IV International Conference on Particle-based Methods – Fundamentals and Applications
PARTICLES 2015
E. Oñate, M. Bischoff, D.R.J. Owen, P. Wriggers & T. Zohdi (Eds)

DISCRETE ELEMENT MODELLING OF GRAIN SIZE SEGREGATION IN BI-DISPERSE GRANULAR FLOWS DOWN CHUTE

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Key words: Granular Flow, DEM, Segregation.

Abstract. Three-dimensional DEM simulations of size segregation in granular flows down chute are presented. Different cubic bi-disperse samples are generated by pluviation, on the rough base formed by randomly placed particles. Periodic boundaries are applied to the flow direction and the two sides. Parametrical studies involving slope angle, width, volume fraction, and coefficient of friction are systemically performed. In all presented cases, steady, fully developed (SFD) state is achieved, where the kinetic energy and fractional volume distribution remain constant. From the macroscopic view, segregations are completed in the SFD state with slightly different extents and a thick layer of pure coarse grains appears on the top of the flow. The profiles of volume fractions are calculated and presented by shear layers. In addition, the trajectories of individual particles are tracked and analysed, showing clearly the contact conditions and shear history experienced by individual particles. It is found that the connectivity of small particles is generally at a lower level than that of the large ones, indicating a high probability of small particles dropping into voids under gravity is higher. On the other hand, the large particles experience a significant increase of connectivity as they migrate through the layer of small particles.

1 INTRODUCTION

Grain segregation due to the variation of particle size, shape, density or other properties is commonly found in industrial processes and in the nature. Grain size segregation is the most effective one among all types of segregation [1], which can be vital in mineral processing procedures but it has an adverse effect on pharmaceutical manufacture and powder production where uniform mixing is desired [2]. Examples of size segregation in nature include the reverse grading of geo-materials in avalanches and debris flows [3]. It may exacerbate the destructiveness of such natural hazards, as it produces higher debris erosive power, longer runout distance and potentially higher impact force [4–7].

Size segregation occurs in many different scenarios and different mechanisms have been proposed in experimental and numerical studies. For instance, the three main mechanisms identified in vibration-induced segregation are convection, inertia and buoyancy [8–15]. For shear-induced segregation under gravity, e.g. in a rotating drum, percolation-based hypothesis states that small particles fall preferentially under gravity through the shear flow as a sieve [16–22], and other driving factors include porosity gradients and velocity gradients [23]. Another common situation for shear-driven segregation under gravity is the chute flow on a slope, or a heap [18]. Apart from the kinetic sieving mechanism in the direction normal to the base, secondary circulation in lateral direction [2] and recirculation near the bouldery front of the chute flow [4,24] are also reported in both small- and large-scale experiments. The recirculation and lateral transport of coarse grains may explain the formation of levees in the run-out of debris flows and avalanches [3,24,25]. In the granular flow down a rough plane, fingering instability, as a consequence of the frontal accumulation of coarse grains, has been reported [26–28]. Stratification is another phenomenon related to size segregation, which can be observed on the surface of a pile in the occurrence of avalanches [16,29–31]. Moreover, some researchers have studied the influence of interstitial water and other viscous fluid, and revealed that the viscous effect and buoyancy effect hinder the separation of different sizes [2,27,32].

The focus of the current work is on the size segregation in dense granular chute flows, which is generally explained by kinetic sieving and squeeze expulsion (after [33]). The basic idea of the two mechanisms is that small grains preferentially fall through the local voids underneath, which are randomly opened by the shearing down chute. The imbalance in contact force and the mass conservation normal to the base lead the larger grains to drift towards the top of the flow. Over decades, experimental studies have been carried out and provided evidences for these hypotheses [2,24,33–35]. The major measurements in experiments are the profiles of solid fractions and velocities from the side view, and the deposit granulometry. However, at present the measurements of phase fractions and velocities in the bulk of dynamic flows still remain a challenge, which hinders the collection of evidences to support the proposed mechanisms.

