MODELING OF PARTICLE SIZE SEGREGATION: CALIBRATION USING THE DISCRETE PARTICLE METHOD

ANTHONY THORNTON

Department of Mechanical Engineering : Multi-Scale Mechanics,
Department of Mathematics : Numerical Analysis and Computational Mechanics
University of Twente, P.O. Box 217
7500 AE Enschede, The Netherlands
e-mail: a.r.thornton@utwente.nl,
http://www2.msm.ctw.utwente.nl/athornton/

THOMAS WEINHART

Department of Mechanical Engineering : Multi-Scale Mechanics,
Department of Mathematics : Numerical Analysis and Computational Mechanics
University of Twente, P.O. Box 217
7500 AE Enschede, The Netherlands
e-mail: t.weinhart@utwente.nl,
http://wwwhome.math.utwente.nl/~weinhartt/

STEFAN LUDING

Department of Mechanical Engineering : Multi-Scale Mechanics,
University of Twente, P.O. Box 217
7500 AE Enschede, The Netherlands
e-mail: s.luding@utwente.nl,

ONNO BOKHOVE

Department of Mathematics : Numerical Analysis and Computational Mechanics
University of Twente, P.O. Box 217
7500 AE Enschede, The Netherlands
e-mail: o.bokhove@utwente.nl,

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Over the last 25 years a lot of work has been undertaken on constructing continuum models for segregation of particles of different sizes. We focus on one model that is designed to predict segregation and remixing of two differently sized particle species. This model contains two dimensionless parameters, which in general depend on both the flow and particle properties. One of the weaknesses of the model is that these dependencies are not predicted; these have to be determined by either experiments or simulations.

We present steady-state simulations using the discrete particle method (DPM) for bi-disperse systems with different size ratios. The aim is to determine one parameter in the continuum model, i.e., the segregation Péclet number (ratio of the segregation velocity to diffusion) as a function of the particle size ratio.

Reasonable agreement is found; but, also measurable discrepancies are reported;

mainly, in the simulations a thick pure phase of large particles is formed at the top of the flow. In the DPM contact model, tangential dissipation was required to obtain strong segregation and steady states. Additionally, it was found that the Péclet number increases linearly with the size ratio for low values, but saturates to a value of approximately 7.35.

Keywords: Granular materials; DPM (DEM); Segregation; Continuum approach.

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1. Introduction

Many industrial processes use materials in a granular form, as they are easy to produce and store. A common industrial problem, especially in the food and pharmaceutical industry, is generating a consistent blend thus suppressing the natural tendency of mixed granular materials to segregate (e.g. see Refs 14, 31, 39). Generating high-quality homogeneous mixtures on an industrial scale is difficult and this fact is illustrated by the large number of different types of mixers available e.g. tumbling-, ribbon-blade-, rotating-, pneumatic-, air-jet-mixers; each with numerous competing designs. Understanding segregation and mixing in these types of apparatus remains an active area of research in both academia and industry. Additionally, segregation during transport and processing represents a huge problem in many other industrial processes, but also, remains poorly understood.

There are many mechanisms for the segregation of dissimilar grains in granular flows,[4] including inter-particle percolation,[6,19] convection,[8,11,30] density differences, collisional condensation,[20,30] differential air drag, clustering,[35] ordered settling and temperature driven condensation;[19,30] however, segregation due to size-differences is often the most important.[10] This study will focus on dense granular chute flow where *kinetic sieving*[32,37] is the dominant mechanism for particle-size segregation. The basic idea is: that as grains avalanche down-slope, the local void ratio fluctuates and small particles fall into the gaps that open up beneath them, as they are more likely to fit into the available space than the large ones. The small particles, therefore, migrate towards the bottom of the flow and lever the large particles upwards due to force imbalances. This was termed squeeze expulsion by Savage and Lun.[37] In frictional flows this process is so efficient that segregated layers rapidly develop, with a region of 100% large particles separated by a concentration jump from a layer of 100% fine particles below.[37,40,42] An experiment with two different density and sized particle species is illustrated in Figure 1, reproduced from Thornton's PhD thesis.[40] It shows the flow of red, large, dense, particles and white, small, less dense, particles from a hopper containing an approximately homogeneous mixture. A region of nearly pure, large, particles is formed near the free-surface, immediately on exiting the gate of the hopper. This layer grows in thickness as the material flows down the slope, due to the downward percolation of the smaller material. As the small material percolates, squeeze expulsion forces the large particles back upwards, forming a similar growing layer of nearly pure, small particles at the bottom of the flow. This process continues until these pure regions meet and the

