

ON THE CONTINUUM MODELLING OF SEGREGATION OF GRANULAR MIXTURES DURING HOPPER EMPTYING IN CORE FLOW MODE

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Key words: Computational Fluid Dynamics, Continuum Modelling, Micromechanical Parametrisations, Granular Material, Core Flow, Segregation

Abstract. *In this paper, the application of a continuum model is presented, which deals with the discharge of multi-component granular mixtures in core flow mode. The full model description is given (including the constitutive models for the segregation mechanism) and the interactions between particles at the microscopic level are parametrised in order to predict the development of stagnant zone boundaries during core flow discharges. Finally, the model is applied to a real industrial problem and predictions are made for the segregation patterns developed during mixture discharge in core flow mode.*

1 INTRODUCTION

In the past few decades, significant effort has been put into understanding the physics and mechanics of granular material flow and a number of mathematical and numerical models have been developed for its description¹⁻¹¹. Both granular dynamics models at the micro-scale^{6,10} and continuum mechanics model at the macro-scale^{7,8} have been developed over the years in an attempt to accurately represent flow characteristics. However, none of these have been entirely successful; while the former require considerable amounts of computing time and memory to simulate large scale processes that involve a very large number of discrete

particles, the latter lack essential information on particle-particle interactions and material parameters at the microscopic level in order to be able to simulate granular processes which involve complex material behaviour, i.e. particle size segregation.

Granular material discharge from bins/hoppers occurs in either *mass flow* mode, where all material regions in the domain are in motion, or *core flow* mode, where there is a flowing material channel above the orifice of the emptying vessel and stagnant material zones further away from it. When a vessel discharges in core flow mode, initially, the flowing zone is confined to a narrow channel above the orifice. Gradually, the flowing zone reaches the top surface (the timescale in which this occurs is very small compared to the latter stages of discharge) and its sides steepen until the material angle of repose is reached. Then, it begins to descend slowly, with material rolling down the interface into the flowing channel and the flowing core becoming wider. The discharge stops once the top surface of the stagnant zone boundary intersects the plane of the orifice and no more material exits the vessel. Figure 1 shows the evolution with time of the flow-no flow boundary during the discharge of a flat bottomed bin. It is industrial common practice to use semi-empirical engineering criteria in order to determine a priori whether a hopper goes into core flow or mass flow¹².

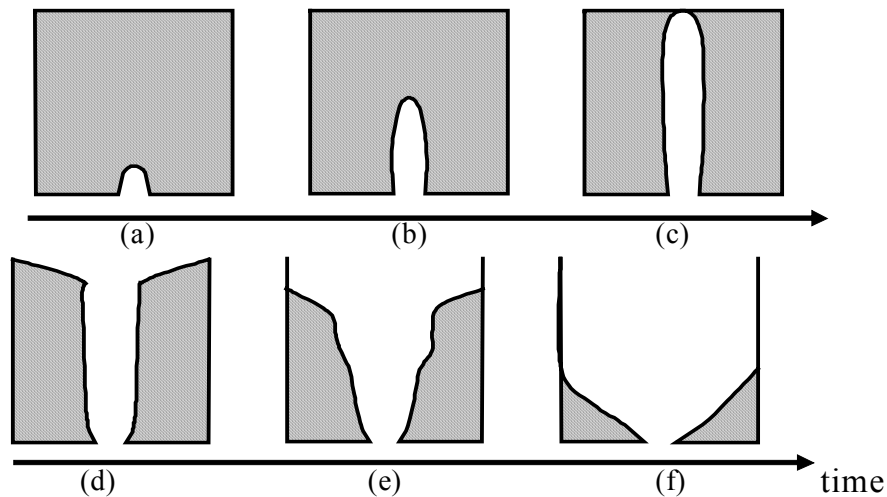


Figure 1: Development with time of the stagnant zone boundaries (dashed lines) during core flow discharge from a flat bottomed vessel

Recently, a continuum model was presented^{9 11}, which set the framework of the correct representation of the flow of granular mixtures, through the derivation and inclusion in the macroscopic equations (i.e. mass and momentum transfer) of micromechanical parametrisations, in order to connect key flow parameters to material properties. In this way, hopper discharges in mass flow mode, as well as hopper charges and subsequent particle size segregation could be effectively modelled. The developed models were validated against existing experimental data. However, material discharges in core flow mode are more complicated to model, due to the lack of reliable methodologies for the prediction of the

development of stagnant zone boundaries.