Recently, discrete element (particle) modelling (DEM or DPM) of bi-disperse granular flows has been reported, which allows a more detailed description of particle velocities, volume fractions and contact forces. The results from this sort of modelling are also interpreted in the macroscopic perspectives, e.g. the rheology of the flow [36,37], the profile of phase fractions [37–40], the kinetic energy [41] and the centre of mass for each species [5,42]. While most published simulations are performed in two dimensions [36,41,42], three-dimensional modelling may be able to provide more information in the lateral direction as segregation is not a pure gravity-driven process [37,39]. On the other hand, the inter-particle interactions, grain packing patterns and the flow rheology are inherently different in a three-dimension configuration.

In this paper, three-dimensional DEM simulations of grain size segregation are performed to study the micro-mechanical behaviour of segregation process. It is important to be able to identify how the segregation develops and to understand the effect of slope angle, width, volume fraction, and coefficient of friction on the degree of segregation. Sample creation and the approach to modelling a steady, fully developed flow are introduced in Section 2. A function is defined to measure the degree of segregation in the shear-dilated flows. In Section 3 and 4, simulation results are interpreted in both macroscopic and microscopic perspectives. The parametric studies, the fraction profile of large grains by different layers and the trajectories of individual particles are presented in sequence.

2 DEM SIMULATIONS

The DEM simulations presented here are performed using the open-source LIGGGHTS code [43], adopting Hertz contact model where Young's modulus E, Poisson ratio υ, the coefficient of friction μ and the coefficient of restitution e are the major parameters specified in material properties. Bi-disperse cubic samples in periodic cells are created to study infinitely long and wide chute flows [44,45]. One typical sample is shown in Figure 1, where a layer of large particles and small particles are poured into the boundary box in sequence under gravity, hence the distribution of geostatic stress as indicated by colours (the transition from red to blue indicates the highest to the lowest stress). The rough base (brown in colour) is constructed by fixing spheres, which are identical to a slice of randomly distributed small particles from the bulk, on the bottom of the box. Periodic boundaries are imposed to the flow directions and the two sides, while the top of the box is unbounded, allowing a free surface of the flow. To achieve flows down an inclined plane, the sample is tilted in xy plane to the target slope angle θ. The local coordinates shown in Figure 1 indicate that the x direction is the flow direction along the slope, while the y direction is normal to the inclined plane.

In all generated flows in this study, the steady, fully developed (SFD) state is achieved, where the kinetic energy and fractional volume distribution remain constant. Segregations are completed before the SFD state with slightly different extents and a thick layer of pure coarse grains appears on the top of the flow. In order to measure the degree of segregation being completed in the final steady state, a function of time is defined by considering the evolution of the centres of mass for the two types of particles. The degree of segregation $\alpha(t)$ is given by

$$\alpha(t) = 0.5 \times \left(1 - \frac{c_{1,t} - c_{2,t}}{c_{1,0} - c_{2,0}}\right) \tag{5}$$

where t is time, and c_1, c_2 are the y-coordinates of the centre of mass for small particles and large particles, respectively. The suffixes 0 and t denotes the initial state and the time t under consideration. The definition of $\alpha(t)$ considers the relative changes of c_1 and c_2, as the sample may be dilated under shear and both c_1 and c_2 may increase due to the dilation. The initial condition is thus $\alpha_0 = \alpha(0) = 0$. If $c_1 = c_2$, then $\alpha = 0.5$, meaning that the two groups of particles are uniformly mixed. The final state is denoted as $\alpha_\infty = \alpha(\infty)$, and $\alpha_\infty = 1$ if totally complete segregation occurs. However, this will not happen either in reality or in numerical simulations, because the diffusive mixing found in bi-disperse granular flows would prevent the fully-completed segregation [35].