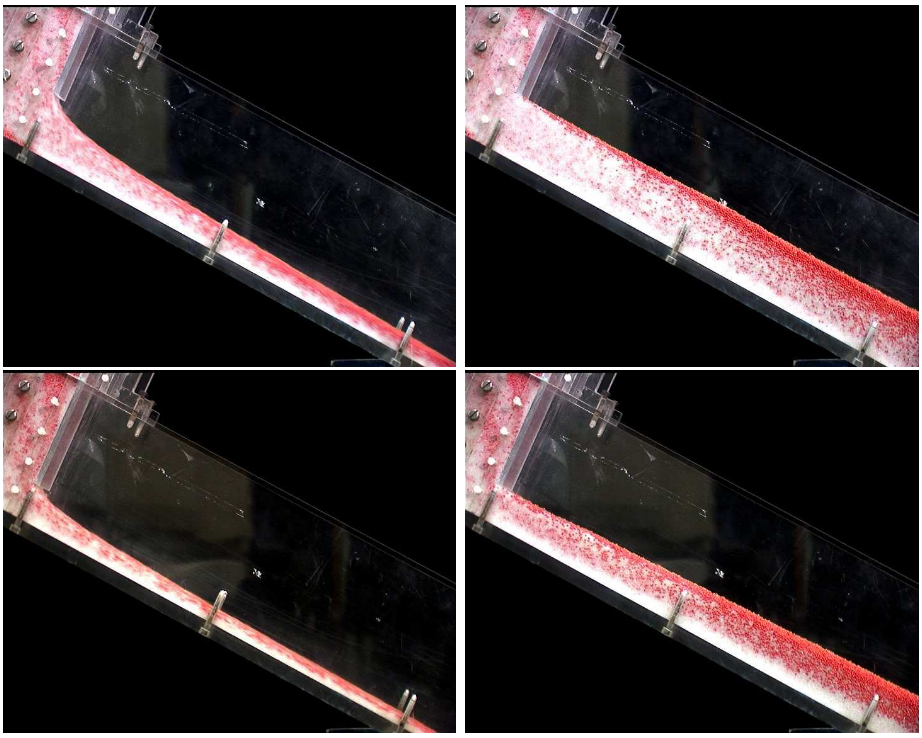

Fig. 1. A series of snapshots from experiments consisting of a 1:1 mixture, by volume, of sugar (red) and glass (white) particles down an inclined plane. The chute is made of perspex and is 5.1cm wide and 148cm long with an incline of 26° to the horizontal. The end of the chute was closed and hence a shock wave is generated when the material reaches the bottom. This shock propagates up the chute until reaching the hopper. As the shock passes, the depth of the flow is seen to increase in thickness. The images on the left-hand side show the material flowing before any material has reached the bottom and generated a shock wave. The images on the right are for the final deposit once the flow has come to rest. The top panels are for a gate height (initial depth) of 5cm and the bottom panels 3cm. The sugar (red) particles have density 1.2041 ± 0.0022g/cm^3 and diameter 1.5165 ± 0.1093mm; whereas the glass (white) particles have a density 2.4913 ± 0.0069g/cm^3 and diameter 0.7180 ± 0.0861mm. The screws from the base of the chute into the side walls are 18cm apart. Images taken from Thornton's Ph.D. Thesis.[40]

flow is inversely graded with large material above small. In this experiment density differences between the particles do add weak additional buoyancy forces that aid the segregation; but, this effect is secondary.[10] The original experiments of Savage & Lun[37] and Vallance & Savage[42] used particles that only differed in size. An image from these experiments can be found in Thornton, Gray and Hogg[41] and clearly shows the same structure with strong inverse grading.

In this publication we will use the Discrete Particle Method (DPM), e.g. see Refs 7, 26, 44, also known as the Discrete Element Method, to investigate segregation in dense granular chute flows. The ultimate aim is to use DPM to both validate the assumptions of kinetic sieving based segregation models, and to aid with the calibration of the free parameters that appear in these models. Despite the large number of discrete particle simulations of segregation in industrial chutes, and other apparatus, very few systematic studies have been performed for straightforward chute flows. Using simple chute geometries allows the results to be more easily compared to continuum theories enabling the determination of macro-parameters as a function of the DPM micro-parameters. We take the first step in this direction by investigating how the ratio of the strength of segregation to diffusion depends on the size ratio.

In summary, we will address three questions: *(i)* what is the minimal DPM contact model required to get segregation similar to that seen in experiments, *(ii)* how does the ratio of segregation to diffusion depend on the size ratio and *(iii)* how do our DPM results compare with a continuum theory, previously reported Monte Carlo simulations and experimental results?

2. The Discrete Particle Method

Many researchers have used DPM simulations to investigate segregation in a variety of situations and in this publication we give a brief overview. DPM has been used to investigate: density segregation in rotating cylinders;[23] flow of sintered ore and coke into blast furnaces;[33,34,46] size-segregation of magnetic particles in chutes;[47] numerous powder pharmaceutical applications including transport, blending, granulation, milling, compression and film coating;[22] and, sieving or screening.[5,25] However, of particular interest to this research, is the investigation of steady-state segregation profiles for varying density and size differences in chute flows by Khakhar *et al.*[24] They used DPM to investigate density effects and Monte Carlo simulations for different sized particles.

We use a DPM to perform simulations of a collection of bi-dispersed spherical particles of different diameters d_s and d_l, with the same density ρ; each particle i has a position $\boldsymbol{r}_i$, velocity $\boldsymbol{v}_i$ and angular velocity $\boldsymbol{\omega}_i$. It is assumed that particles are spherical, soft, and the contacts are treated as occurring at single points. The relative distance between two particles i and j is $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$, the branch vector (the vector from the centre of the particle to the contact point) is $\boldsymbol{b}_{ij} = -(d_i - \delta^n_{ij})\hat{\boldsymbol{n}}_{ij}/2$, the unit normal is $\hat{\boldsymbol{n}}_{ij} = (\boldsymbol{r}_i - \boldsymbol{r}_j)/r_{ij}$, and the relative velocity is $\boldsymbol{v}_{ij} = \boldsymbol{v}_i - \boldsymbol{v}_j$. Two particles are in contact if their overlap,

$$\delta^n_{ij} = \max(0, (d_i + d_j)/2 - r_{ij}),$$

is positive. The normal and tangential relative velocities at the contact point are given by

$$\boldsymbol{v}^n_{ij} = (\boldsymbol{v}_{ij} \cdot \hat{\boldsymbol{n}}_{ij})\hat{\boldsymbol{n}}_{ij}, \quad \text{and} \quad \boldsymbol{v}^t_{ij} = \boldsymbol{v}_{ij} - (\boldsymbol{v}_{ij} \cdot \hat{\boldsymbol{n}}_{ij})\hat{\boldsymbol{n}}_{ij} + \boldsymbol{\omega}_i \times \boldsymbol{b}_{ij} - \boldsymbol{\omega}_j \times \boldsymbol{b}_{ji}.$$