So far, one of the more successful approaches for the determination of the stagnant zone boundaries was that of the *kinematic model*^{13 14}. The kinematic model derives from statistical mechanics and assumes a linear relationship between the horizontal velocity and the horizontal gradient of the vertical velocity. This relationship depends only on one empirical material parameter, the *kinematic constant*, which has dimensions of length and can be correlated to the height of the stagnant zone. In order to enable modelling under unsteady state conditions, a modified kinematic model was developed to account for the changing shape of the flowing zone and the dilation occurring at the initiation of the flow¹⁵. The modified kinematic model was utilised to model mono-sized material discharges from flat-bottomed hoppers.

Recently, the developed continuum framework was implemented with the modified kinematic model and extended, in order to enable the modelling of core flow discharges of multi-component granular mixtures from hoppers that incorporate conical sections¹⁶. The model was validated with the use of available experimental data. In the present paper, the developed framework is utilised in order to simulate a real industrial process (the discharge in core flow mode of a granular mixture from a hopper) and make predictions about the particle size segregation and the subsequent mixture composition at the outlet. In this way, the capability of the model is demonstrated to realistically represent real-life industrial applications and its utilisation is discussed for the *a priori* prediction of the evolution of a process.

2 THE CONTINUUM MECHANICS FRAMEWORK

The continuum mechanics framework is employed to solve the conservation equations for mass, momentum and energy for a multi-species granular mixture. The full set of equations was solved using PHYSICA, a three-dimensional, unstructured, finite-volume modular suite of software, developed at the University of Greenwich¹⁷. For reasons of simplification, one-phase flow was assumed (where the properties of the different mixture components were averaged), so that only one momentum equation for the bulk was solved. Moreover, energy equations need not be solved, since changes in granular temperature were accounted for directly within the micromechanical framework.

2.1 Mass conservation

The calculation of each of the individual material components f_i (fractional volume of component- i in control-volume, $0.0 \leq f_i < 1.0$ and total material fraction = $\sum f_i \leq$ maximum packing fraction < 1.0) is performed through the solution of the equation:

$$\frac{\partial f_i}{\partial t} + \nabla \cdot (f_i \vec{u}_b + \vec{J}_{seg\ i}) = 0 \quad (1)$$

where \vec{u}_b is the bulk velocity vector and $\vec{J}_{seg\ i}$ is the segregation ‘‘drift’’ flux, which describes the motion of each individual component relative to each other. Particle size segregation might occur owing to three mechanisms: (a) *shear-induced segregation*, due to gradients of

bulk strain rate (mostly for the coarser components of the mixture); (b) *diffusion*, due to concentration gradients (mostly for the finer components of the mixture – the response mechanism to shear-induced segregation); (c) *gravity-driven spontaneous percolation*, a mechanism which tends to drive the fine components of a granular mixture in the direction of gravity through any existing void spaces in the coarse phase matrix-this process does not depend on any thermodynamic property of the mixture.

Functional forms for the three segregation fluxes, involving characteristic transport coefficients of each mechanism, have been extracted within a micromechanical framework using principles of kinetic theory and the Discrete Element Method (DEM). A more detailed description on the functional forms of the three individual segregation fluxes and the calculation method of the transport coefficients can be found in previous works^{9 18}. For the discretization and solution of the mass conservation equation a Total Variation Diminishing (TVD) based scheme (Scalar Equation Algorithm – SEA¹⁹) was used.