After defining the degree of segregation, parametrical studies, including the sample size, slope angle, the volume fraction of small particles, and the coefficient of friction, are systemically performed. The length L and the height H of the sample have been studied in [42], following which $L = H = 40d_1$ is chosen in the current work. Here, d_1 is the diameter of small particles. In addition, it has been found in this study that sample size effects can be ignored with a sample measuring $W = 40d_1$ in width. On the other hand, since the influence of Young's modulus and Poisson ratio are not the focus of the current study, and the influence of the

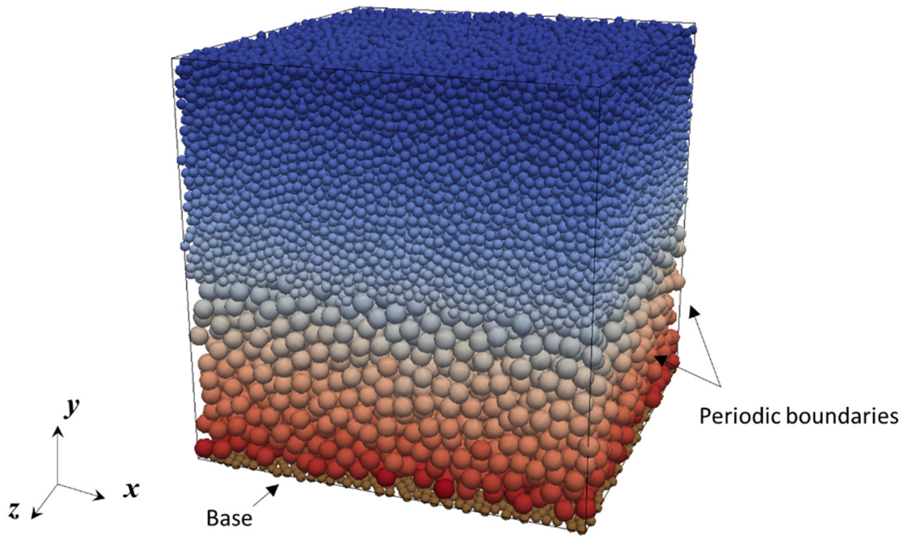

Figure 1: A bi-disperse sample with a rough base and periodic boundaries

coefficient of restitution is not significant in dense granular flows [44], these three parameters are fixed in the presented cases, i.e. E = 5MPa, υ = 0.45 and e = 0.4. The diameters of small and large particles adopted in this study are d_1 = 0.005m and d_2 = 0.01m, respectively.

All modelled cases are divided into three groups for different slope angles θ, friction coefficients μ and volume fractions of small particles ϕ_1 (Table 1). The volume fraction ϕ_1 is calculated from the height ratio of the two layers, i.e. h_1/h_2. The numbers of the two types of particles (n_1 and n_2) are also listed.

Table 1: Simulations performed

Group	θ (°)	μ	h_1/h_2	ϕ_1	n_1	n_2
I	21.5–30	0.4	1	0.53	2273	20361
II	25	0.1–0.5	1	0.53	2273	20361
III	25	0.1–0.5	0.5–3	0.27–0.69	10431–27037	3508–1484

3 RESULTS: MACROSCOPIC PERSPECTIVE

3.1 Degree of segregation

For the cases of Group I, the evolution of degree of segregation with increasing slope angle is shown against time in Figure 2. It is observed that after a short period of delay, segregation starts at 18–20 seconds. By checking the snapshots of the simulations, the delay is attributed to the rearrangement of particles and the dilation of the sample as a whole. The segregation is completed faster with higher slope angle, because the x-component of gravity is higher and it accelerates the flow. In all cases, the segregation process gets slower at a later stage and approaches to a steady state where α remains constant. The final degrees of segregation (α_∞)

are nearly converged at around 200s.

For Group II, keeping the same slope angle (25°), the degree of segregation is plotted against different coefficients of friction, as shown in Figure 3. Similar results can be found for other slope angles. It is observed that a hinge point appears at around 58s, before which the case with lower μ evolves slightly faster, while after that the case with higher μ climbs higher. The hypothesis is that for the low friction case, the rearrangement of particles occurs faster in the first stage, and the small particles can percolate through the opened voids more easily as there are more sliding occurring. Meanwhile, the reason behind the correlation of μ and α_∞ is yet under investigation.