Particles are assumed to be linearly viscoelastic; therefore, the normal and tangential forces are modeled as a spring-dashpot with a linear elastic and a linear dissipative contribution.[7,26] Hence, the normal and tangential forces, acting from j

on i, are given by

$$\boldsymbol{f}_{ij}^n = k^n \delta_{ij}^n \hat{\boldsymbol{n}}_{ij} - \gamma^n \boldsymbol{v}_{ij}^n, \quad \boldsymbol{f}_{ij}^t = -k^t \boldsymbol{\delta}_{ij}^t - \gamma^t \boldsymbol{v}_{ij}^t,$$

where k^n and k^t are the spring constants and, γ^n and γ^t the damping constants. The elastic tangential displacement, $\boldsymbol{\delta}_{ij}^t$, is defined to be zero at the initial time of contact, and its evolution is given by

$$\frac{d}{dt}\boldsymbol{\delta}_{ij}^t = \boldsymbol{v}_{ij}^t - r_{ij}^{-2}(\boldsymbol{\delta}_{ij}^t \cdot \boldsymbol{v}_{ij})\boldsymbol{r}_{ij}, \tag{1}$$

where the second term corrects for the rotation of the contact, so that $\boldsymbol{\delta}_{ij}^t \cdot \hat{\boldsymbol{n}}_{ij} = 0$. When the tangential to normal force ratio becomes larger than the microscopic friction coefficient, μ^p, the tangential spring yields and the particles slide, truncating the magnitude of $\boldsymbol{\delta}_{ij}^t$ as necessary to satisfy $|\boldsymbol{f}_{ij}^t| < \mu^p |\boldsymbol{f}_{ij}^n|$. A more detailed description of the contact law used can be found in Weinhart *et al.*[44] and for a detailed discussion of contact laws, in general, we refer the reader to the review by Luding.[26]

The total force on particle i is a combination of the contact forces $\boldsymbol{f}_{ij}^n + \boldsymbol{f}_{ij}^t$ between all particle pairs i, j, currently in contact, and external forces, which for this investigation will be limited to only gravity. We integrate the resulting force and torque relations in time using Velocity-Verlet[2] and forward Euler with a time step $\Delta t = t_c/50$, where t_c is the contact duration[26] given by

$$t_c = \pi \Big/ \sqrt{\frac{k^n}{m_{ij}} - \left(\frac{\gamma^n}{2m_{ij}}\right)^2}, \tag{2}$$

with reduced mass $m_{ij} = m_i m_j/(m_i + m_j)$. The base is composed of fixed particles, which are endowed with an infinite mass and, thus are unaffected by body and contact forces: they do not move.

Obtaining macroscopic fields from DPM simulations is a non-trivial task, especially near a boundary. We will use an advanced and accurate spatial coarse-graining procedure.[3,12] For the present study, we only require the volume of the small particles,

$$V^s(\boldsymbol{r}, t) = \frac{\pi}{6} d_s^3 \sum_{i \in \mathcal{S}} \mathcal{W}(\boldsymbol{r} - \boldsymbol{r}_i(t)), \tag{3}$$

and the total particle volume

$$V(\boldsymbol{r}, t) = \frac{\pi}{6} \sum_i d_i^3 \mathcal{W}(\boldsymbol{r} - \boldsymbol{r}_i(t)), \tag{4}$$

where $\mathcal{W}$ is a coarse-graining function, and $\mathcal{S}$ denotes the set of small particles. In this publication $\mathcal{W}$ is taken to be a Gaussian of width, or variance, $d_s/2$, i.e.,

$$\mathcal{W}(\boldsymbol{r} - \boldsymbol{r}_i(t)) = \frac{1}{(\sqrt{2\pi} d_s/2)^3} \exp\left(-\frac{|\boldsymbol{r} - \boldsymbol{r}_i(t)|^2}{2(d_s/2)^2}\right). \tag{5}$$

For information on how to construct other fields, we refer the reader to Goldhirsch[12] and for an extension that is still valid near a boundary see Weinhart *et al.*[45]

3. Continuum model of segregation

The first model of kinetic sieving was developed by Savage and Lun,[37] using a statistical argument about the distribution of void spaces. This model was able to predict steady-state size distributions for simple shear flows with bi-dispersed granular materials. Later, Gray and Thornton[18,40] developed the same structure from a mixture-theory framework. Their derivation has two key assumptions: firstly, as the different particles percolate past each other there is a Darcy-style drag between the different constituents (i.e., the small and large particles) and, secondly, particles falling into void spaces do not support any of the bed weight. Since the number of voids available for small particles to fall into is greater than for large particles, it follows that a higher percentage of the small particles will be falling and, hence, not supporting any of the bed load. In recent years, this segregation theory has been developed and extended in many directions: including the addition of a passive background fluid,[40,41] the effect of diffusive remixing,[16] and the generalisation to multi-component granular flows.[15] We will use the two-particle size segregation-remixing version derived by Gray and Chugunov;[16] however, it should be noted that Dolgunin and Ukolov[9] were the first to suggest this form, by using phenomenological arguments. The bi-dispersed segregation-remixing model contains two dimensionless parameters, which in general will depend on flow and particle properties; examples include: size-ratio, material properties, shear-rate, slope angle, particle roughness, etc. One of the weaknesses of the model is that it is not able to predict the dependence of its parameters on the particle and flow properties; these have to be determined by either experiments or DPM simulations.

Kinetic-sieving models work best in dense, not too energetic flows, where enduring contacts exist. For more energetic flows kinetic theory is more appropriate and segregation models derived from this framework are applicable, examples include, Jenkins;[20] Jenkins and Yoon;[21] and, Alam, Trujillo and Herrmann.[1] Using DPM, it is possible to systematically increase the kinetic energy of the flows and investigate the transition between dense and kinetic regimes, but this is beyond the scope of the current investigation, where we only consider the dense regime.