2.2 Momentum conservation

The momentum conservation equation for the bulk (for the solution of which a SIMPLE-based algorithm and a conjugate gradient iterative solver were employed) may be written as:

$$\rho_b \frac{\partial \vec{u}_b}{\partial t} + \nabla \cdot (\rho_b \vec{u}_b \vec{u}_b) = -\vec{\nabla} p + \nabla \cdot (\mu_b \vec{\nabla} \vec{u}_b) + \vec{S} \quad (2)$$

where p is the pressure and \vec{S} is a source term (i.e. gravity, etc.). The parameters ρ_b and μ_b are the bulk material density and pseudo-viscosity (equivalent to fluid viscosity), respectively. They are calculated through averaging of the properties of the mixture components, ρ_{gran} and μ_{gran} (solids density and pseudo-viscosity of granular material) and air ρ_{air} and μ_{air} (density and viscosity of air):

$$\rho_b = \sum_i f_i \rho_{\text{gran}} + (1 - \sum_i f_i) \rho_{\text{air}} \quad (2a)$$

$$\mu_b = \sum_i f_i \mu_{\text{gran}} + (1 - \sum_i f_i) \mu_{\text{air}} \quad (2b)$$

The role of the pseudo-viscosity in the momentum equation is crucial in dictating the evolution of the flow. The higher its value, the less mobile the material becomes, causing deceleration of the flow. If different regions of the material domain were to experience different shear forces at different times, this would affect the material flowability, causing it to flow more slowly in the regions where the pseudo-viscosity is higher (i.e., the shear forces acting like friction forces to the flow). In this way, if the evolution of the stagnant zone boundaries during core flow could be determined, the granular material pseudo-viscosity could be the controlling parameter to force the flow to cease in stagnant regions on the timescale of the simulation. For this reason, the modified kinematic model¹⁵ was employed, in order to determine the temporal evolution of the stagnant zone boundaries.

3 THE EVOLUTION OF THE STAGNANT ZONE BOUNDARY

As mentioned, the kinematic model¹³ assumes a linear relationship between the horizontal velocity and the horizontal gradient of the vertical velocity. This relationship depends only on empirical material parameter B , called the *kinematic constant*, which has dimensions of length. Initially, an approximate solution of the velocity distribution is obtained by considering the discharge from a point sink in a semi-infinite medium. By expressing the velocity in terms of the stream function and integrating the relation obtained along a streamline, the time taken for a particle originally at any location in a bin to reach the outlet can then be calculated. From this and by making allowance for the voidage changes that occur at the initiation of the motion, the stagnant zone boundary at time T obeys the equation:

$$T = \frac{2B\pi z^2 \Delta\rho}{Q\rho_{fl}} \exp\left(\frac{r^2}{4Bz}\right) \quad (3)$$

where r and z are cylindrical coordinates expressing radial and vertical distances, respectively, of a particle from the hopper outlet (measured from the outlet centre), Q is the discharge volumetric flow rate, $\Delta\rho$ is the change of material bulk density which accompanies the initiation of the motion (i.e. the difference between the bulk densities of stagnant and flowing material regions), ρ_{fl} is the bulk density of the flowing material region and B is the kinematic constant. It has been argued that in the case of multi-component mixtures, B should be equal to the average of all particle diameters¹⁶. The ratio $\Delta\rho/\rho_{fl}$ was taken as 0.1 and was kept constant for all performed simulations. The discharge volumetric flow rate Q through a circular outlet under free-fall conditions is given by $0.58g^{1/2}d_{out}^{5/2}$ (for flat bottomed bins) or $0.58g^{1/2}d_{out}^{5/2}(\tan a)^{-0.35}$ (for hoppers with conical sections of hopper half-angle a), where d_{out} is the outlet diameter and g is the gravitational constant.