In the simulations of Group III, it is found that α_∞ does not change with different volume fractions of small particles (ϕ_1). The results are plotted in Figure 4, in comparison with the data from previous 2D simulations [42]. The y-axis $(c_\infty - c_0)$/H is the normalized migration distance of the center of mass of large particles. The slope of the solid and dashed lines then represents the final degree of segregation, following the definition in [42], which is equivalent to Equation (5) if the dilation of sample in the SFD stage is neglected. The solid line is obtained using extrapolated values in [42] for comparison, since there is no distribution width for the two sizes in the current study. The dashed line is the fitting line of all $\mu = 0.5$ cases in the current 3D simulation results (i.e. the red hollow symbols in Fig. 4). The solid red circle is considered as an outlier. It is found that in 3D simulations the final degree of segregation α_∞ is lower than that in 2D. It indicates that segregation is completed more easily in 2D, partially attributed to the fact that in a two-dimensional configuration, the local voids fractions are higher and the movements in the other direction are constrained, promoting the upward migrations. Although the results for different volume fractions and slope angles converge to a single straight line, α_∞ increases with increasing μ for all different values of ϕ_1, which agrees with the findings in Figure 3.

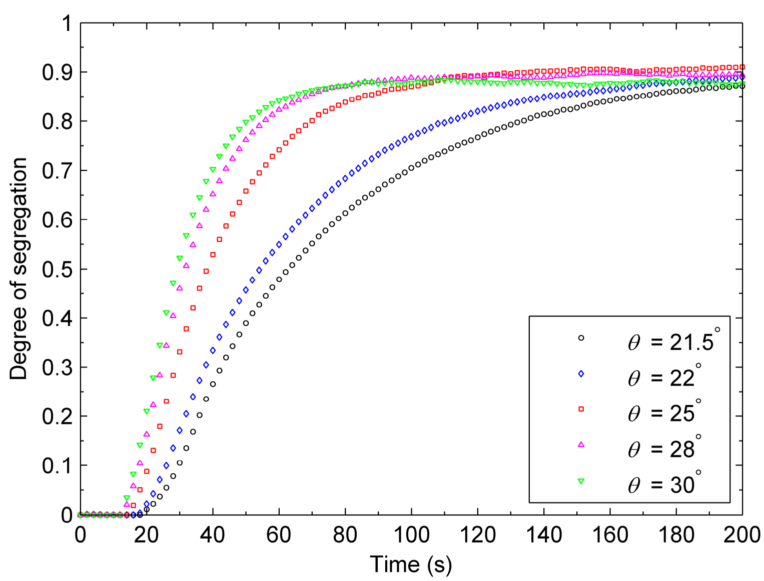

Figure 2: Degree of segregation with different slope angles ($\mu = 0.4$)

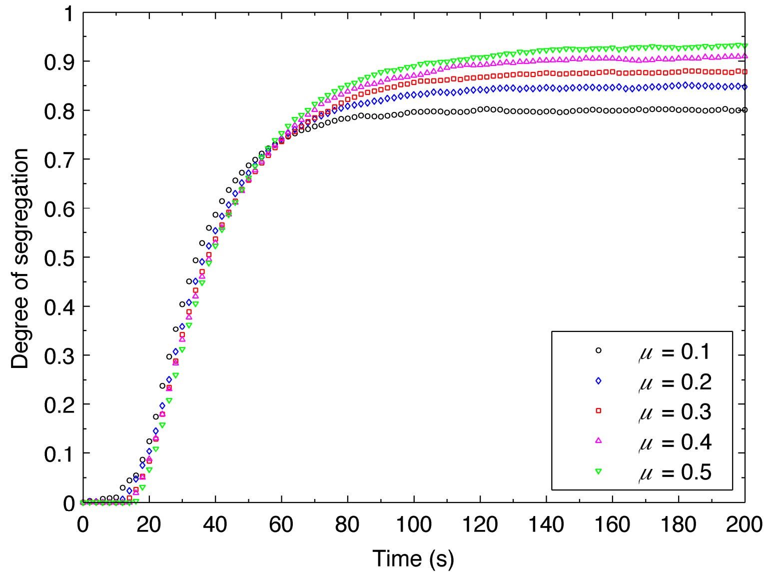

Figure 3: Degree of segregation with different coefficients of friction ($\theta = 25°$)