The two-particle segregation-remixing equation[16] takes the form of a non-dimensional scalar conservation law for the small particle concentration ϕ as a function of the spatial coordinates $\hat{x}, \hat{y}$ and $\hat{z}$; and, time $\hat{t}$,

$$\frac{\partial \phi}{\partial \hat{t}} + \frac{\partial}{\partial \hat{x}} (\phi \hat{u}) + \frac{\partial}{\partial \hat{y}} (\phi \hat{v}) + \frac{\partial}{\partial \hat{z}} (\phi \hat{w}) - \frac{\partial}{\partial \hat{z}} (S_r \phi (1 - \phi)) = \frac{\partial}{\partial \hat{z}} \left(D_r \frac{\partial \phi}{\partial \hat{z}} \right), \tag{6}$$

where S_r is the dimensionless measure of the segregation-rate, whose form in the most general case is discussed in Thornton, Gray and Hogg[41] and D_r is a measure of the diffusive remixing. In Eq. (6), ∂ is used to indicate the partial derivative, $\hat{x}$ is the down-slope coordinate, $\hat{y}$ the cross-slope and $\hat{z}$ normal to the base coordinate; furthermore $\hat{u}, \hat{v}$ and $\hat{w}$ are the dimensionless bulk velocity components in the $\hat{x}, \hat{y}$ and $\hat{z}$ directions, respectively. The conservation law (6) is derived under the assumption of uniform total granular volume fraction and is often solved subject to the condition that there is no normal flux of particles through the base or free surface of the flow.

3.1. *Steady-state solution*

We limit our attention to small-scale DPM simulations, periodic in the x and y-directions, and investigate the final steady-states. Therefore, we are interested in a steady-state solution to (6) subject to no-normal flux boundary condition, at $\hat{z} = 0$ (the bottom) and 1 (the top), that is independent of $\hat{x}$ and $\hat{y}$. Gray and Chugunov[16] showed that such a solution takes the form,

$$\phi = \frac{\left(1 - e^{(-\phi_0 P_s)}\right) e^{(\phi_0 - z) P_s}}{1 - e^{(-(1-\phi_0) P_s)} + \left(1 - e^{-\phi_0 P_s}\right) e^{(\phi_0 - z) P_s}}, \tag{7}$$

where $P_s = S_r / D_r$ is the segregation Péclet number and ϕ_0 is the mean concentration of small particles. This solution represents a balance between the last two terms of (6) and is related to the logistic equation. In general, P_s will be a function of the particle properties, and we will use DPM to investigate the dependence of P_s on the particle size ratio

$$\sigma = d_s / d_l. \tag{8}$$

It should be noted that σ has been defined such that it is consistent with the original theory of Savage and Lun;[37] however, with this definition only values between 0 and 1 are possible. Therefore, we will present the results in terms of σ^{-1} which ranges from 1 to infinity. The useful property of the steady-state solution (7) is that the profile is only a function of the total small particle concentration ϕ_0 and P_s: It allows P_s to be determined from a simple periodic box DPM simulation.

3.2. *Non-dimensionalisation of the DPM results*

The DPM results presented in Section 4 will be averaged in the x- and y-directions and hence, we will obtain local volumes of both the total granular (4) and small particles (3) as a function of z only. For comparison with the non-dimensional analytical solution (7) the results will be non-dimensionalised by the scaling

$$\hat{z} = (z - b)/(s - b) \quad , \quad \phi = V^s / V, \tag{9}$$

where b is the location of the base of the flow, s the location of the free surface and V^s and V are given by equations (3) and (4), respectively. Hence, the mean concentration, ϕ_0, of small particles is given by

$$\phi_0 = \frac{1}{s - b} \int_b^s \phi(z)\, \mathrm{d}z = \int_0^1 \phi(\hat{z})\, \mathrm{d}\hat{z}. \tag{10}$$

It is then possible to directly compare (7), obtained subject to the no-normal flux condition at $\hat{z} = 0, 1$, with the steady-state volume fraction profiles, $\phi(z)$, obtained from the simulations. Then, Eq. (7) allows the determination of P_s as a function of the parameters of the contact model.

The free surface of the flow is not clearly defined in a DPM simulation and here two different definitions will be considered. Weinhart *et al.*[44] investigated how to consistently define the base and free-surface locations for flows over rough bottoms. Following their results we define both the base and free surface via the downward normal stress, σ_{zz}. For steady uniform flows, it follows directly from the momentum equations that the downward normal stress is lithostatic, i.e., it balances the gravitational weight. Thus, $\sigma_{zz}(z)$ has to decrease monotonically from a maximum at the base to zero at the free-surface. However, in order to avoid effects of coarse graining or single particles near the boundary, we cut off the stress $\sigma_{zz}(z)$ on either boundary by defining threshold heights

$$z_1 = \min\{z : \ \sigma_{zz} < (1-\kappa) \max_{z\in\mathbb{R}} \sigma_{zz}\} \quad \text{and} \tag{11a}$$

$$z_2 = \max\{z : \ \sigma_{zz} > \kappa \max_{z\in\mathbb{R}} \sigma_{zz}\} \tag{11b}$$

with $\kappa = 0.01$. We subsequently linearly extrapolate the stress profile in the interval (z_1, z_2) to define the base, b, and surface location, s, as the height at which the linear extrapolation reaches the maximum and minimum values of σ_{zz}, respectively,

$$b = z_1 - \frac{\kappa}{1-2\kappa}(z_2 - z_1); \text{ and } \ s_f = z_2 + \frac{\kappa}{1-2\kappa}(z_2 - z_1), \tag{11c}$$

here the subscript f indicates that this is a definition of the free-surface location.