Equation (3) though, fails to represent accurately later stages of the discharge, when the flowing zone reaches the upper free surface or the side walls and begins to descend. In those stages, the equation of the stagnant zone boundary is modified¹⁵ near the upper free surface and the walls in order to be consistent with observations¹² and allow the top surface to be at the material angle of repose. For this reason, the upper sides of the flow channel boundary are defined as a conical surface at the angle of repose and the equation describing the stagnant zone boundary at time T (assuming volume balance) becomes:

$$QT = \pi R_{cyl}^2 h + \frac{\pi}{3} R_{cyl}^3 \tan \varphi \quad (4)$$

where R_{cyl} is the hopper radius, h is the height of the outer edge of the top free surface below the original level and φ is the material angle of repose. For the derivation of this equation, it is assumed that the flowing channel is always maintained filled and that the top air-material interface between wall and outlet axis is always maintained at the angle of repose.

In the case of a hopper with a conical section, equation (4) needs to be modified for the final stages of the discharge, within the conical section, to account for the different volume balance. In this case, the equation which describes volume balance becomes:

$$QT = \pi R_{\text{cyl}}^2 H_{\text{cyl}} + \pi \frac{h - H_{\text{cyl}}}{3} (R_{\text{cyl}}^2 + R_{\text{cyl}} r_c + r_c^2) + \frac{\pi}{3} r_c^3 \tan \varphi \quad (5)$$

where H_{cyl} is the cylindrical section height and radius r_c is related to known quantities through the equation $r_c = R_{\text{cyl}} - (h - H_{\text{cyl}}) \tan a$.

The position of the final stagnant zone may be determined by following the straight line at the material angle of repose, which intersects the plane of the hopper outlet, as in Figure 1(f). Material below that line is retained indefinitely in the hopper.

4 SOLUTION PROCEDURE

In order to start a simulation of discharge, the initial (and already segregated) fill state of the granular mixture should be accounted for. This may be obtained directly through the use of an experimental device called the *segregation tester*, which provides details of the material composition radial distribution during the filling process of a hopper and the resulting radial segregation patterns²⁰. The segregation tester consists of a rotating transparent mixer and a parallelepiped section underneath the mixer, which is adjusted to an inclination representing the material angle of repose (see Figure 2). The parallelepiped section is divided into 5 compartments, which can be separated after the end of the filling process, so that material may be analysed from each compartment separately.

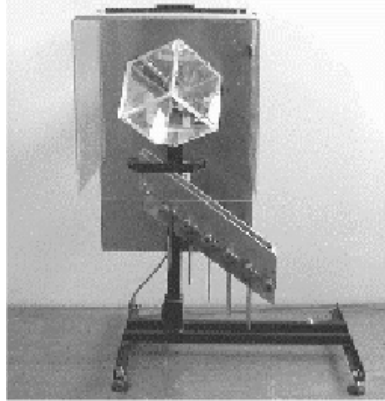


Figure 2: Segregation Tester

During the simulation of discharge of an N-component granular mixture, three momentum equations (corresponding to x-, y- and z-directions) and N mass conservation equations (including the appropriate parametrisations for particle size segregation⁹) were solved in each cell of the computational domain. As has already been mentioned, the flow may be controlled via the granular dynamic pseudo-viscosity term μ_{gran} of equation (2b). At the onset of the simulation the evolution of the flow-no flow boundary can be determined via equation (3) and the modifications applied via equations (4) and (5) for the later stages of the discharge. In this way, the critical times T for all material regions in the domain may be determined, which correspond to the time intervals after which these regions are allowed to flow. Initially, everywhere in the domain μ_{gran} was set to a very high value ($10^6 \text{ m}^{-1} \text{ kg s}^{-1}$, obtained by trial and error), which stops the material from flowing. When in a material region simulation time

reached the critical time T , then in that region a different pseudo-viscosity (one that allowed flow) was employed. A constitutive equation for this pseudo-viscosity was obtained based on the Drucker-Prager yield criterion¹¹. In order to avoid numerical instabilities at the transition between flowing and non flowing parts due to high velocity gradients, a thin transition region between them was considered. In this region, the viscosity was assumed to vary linearly between its no flow value and its average value within the flowing region.