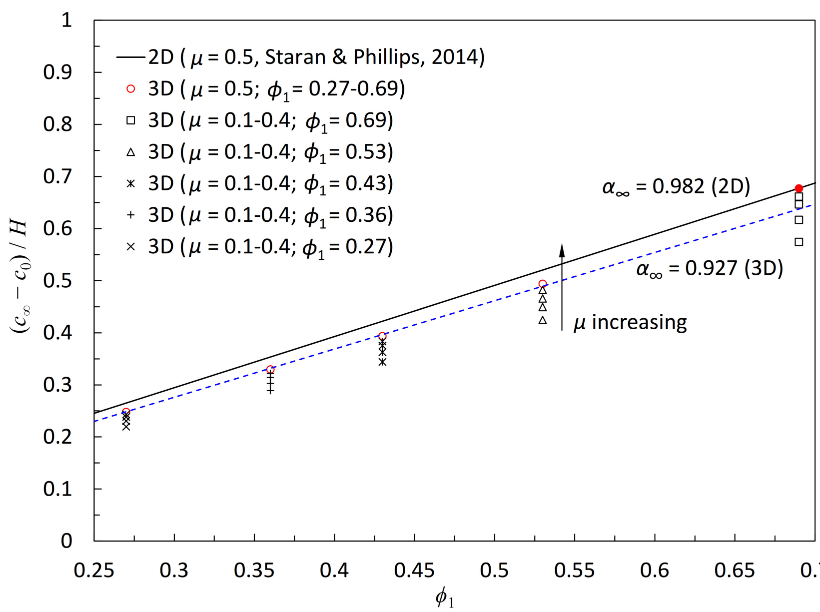

Figure 4: Final degree of segregation for various cases, compared to 2D simulations

3.2 Profile of volume fractions

Granular flows under shear exhibit layered behaviours because of the velocity gradients between different layers [46]. In bi-disperse flows, the evolution of the volume fractions of different species is also of interest during the mixing and segregation. Therefore, the volume fractions of large particles are averaged over different horizontal shear layers along the height of the sample. The case with $\mu = 0.4$, $\theta = 25°$ and $\phi_1 = 0.53$ is presented in the followed sections as an example. The profiles of fractional volumes are shown in Figure 5 for different time steps. Basically, three main stages can be identified, i.e. the initial stage (t = 0s) where large particles only appear in the lower half of the sample, the mixing/segregation stage (t < 100s) and the steady state (t > 100s) where the profiles get converged. The profile at t = 40s is nearly vertical in the bulk, indicating that the two groups are fully mixed, where the S-shape in the SFD state is consistent with the prediction of the mathematic model proposed in [35].