In granular chute flows there is a layer of saltating particles towards the top of the flow, where the density decreases with height. This effect is confirmed in the simulations presented here, see Figure 5. Gray and Chugunov[16] suggested that the theory should not be fitted over the less dense region and defined the top of the flow as the point where the density starts to decrease. Therefore, we will also use

$$s_d = (1-2\kappa) \max \rho \tag{12}$$

to define the surface between the dense and less dense regions, where ρ is the density of the flow. An illustration of the demarcation between dense and less dense flow is shown in Figure 5. We will use the notation $\hat{z}_f$ to indicate the scaling based on the free-surface location and $\hat{z}_d$ on the location of the dense basal layer.

4. Previous comparison to the theory

The original theory of Thornton and Gray[18,40] has been used to investigate shear-driven segregation in an annular Couette cell.[13,28,29] In the papers cited the segregation rate is assumed to be proportional to the local shear rate and the experimentally determined velocity profiles are used to solve the continuum model. In these experiments it was not possible to monitor the local volume fraction of the small particles directly, and it had to be inferred via the measured expansion and compaction of the sample. They found good agreement between model and theory in the initial phase, but at later times the segregation rate exponentially slowed down, which is not captured by the model. Additionally, they observed an increase in the thickness of the sample as the particle profile evolved (Reynolds dilatancy); this effect

Table 1. List of the values used in the contact model. Parameters k, γ are chosen such that for a small-small collision the restitution coefficient $r_c = 0.6$ and $t_c = 0.005\sqrt{d_s/g}$. For details of the contact model refer to Section 2.

ρ	$2400\,\mathrm{kg\,m^{-3}}$	k^n	$29.00\,\mathrm{N\,m^{-1}}$
g	$9.8\,\mathrm{m\,s^{-2}}$	k^t	$2/7k^n$
d_s, d_{base}	$0.6\,\mathrm{mm}$	$\gamma^n,\ \gamma^t$	$0.0017\,\mathrm{s^{-1}}$
d_l	$(1.1-2)d_s$	μ^p	0.5

is also not included in the model. The measured segregation rates were found to be non-monotonic in particle size-ratio; however, they considered very large size-ratios (up-to $\sigma^{-1} = 4$) for which the kinetic sieving process is known to start breaking down. Savage and Lun[37] showed that percolation effects are evident for $\sigma^{-1} > 2$ and stated that spontaneous percolation occurs for $\sigma^{-1} > 6.464$, i.e., small particles could percolate through the matrix of larger particles simply as a result of gravity, even in the absence of any shear.

Recently, chute experiments have been performed with a binary mixture of spherical glass particles with size-ratio of $\sigma^{-1} = 2$ down an incline of 29 degrees.[43] In these experiments it was very difficult to produce steady flow conditions and a dependence of the Péclet number on other parameters was observed. For these flow conditions Péclet numbers in the range 11-19 were reported.

Marks and Einav[27] used a cellular automata model to investigate segregation in granular chute flows. They found good agreement between the model and their simulations. For simple shear configurations they found sharp jumps in concentration as predicted by the original low-diffusion theory.[18,40]

Khakhar, McCarthy & Ottino[24] performed a detailed investigation of segregation, by both size and density differences in granular chute flows. For equal density different size particles they used Monte Carlo techniques to obtain steady-state profiles. Gray and Chugunov[16] fitted this data to the steady-state solution (7). They found that for inelastic particles with $\sigma^{-1} = 1.11$, on an incline of 25^o, a Péclet number of 4 matched the data best. It should be noted that they did not fit across the entire layer of the flow, but from the top of the dense avalanching layer. Gray and Chugunov[16] used an ad-hoc position for the location of the dense avalanching layer; we however, will use definition (12).

5. Measured segregation rates

Simulations were run with the parameters given in Table 1. The parameters of the normal forces were such that the restitution coefficient, for a collision between two small particles, is

$$r_c = \exp^{-6t_c\gamma^n/(\pi d_s^3\rho)} = 0.6$$

and the collision time $t_c = 0.005\sqrt{d_s/g}$ for the small particles, where $\sqrt{d_s/g}$ is the small particle diameter to gravitational acceleration timescale. In total ten simu-

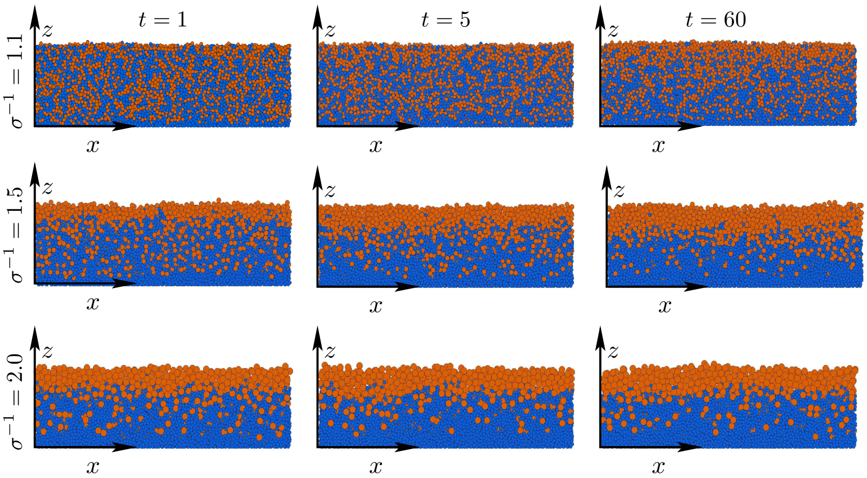

Fig. 2. A series of snapshots from the DPM simulations with large (orange) and small (blue) particles. The rows correspond to distinct particle sizes and columns to different times. Along the top row $\sigma^{-1} = 1.1$, middle row $\sigma^{-1} = 1.5$ and bottom row $\sigma^{-1} = 2$; whereas, the left column is for $t = 1$, middle $t = 5$ and right $t = 60$.