5 RESULTS AND DISCUSSION

The numerical model was used to simulate a real industrial application, i.e. the core flow discharge of a ternary granular mixture from a cylindrical storage hopper with a conical section. Particular emphasis was put in the prediction of material size segregation occurring during the discharge process, in order to be able to evaluate a priori the segregation behaviour of a mixture of a given composition during emptying of that particular hopper. The material used was granulated sugar. The hopper dimensions and bulk material properties are summarized in Table 1. Hoppers of these specifications are commonly met in plants in a number of sectors of the process engineering industry. Since the studied discharges were centric (i.e. the outlet was located around the central axis of symmetry of the hopper), for reasons of simplicity and due to the observed symmetry of the flow around the hopper central axis, a semi-3D geometry, of a hopper slice of 5° angle around the central axis of symmetry, was chosen as the most appropriate geometry for the performed simulations.

| Parameters | |
|---|--------------------------------------|
| Cylindrical section height | 37.5 cm |
| Ratio of cylindrical section height to conical section height | 18.75 |
| Ratio of cylindrical section diameter to outlet diameter | 5 |
| Ratio of cylindrical section height to cylindrical section diameter | 1.07 |
| Material | granulated sugar |
| Solids density | 1660 kg/m ³ |
| Bulk density | 700 kg/m ³ |
| Angle of repose | 37° |
| Angle of friction between the particles and hopper wall | 22° |
| Volumetric discharge rate | 4×10 ⁻⁴ m ³ /s |

Table 1: Parameters used in the simulations

The particle size distribution of the bulk material was divided into three separate size classes: large particles (particle diameter from 1 to 1.4 mm), intermediate particles (particle diameter from 0.5 to 1 mm) and small particles (particle diameter smaller than 0.5 mm). Simulations were performed for two different initial compositions of the feed mixture, in order to investigate the effect of the initial size distribution of the mixture on the overall

segregation characteristics during emptying of the hopper. The first mixture consisted of 36.4% small, 62.1% intermediate size and 1.5% large particles, while the second mixture was composed of 34.5% small, 64.7% intermediate size and 0.8% large particles. The small may be considered as the *finer phase* of the mixture, while the intermediate and large particles may be considered as the *coarser phase* of the mixture.

The hopper was centrally filled from the top, with the top free surface of the material inclined at the material angle of repose. The experimental segregation tester was used to characterize the material radial segregation resulting from filling and the experimentally measured composition was used as the starting material distribution in the hopper.

Before simulating segregation during discharge, it was necessary to quantify the segregation propensity of the bulk material. In a previous work⁹, segregation transport coefficients were rigorously calculated using DEM analysis and were then directly imported in the continuum framework. For the purpose of this paper, an approximate method of calculation of those coefficients was used. This method consisted in calibrating the segregation transport coefficients through a series of simulations, which mimicked the segregation tester experiment in an attempt to reproduce the segregation pattern measured in the tester. The transport coefficients which best matched the experimentally observed segregation pattern were then selected and used in the emptying simulations. The mesh of the segregation tester is shown in Figure 3a.

Figure 4 shows the particle size distributions measured in the tester along the inclined heap line, which was equally divided into five slots (1 to 5). Also shown are the distributions obtained using the numerical model, which gave the best match with the experimental results. The adjusted values of the predominant segregation transport coefficients are given in Table 2 for the two mixtures.

