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Predictions of segregation of granular material with the aid of PHYSICA, a 3-D unstructured finite-volume modelling framework

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SUMMARY

In this paper a continuum model for the prediction of segregation in granular material is presented. The numerical framework, a 3-D, unstructured grid, finite-volume code is described, and the micro-physical parametrizations, which are used to describe the processes and interactions at the microscopic level that lead to segregation, are analysed. Numerical simulations and comparisons with experimental data are then presented and conclusions are drawn on the capability of the model to accurately simulate the behaviour of granular matter during flow. Copyright © 2002 John Wiley & Sons, Ltd.

KEY WORDS: granular material; segregation; continuum modelling; micro-physical parametrizations

1. INTRODUCTION

In recent years significant effort has been put in the modelling of granular flows using a continuum mechanics approach (e.g. References [1, 2]). Although these models are partially successful in capturing some characteristics of the flow, they lack essential information on material parameters, which are needed to account for the interactions between different particles. Thus, they cannot be used to simulate processes of great importance in the process engineering industry (i.e. hopper filling/emptying, pneumatic conveying, etc.), where these particle–particle interactions might lead to phenomena such as particle size segregation.

On the other hand, granular dynamics and micro-physical models are able to describe successfully the flow of granular material by accounting for particle–particle interactions at the microscopic level (e.g. Reference [3]). However, due to the complexity of the simulated processes, these models can only be applied to a small number of discrete particles. Therefore, such models would not be suitable for large-scale process modelling as they require consid-

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erable amounts of computing time to simulate processes that involve very large numbers of particles.

In the present paper it is argued that the various transport processes, which arise from the micro-physical properties of the different particle species in a multi-component granular mixture, can be parametrized and employed in a continuum framework in the form of constitutive equations. In this way, the continuum theory is provided with the necessary information about the micro-physics of each individual particle species, thus enabling the flow modelling of multi-component granular mixtures.

This work describes the continuum framework and the micro-physical parametrizations that are employed to account for mixture phases separation during material flow. Examples of the model predictions for different flow conditions and comparisons with experimental data are presented and conclusions are drawn on the capability of the model to realistically predict and quantify size segregation in granular flows.

2. THE CONTINUUM FRAMEWORK

The full set of flow equations was solved using PHYSICA, a finite-volume code developed at the University of Greenwich [4]. The PHYSICA toolkit is a fully unstructured-mesh modular suite of software for the simulation of coupled physical phenomena in three spatial dimensions and time. Its data structures allow for vertex-based tetrahedral, pentahedral, hexahedral and cell-centred polyhedral elements to be used. A choice of differencing schemes, such as central differencing, upwinding, hybrid, power law, exponential, is offered in the code and the Rhie–Chow interpolation method [5] is employed to avoid the possibility of checkerboard velocity and pressure fields. The code uses SIMPLE-based algorithms for the solution of the flow equations (see e.g. Reference [6]) and different iterative solvers (i.e. conjugate gradients, Gauss–Seidel, Jacobi) may be invoked for the numerical solution of the discretized equations. PHYSICA has also been recently implemented with a range of turbulence models, source-based solidification/melting algorithms and elasto-visco-plastic solid mechanics models, and has been successfully applied to problems involving complex interactions of physical behaviour over arbitrarily unstructured domains (see e.g. References [7, 8]).

2.1. Continuum model equations

The continuum framework is employed to solve the conservation equations for mass, momentum and energy. For the modelling of an N-species granular mixture, $3N+3$ momentum (in the x-, y- and z-direction) and $N+1$ energy equations, for each of the mixture N-components and the surrounding air. However, for reasons of simplification, only three momentum equations for the bulk (the sum of all N-species and air in a control-volume) were solved. Moreover, an equation for energy was not solved. Instead, energy-linked flow parameters were accounted for by the micro-physical constitutive models, through which the granular temperature of the flow was directly linked to the bulk velocity gradients through kinetic/theoretical considerations [9]. The consistency and effectiveness of these simplifications will be discussed during the presentation of the results.

Thus, the momentum equation, i.e. in the x-direction, may be written as

$$\rho_b \frac{\partial u_b}{\partial t} + \rho_b \left(u_b \frac{\partial u_b}{\partial x} + v_b \frac{\partial u_b}{\partial y} + w_b \frac{\partial u_b}{\partial z} \right) = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}\left(\mu_b \frac{\partial u_b}{\partial x} \right) + \frac{\partial}{\partial y}\left(\mu_b \frac{\partial u_b}{\partial y} \right) + \frac{\partial}{\partial z}\left(\mu_b \frac{\partial u_b}{\partial z} \right) + S_x \quad (1)$$