lations were performed for values of $\sigma^{-1} = d_l/d_s$ from 1.1 to 2.0 in steps of 0.1. Initially, only normal forces were 'turned on' in the contact model, but these flows did not settle to a stable steady state. Also, with only normal forces the flow occasionally spontaneously compacted, reducing its thickness by around 15% and then slowly dilated back to approximately its original density; this effect has not been observed in experiments. For this reason tangential forces were added to the contact model with $k^t = 2/7k^n$, $\gamma^t = \gamma^n$, and $\mu = 0.8$. Including the tangential forces had three effects: *i*) the flow settled to a steady state, *ii*) the compaction effect was not observed and *iii*) the degree of segregation was increased. It should be noted that we also performed simulations with only normal forces and tangential dissipation. This was sufficient to remove most of the problems; however, the flow was not quite fully steady and the segregation was slightly weaker. We therefore concluded, that for the process of segregation in granular chute flows including both tangential and normal forces leads to better overall behaviour. From this point onwards, only simulations containing both normal and tangential forces will be considered, with parameters as given in Table 1.

Figure 2 shows a series of images from the DPM simulations at different times and values of σ^{-1}. The simulations take place in a box, which is periodic in x and y, is $5d_s$ wide and $83.3d_s$ long, inclined at an angle of 25^o to the horizontal. The base was created by adding fixed small particles randomly to a flat surface. The simulations are performed with 5000 flowing small particles and the number of large particles is chosen such that the total volume of large and small particles

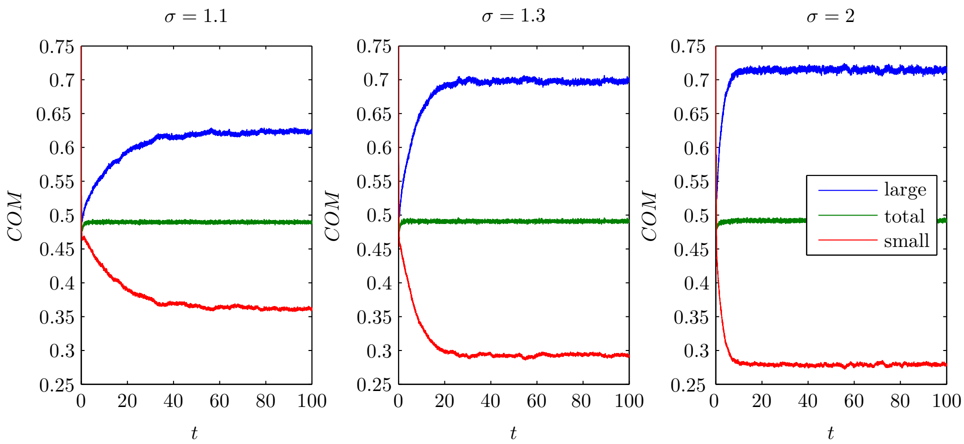

Fig. 3. Centre of mass (COM), scaled by the flow height, of the small particles (red), large particles (blue) and bulk (green) as a function of time. Plots are shown for $\sigma^{-1} = 1.1, 1.3$ and $\sigma^{-1} = 2$. From the plots it is clear all simulations are in steady state by $t = 50$.

is equal, i.e., $\phi_0 = 0.5$ (to within the volume of one large particle). The initial conditions are randomly distributed without checking for overlaps; this creates a good homogeneous distribution of particles, but it does mean there are a few large initial overlaps. The initially large stored potential energy, causes a small 'explosion' of particles in the first few time steps, but it is quickly dissipated and has no effect on the long-term evolution of the flow. To investigate the early evolution of the segregation $t < 1$, such initial conditions do not suffice and more care is required to prepare an initially well mixed configuration.

Qualitatively it can be seen from Figure 2 that the larger σ^{-1} the stronger the segregation. For the cases $\sigma^{-1} = 1.5$ and $\sigma^{-1} = 2$ a thick pure phase of large particles is formed at the top of the flow, but no equivalent thick pure small phase is formed at the base. At the base a very thin pure layer of small particles is formed which is at most two particle layers thick. This is due to the base comprising of small particles and, hence, only small particles can fit in the gaps in the basal surface. For the case $\sigma^{-1} = 1.1$ some segregation can be observed; but, no pure layers are formed at either the top or the bottom.

Due to the use of a periodic box, no direct comparison with the large number of low-diffusion ($P_s \to \infty$), two-dimensional, analytical solutions, that have been previously published,[17,18,29,38,40,41] can be made. However, if the flow is computed until it reaches a steady state, a comparison with the steady-state solution for the diffusion case (finite P_s), presented by Gray and Chugunov,[16] can be performed. This steady state only depends on the volume fraction of small particles and the Péclet number of the flow, as given by Eq. (7). To confirm the flow is in steady state, the vertical centre of mass (COM) of the small and large particles is computed. Three examples are shown in Figure 3. As can be seen, initially the COM of the small particles quickly decreases, while the COM of the large particles rises. This