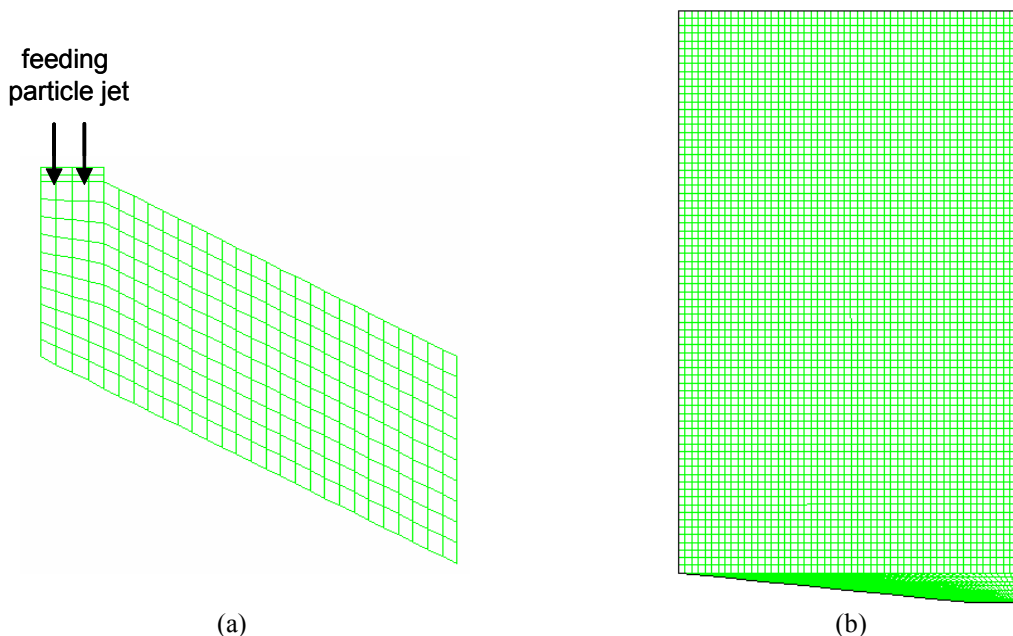


Figure 3: Computational mesh of (a) the segregation tester and (b) the cylindrical hopper

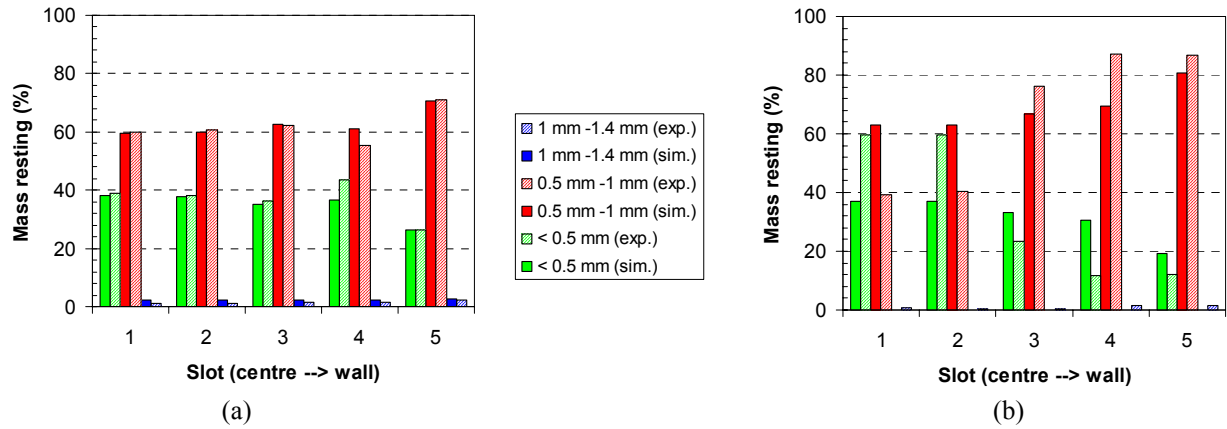


Figure 4: Segregation profiles measured in the segregation tester and obtained from the numerical model for (a) mixture 1 and (b) mixture 2

| Parameters | Mixture 1 | Mixture 2 |
|---|--------------------|--------------------|
| Shear-induced segregation coefficient of large particles (m^2/s) | 5×10^{-6} | 2×10^{-5} |
| Shear-induced segregation coefficient of intermediate particles (m^2/s) | 5×10^{-6} | 2×10^{-5} |
| Diffusion coefficient of small particles (m^2/s) | 10^{-6} | 7×10^{-6} |