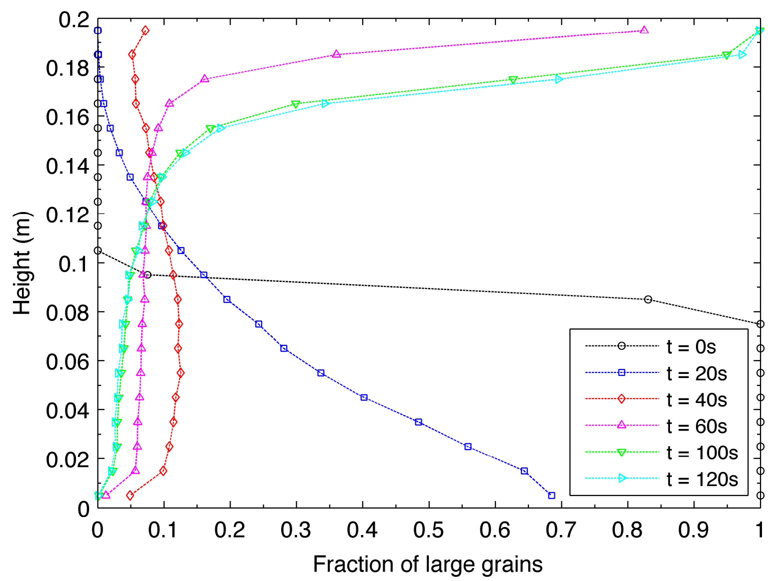

Figure 5: Profiles of volume fraction of large grains at different time

4 RESULTS: MICROSCOPIC PERSPECTIVE

The contact history and trajectory in y-direction are tracked on a randomly picked small particle that is initially in the top layer of the flow (Figure 6). The red line shows that after being lifted by the overall dilation before 20s, the particle is continuously dropping (despite the random fluctuation) throughout the whole simulation and finally reaches the base. On the other hand, the connectivity (i.e. the number of contacts acting on the particle) remains low (or normal level) during the whole process, with an average value about 3. It indicates that the small particle is subjected to less contacts, and has a higher chance to find voids opened by the shear flow. These findings provides microscopic evidence for the proposed kinetic sieving mechanism, which hypothesizes that the small particles can preferentially percolate through the voids [33].

Similar analysis is done for a typical large particle that is initially located at the base. The evolution of its elevation in Figure 7 shows that the upward migration is initiated at t = 20s, and it then migrates rapidly to the top of the flow. Fluctuations are observed when it stays in the top layer in the SFD state. Correspondingly, a clear trend of connectivity is identified (Fig.7). When