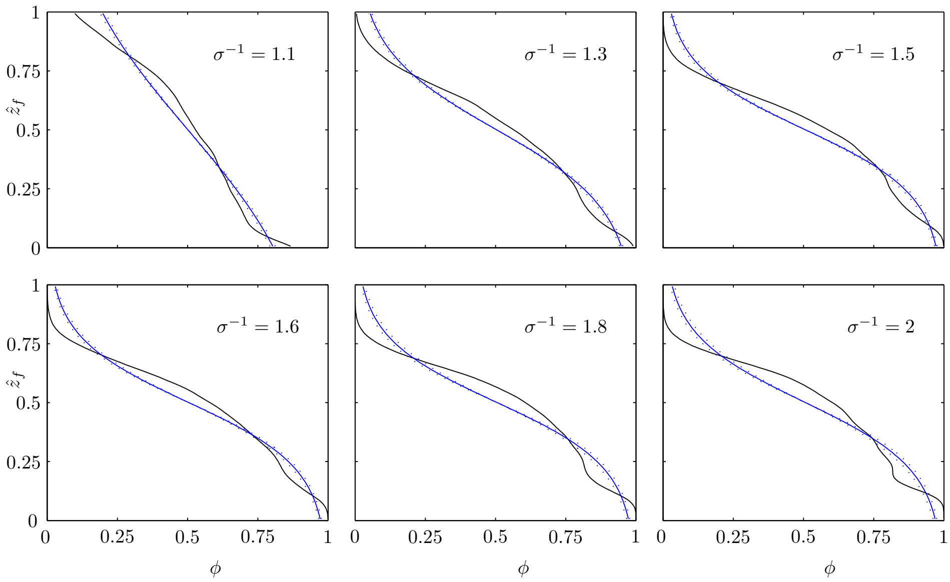

Fig. 4. Plots of the small particle volume fraction ϕ as a function of the scaled depth $\hat{z}_f$. The black lines are the coarse-grained DPM simulation data and the blue lines are the fit to Eq. (7) produced with MATLAB's non-linear regression function. For the fit only P_s is used as a free parameter. Dotted lines shows the 95% confidence intervals for the fit.

process slows down and eventually the COM becomes stable. For all the values of σ^{-1} considered, the COM of the small particles reaches a constant value by $t = 50$. Therefore, to obtain good statistics about the z dependence of ϕ, the data will be averaged in both x and y and over the interval $t \in [90, 100]$; examples of these averaged coarse-grained depth profiles are presented in Figure 4.

In Figure 3 the bulk COM is also plotted and it is clear that this remains roughly at the same depth while the segregation process is taking place. In the larger size-ratio cases a change in the bulk COM can be seen between the homogeneous mixed initial conditions and the final segregated state. This effect is expected due to the compaction effects that are present in the mixed states, for large size ratios; but, currently this effect is not taken into account in the continuum model, which is one area where it could be improved. This change in the flow thickness (centre of mass) was also observed in the previous shear-driven size-segregation experiments.[13,28]

Additionally, from Figure 3 it is clear that the smaller σ^{-1}, the longer it takes for the flow to reach steady state. This is an indication that the segregation rate S_r is weaker for a smaller size difference, i.e. low σ^{-1}, and this lower S_r could be the source of the lower Péclet number.

Figure 4 shows a fit of Eq. (7) to the small particle volume fraction for several cases. The fit is performed using non-linear regression as implemented in MATLAB. The fit is reasonable in all cases, especially considering there is only one degree of freedom, P_s. From these plots it is clear that the degree of segregation is stronger

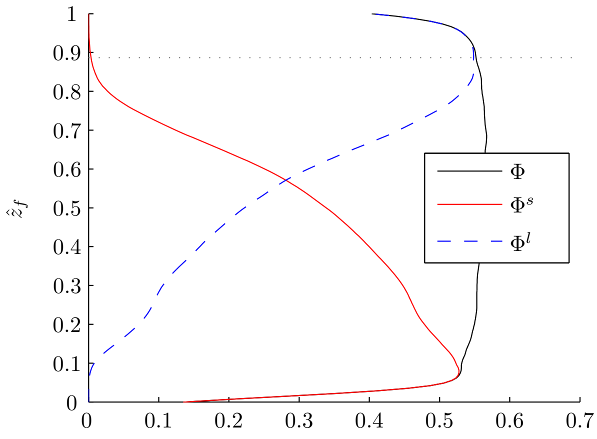

Fig. 5. Plot of the volume fraction of both the small, Φ^s and large particles, Φ^l and the bulk solids volume fraction, Φ, for the case $\sigma^{-1} = 1.6$. The dotted line shows the location between the basal dense layer and the upper more dilute region as given by definition (12).

as the size ratio is increased. Also, for $\sigma^{-1} > 1.3$ a measurable pure phase of large particles is generated at the top of the flow. This layer becomes thicker as the size-ratio is increased. From the plots it can be seen that at the bottom, the flow becomes very rich in small particles; but, only a thin (2 particle layers) pure phase is observed. This stronger segregation at the top, compared to the bottom of the flow is often observed in experiments, see Figure 1; but, is not captured by the current theory. Finally, in each case an inflection in the profile is observed towards the base, which is also not predicted by the theory; however, this has been observed before in the Monte Carlo simulations of Khakhar, McCarthy & Ottino,[24] replotted in terms of volume fraction by Gray and Chugunov.[16]

Gray & Chugunov[16] have previously noted that their theory does not capture the perfectly pure region at the top of the flow and proposed only fitting to the dense basal layer. A typical density profile is shown in Figure 5 and the decrease in density reported by Gray and Chugunov[16] can be observed towards the top of the flow. Therefore, we use (12) to define the transition between the dense basal layer and the more dilute layer above (indicated by the dotted line on Figure 5). Fits to this scaling were also performed. When scaling by the location of the basal layer a higher value of $\phi_0 > 0.5$ was computed, as these fits do not include the large particles in the upper part of the flow. The measured Péclet number for each type of fit is shown in Figure 6 and from the error bars (95% confidence bounds) it can be seen that both fits have approximately the same accuracy. Therefore, nothing is gained by only fitting to the dense basal layer. Also, only fitting to this layer has the added problem that at the interface, between the dense and less dense layer, s_d, the no-flux condition does not hold, i.e., there is a transfer of particles between these two layers. Finally, the trend is the same for both fittings, but scaling by the