Table 2: Adjusted values of the predominant segregation transport coefficients of the individual mixture components

In both cases, the smallest particles were found to accumulate close to the central feed line (slot 1), whereas the intermediate and large particles were found to accumulate towards the vessel wall (slot 5). Even though the differences in the initial concentrations of the two mixtures were relatively small, noticeable differences were observed in the degree of segregation of the two mixtures. Segregation was more pronounced for the second mixture, which was characterized by lower initial concentration of the smallest particles. This result was reflected in the adjusted segregation transport coefficients, whose values for the second mixture were significantly greater than those for the first mixture. This may be interpreted as follows: the studied mixtures were of moderate size ratios (i.e. the size ratio of the two predominant components of each mixture-small and intermediate particles-did not exceed in general 2:1), hence gravity driven percolation did not constitute a problem. The driving mechanism of size segregation, as already discussed in Section 2, is shear-induced and concerns primarily the coarser phase of a mixture. In this way, it is the coarser particles which will concentrate towards regions of high shear, while the fines will move in the opposite direction in order to fill the voids left by the coarse particles. In the second mixture, due to the higher concentration of coarser particles (more intermediate size particles present than in the first mixture), more coarse particles will move first towards the hopper walls (regions of high

shear), thus leaving the finer particles only the space closer to the central filling axis of the hopper to occupy. In this way, the concentration of the coarser (finer) phase will be higher closer to the hopper wall (central axis of filling) for the second mixture, thus enhancing segregation, as compared to the first mixture.

The average relative error between the numerical and experimental results was 15% and 30% for the first and second mixture respectively. Despite those error levels, the approximate method used here to evaluate the segregation transport coefficients is believed to constitute, for the purpose of the present study, an acceptable alternative to the rigorous but computationally expensive DEM approach used in a previous work.

For the simulation of the discharge process, a non-uniform mesh of 4212 elements was utilised (Figure 3(b)) and a variable time step was used, defined by the CFL criterion (with a maximum CFL number of 0.07). The running time of the discharge simulation was approximately 24 hours on a Pentium III 2.8GHz processor PC. Figure 5 depicts the calculated time evolution of the boundary between the flowing and stagnant zones during the discharge process. Note that no effect of the size distribution of the mixture on the evolution of this boundary was considered in the present work. In the early stages of the discharge, a narrow flowing zone quickly developed upwards and reached the top in less than 1 s. Then, the flowing zone widened and descended slowly, reaching eventually the position of the final stagnant zone (at the angle of repose) at 85.8 s. After that stage, no more material was observed to exit the hopper. This behaviour is in general agreement with experimental observations of core flow discharge¹².

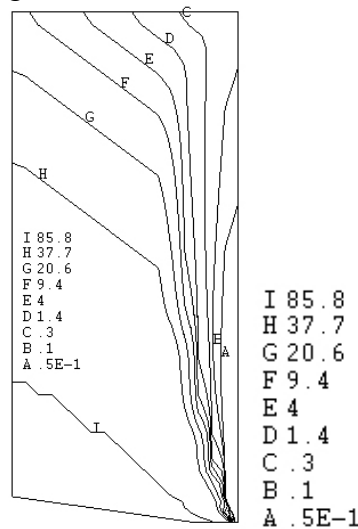


Figure 5: Time evolution of the boundary between the flowing and stagnant zones during the discharge of the hopper.

The variation in the mixture composition, averaged across the hopper outlet, during the discharge is presented in Figure 6, where the composition is plotted as a function of the percentage of mass discharged from the total hopper inventory. Some fluctuations were present in the plot, which may be attributed to a too high sampling rate in the numerical procedure used to average the composition. For both mixtures, no more material could exit

the hopper after 83 % of mass was discharged. The material left in the hopper corresponds to the final region of stagnant material at the bottom corner of the hopper, in agreement with the core flow pattern presented above.