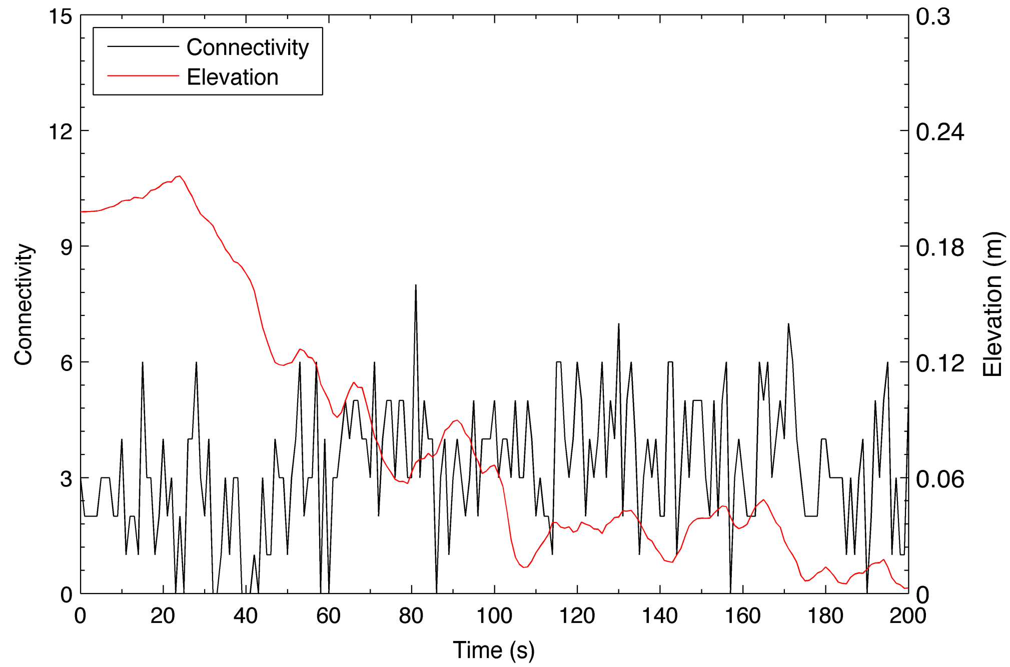

Figure 6: Trajectory and connectivity history of a single small grain

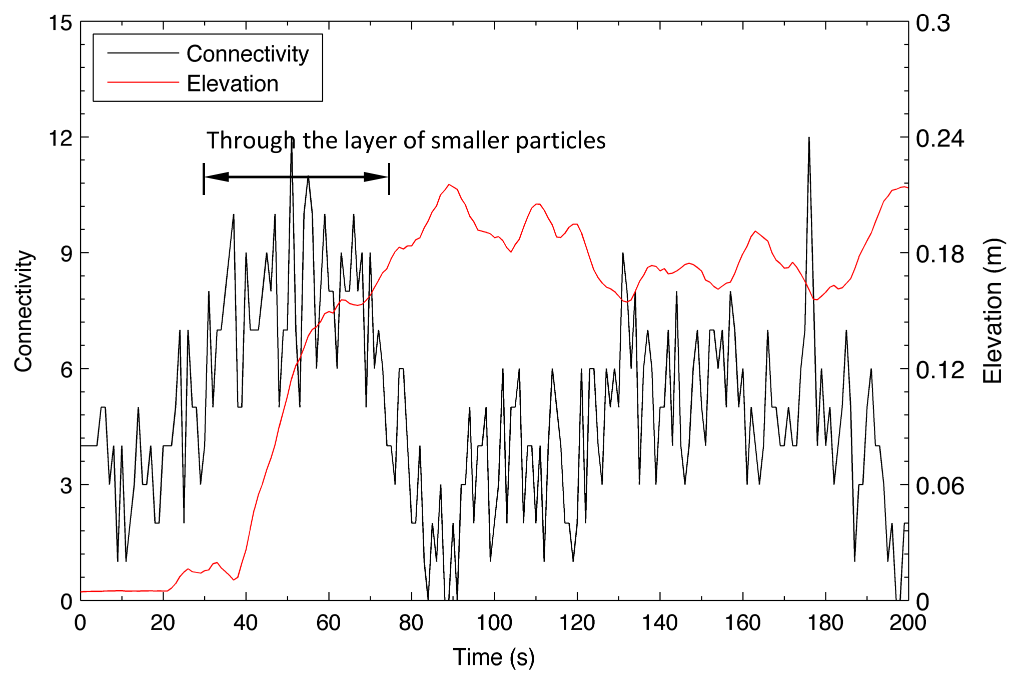

Figure 7: Trajectory and connectivity history of a single large grain

the particle is moving upward, the connectivity becomes significantly higher (8 on average, with peaks at nearly 12), implying that the large grain is mainly surrounded by the small ones. The high connectivity of the large particle moving through the layer of small particles, in conjunction with the rapid upward movement, offers a microscopic interpretation of the squeezing expulsion mechanism [33].

5 CONCLUDING REMARKS

In this paper, three-dimensional DEM simulations of size segregation are presented. Parametric studies have been performed aiming to provide guidance for similar modelling on setting sample size, slope angle and coefficient of friction. The influences of the different parameters on segregation are analysed. It is found that higher slope angle leads to faster segregation, while higher friction coefficient results in a higher final degree of segregation. The results presented with a newly defined degree of segregation, α_∞, are generally in good agreement with the previous 2D studies, as it is converged to a certain value for several different conditions. The comparison also reveals that the degree of segregation is higher in the 2D configuration, as the void fractions are higher and the movements in the other direction are constrained. In the macroscopic perspective, the profiles of volume fraction are presented. On the other hand, one of the major contribution of the current study is to provide microscopic evidences for the reviewed mechanisms (i.e., kinetic sieving and squeeze expulsion), since discrete element modelling produces more detailed information on the behaviour and contact conditions of individual particles. The trajectory of each particle is tracked and analysed, showing clearly the contact conditions experienced by each single particle. It is found that the connectivity of small particles are at a lower level than that of the large ones, indicating a higher probability of small particles dropping into voids under gravity. The large particles experience a significant increase of connectivity when they are migrating through the layer of small particles.

6 ACKNOWLEDGMENT

The work was supported by Research Grants Council of Hong Kong (under RGC/GRF 17203614), and the Research Institute for Sustainable Urban Development at The Hong Kong Polytechnic University. The computation was performed using the HKU Information Technology Services research computing facilities that are supported in part by the Hong Kong UGC Special Equipment Grant (SEG HKU09).

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