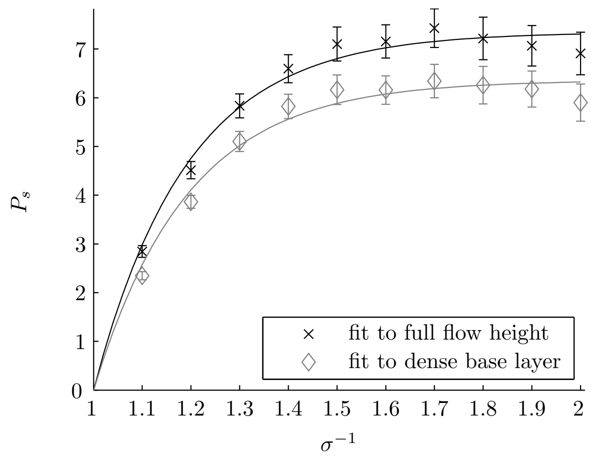

Fig. 6. Plot of the Péclet number, as obtained from the fit of Eq. (7) to the DPM data as a function of particle size ratio σ^{-1}. The crosses indicate data that is scaled using the full flow depth, i.e., $\hat{z}_f$; whereas, for the diamonds the flow is scaled by the thickness of the dense avalanche region, i.e., $\hat{z}_d$.

basal layer does lead to a lower Péclet number, implying a reduction in the degree of segregation. Therefore, we will only consider scaling by the full flow depth from this point onwards, i.e., s_f.

Figure 6 shows the segregation Péclet number, P_s, as a function of σ^{-1}. Even for the smallest size ratio, $\sigma^{-1} = 1.1$, P_s is 2.8, indicating that segregation is almost three times stronger than diffusion. For σ^{-1} between 1.1 and 1.5 it would appear that P_s saturates exponentially to a constant value of around $P_{max} = 7.35$. A fit is shown to

$$P_s = P_{max}(1 - e^{-k(\sigma^{-1}-1)}) \tag{13}$$

where $k = 5.21$ is the saturation constant. Further investigation is required on how P_s depends on other parameters that appear in the contact model. Previously, Gray and Chugunov[16] compared the model to a Monte Carlo result of Khakhar, McCarthy and Ottino[24], in which $\sigma^{-1} = 1.11$, and found that a value of $P_s = 4$ fitted the data best. This is a little larger than the value reported here, but the numerical model and properties are different between the two simulations. Previous chute experiments[43] reported a range of Péclet numbers from 11-19 for $\sigma^{-1} = 2$, which again is larger than the values we find here, but their experiments were performed at a higher inclination angle.

For very high size ratios it does appear the Péclet number is beginning to decrease, as reported by Golick and Daniels;[13] however, the reduction is within the fitting error, therefore, this is not conclusive. We did not go to higher size ratios as it is not expected that the model in its current form will capture the key physics. It does not include the effect of percolation of the small particles, which Savage and

Lun[37] reported needs to be taken into account for values of $\sigma^{-1} > 2$.

6. Conclusions

In summary, we have presented a DPM study of how the Péclet number, P_s, the ratio of particle size-segregation strength to diffusion, depends on the size ratio of the particles. Previously, only a fit to a single simulation had been reported.[16] These DPM simulations were compared with theoretical predictions, but only for steady-states; to a previous Monte-Carlo simulation; and, to experiments.

The main findings of this paper are: *(i)* To get strong segregation and steady profiles it was necessary to 'turn on' the rotational degrees of freedom. This was done by introducing a tangential sliding friction model; however, only adding tangential dissipation produced very similar results. *(ii)* As expected, P_s does increase for larger particle size ratio σ^{-1}, but appears to saturate to a constant value. *(iii)* The results of the DPM were compared to the binary segregation-remixing model of Gray and Chugunov[16]; the agreement was good given the model only has one free fitting parameter, P_s. The major difference between the model and DPM is the slight asymmetry in the segregation, with a thick pure phase of large particles forming at the top; but, only a thin perfectly pure layer of small particles appearing at the base of the flow. The weaker segregation found at the base has previously been observed in experiments and this effect could be captured in the model, by introducing diffusion that is a function of the fluctuation energy of the flow. It is known[36] that the fluctuation energy is stronger towards the base and almost zero at the free surface. Additionally, a small change in the bulk centre of mass was observed between the homogeneous and the segregated state; again this effect is not included in the continuum model. However, it could be incorporated in the three-phase version of Thornton, Gray and Hogg[41] as this explicitly models the air phase and hence, can be extended to allow the bulk granular volume fraction to vary in height and evolve with time. Hence, in the future we aim to use the results of DPM simulations to improve the continuum model.

Further investigations are required to determine how the degree of segregation depends on the parameters of the DPM. Since only steady-state profiles were considered, it was only possible to ascertain the ratio of the strength of the diffusion to the strength of the segregation. To measure these two effects independently time-evolving profiles must be considered, this requires a better procedure to produce the initial configurations. Additionally, the DPM has highlighted two aspects that are not captured by the continuum model: the compaction effect and the asymmetry in the segregation depth profiles.

We have taken the contact model properties of the large and small particles to be the same, i.e., $k^n, \gamma^n, k^t, \gamma^t$ and μ; however, to gain closer agreement with the experiments it may be better to assume the material properties are equal for both particle types, i.e., bulk modulus, coefficient of restitution, etc. and hence the contact properties become size dependent. Finally, this research has shown that

DPM can be used to check and validate the assumptions of continuum segregation models.

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