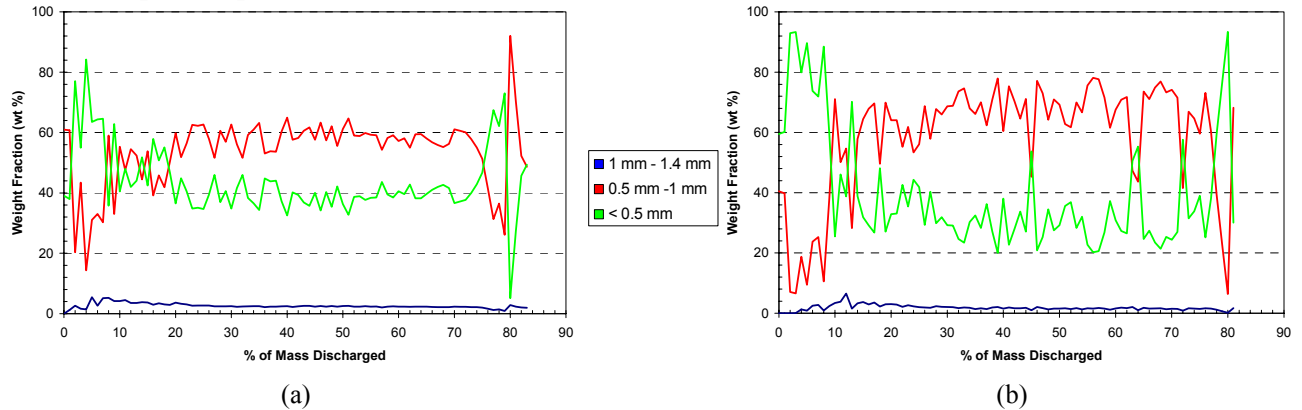


Figure 6: Segregation profiles of the individual mixture component during the hopper discharge for (a) mixture 1 and (b) mixture 2.

Initially, the mixture exiting the hopper exhibited a high proportion of small particles, which was expected considering the initial hopper filling state (i.e. small particles occupied mostly the central region) and the flow pattern during the initial stages of the discharge (i.e. central region first emptied). Then, the fraction of small particles exiting the domain decreased very quickly and became lower than the fraction of intermediate size particles. This result could be attributed to the shear-induced segregation / diffusion processes, which caused the intermediate and large particles to concentrate at fill towards the hopper wall. This effect was more pronounced in the case of the second mixture, which is consistent with the higher segregation degree of the second mixture observed in Figure 4. The discharge eventually reached a quasi-steady state, during which the composition of the mixture exiting the hopper was roughly constant. Near the end of the discharge, the fraction of small particles was observed to increase. This is due to the accumulation of small particles further away from high shear regions (i.e. the flowing zone close to the hopper axis of symmetry) and is consistent with the description of the segregation mechanism given in Section 2. Thus, the presented results clearly demonstrate that the discharge did not lead to a homogeneous mixture, but to a strongly segregated mixture, especially during the early and final stages of the discharge.

6 CONCLUSIONS

- The modified kinematic model for the prediction of the evolution of stagnant zone boundaries during core flow discharge was incorporated into a continuum mechanics framework, in order to model segregation during core flow discharges of granular mixtures. The presented framework has been validated and is already in use by industry for optimisation of existing operations, which involve granular material handling.
- Numerical simulations were performed for a real engineering application in order to

assess the ability of the model to evaluate the segregation behaviour of granular mixtures.

- The performed simulations demonstrated that the two ternary mixtures that were examined exhibited strong tendency to segregate in that particular hopper, especially during the initial and final stages of discharge. If the exhibited behaviour is not the required one at the end of such a process (i.e., different composition is needed), then either the initial mixture composition should be modified, or a different hopper should be used.
- The presented continuum framework with its incorporation of constitutive laws for the description of segregation of granular mixtures during core flow discharges is believed to be unique.

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