situation is in contrast to whatever reported in the previous studies [5, 16, and 17]. The number of convection rolls...
and their movement might be caused by the effect of friction. In this study, it can be said that the effect of convection due to friction dominates over the effect of particle re-organization due to density ratio and dimensionless acceleration. Significantly, a value of friction coefficient between interparticle and that value between the container wall and particle is set to be the same. This is a reason why segregation phenomena do not occur in this study.

4. Conclusion
The objective of this study is to methodically investigate the influences of particle density and dimensionless acceleration on segregation phenomena in two-dimensional granular media subjected to vertical vibrations. For this purpose, Binary granular systems composed of 4000 regular pentagonal particles with different densities were systematically simulated by means of contact dynamics (CD) method via LMG90 software. Under the gravitational force, vertical vibrations were then applied to the mixture. The level of vibration was controlled by a dimensionless acceleration ($\Gamma$). It was found that for all the density ratios under any dimensionless accelerations, segregation coefficient ($H$) is close to zero. In addition, only “Uniform” and “Transition” patterns are observed in terms of the distribution of a collection of all dense particles inside the granular system. These results clearly indicate that no segregation phenomena occur in the vibrated granular systems due to the effects of particle density and dimensionless acceleration. This situation could be explained by the fact that the coefficient of friction between interparticle was set to be the same as the coefficient of friction between particle and wall, leading to an occurrence of convection. The convection occurred here are mixing between normal and reverse convections, when the dimensionless acceleration is greater than 2 for any density ratios. It is interesting to note that the convection rolls do not occur only near the sidewalls of the container as found on the previous studies, but they also move to other areas inside the container. Moreover, more than 2 convection rolls are observed in some periods. In this case, it could be said that the effect of friction causing the convection dominates over the effects of density and dimensionless acceleration. That could be a reason why no segregation was found in this study.

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