where u_b, v_b and w_b are the bulk velocity components in x-, y- and z-direction, respectively, p is the pressure and S_x is a source term (i.e. gravity, wall friction near solid wall boundaries which for granular material is dependent on the normal stress [10], etc.). The parameters ρ_b and μ_b are the bulk material density and pseudo-viscosity (equivalent to fluid viscosity—only in granular material it is not a result of random molecular collisions but slow frictional contacts), respectively, which are calculated by the equations:

$$\rho_b = f\rho_{gran} + (1 - f)\rho_{air} \quad (1a)$$

$$\mu_b = f\mu_{gran} + (1 - f)\mu_{air} \quad (1b)$$

In the above equations, ρ_{air} and μ_{air} are the air density and viscosity, respectively, and ρ_{gran} and μ_{gran} are the granular solids density and pseudo-viscosity, resulting from the material properties of the individual mixture components. The scalar parameter f represents the fractional volume of total material present in a computational control-volume (total solids fraction) and results from the summation of all fractions of the individual material components f_i present in the control-volume. It takes values between 0 (control-volume empty of material) and the maximum allowed packing fraction (always less than unity). The maximum allowed packing fraction is a function of the individual components' shapes, sizes, etc., and is taken as a model-input value, determined through experimental data. There are a number of granular models, which connect the pseudo-viscosity μ_{gran} to local stresses, velocity gradients, material bulk density, etc. [1]. However, for the performed simulations and comparisons with experimental data, it was chosen to determine the pseudo-viscosity via initial calibration of the model to the material flow rate during discharge, a parameter which can be directly calculated in the micro-physical framework [11]. Special consideration was given to appropriate initial/boundary conditions to determine the initial state of granular material that has been resting in bins/hoppers before discharge. For the solution of Equation (1), the SIMPLEC algorithm and a conjugate gradient iterative solver were employed (see e.g. Reference [6]).

The calculation of each of the individual material components f_i in a control-volume was performed through the solution of transport equations, which, in the absence of sinks/sources, may be written as

$$\frac{\partial f_i}{\partial t} + \nabla \cdot (f_i \boldsymbol{u}_b + \boldsymbol{J}_{seg\,i}) = 0 \quad (2)$$

where $\boldsymbol{u}_b$ is the bulk velocity vector and $\boldsymbol{J}_{seg\,i}$ is a 'drift' flux which represents segregation. The term $\boldsymbol{J}_{seg\,i}$ is very important, since it dictates the motion of the individual species in

the bulk and determines the levels of segregation in the mixture. This term will be analysed in the following section. Summation of all individual fractions in a control-volume of the computational domain gives the total solids fraction f. Since the present paper concentrates on the parametrization of $\boldsymbol{J}_{\mathrm{seg}\,i}$, only a brief analysis will be given on the numerical techniques that were employed and tested for the solution of Equation (2). This equation is a donor–acceptor type of equation and is used to predict the material interface (and hence, the levels of segregation) in the domain. For its solution, various schemes were tested (i.e. Van Leer, VOF) and all resulted in significant interface diffusion, due to the complex nature of the flow and the applied irregular meshes. Particular mention should be made to VOF; the conventional donor–acceptor scheme [12] fails when employed in a unstructured irregular mesh with arbitrarily sized control-volumes, especially at the boundaries between control-volumes that are very different in size or isolated material pockets which remain trapped. The development of a fully unstructured VOF scheme, suitable for multi-component flows, is currently under way. Of all the numerical schemes tested, TVD gave the sharpest interface and represented more accurately the segregation levels of the mixtures studied in this paper. All simulations for this work were thus performed using a TVD scheme (SEA algorithm [13]) for the solution of the species transport equations.

3. PARAMETRIZATION OF SEGREGATION FLUXES

The segregation flux was analysed in the micro-physical framework, by using principles of kinetic theory [14]. Starting from the reduced Liouville equation, a generalized Boltzmann equation that included inelastic collision effects was derived by considering conditions for particle chaotic motions. Thus, the non-equilibrium velocity distribution functions were determined for each particle size in a multi-component granular mixture through the use of a generalized Grad moment method. Particle 'drift' velocities were derived and the segregation flux $\boldsymbol{J}_{\mathrm{seg}\,i}$ in Equation (2) was expressed as

$$\boldsymbol{J}_{\mathrm{seg}\,i} = f_i(\mathbf{v}_{\mathrm{D}i} + \mathbf{v}_{\mathrm{S}i} + \mathbf{v}_{\mathrm{P}i}) \tag{3}$$

where $\mathbf{v}_{\mathrm{D}i}$ is the 'drift' velocity of the ith material component due to diffusion, i.e. flow down the ith component fraction gradient; $\mathbf{v}_{\mathrm{S}i}$ is the 'drift' velocity of the ith material component due to shear-induced segregation, the flow of coarser particles in the mixture across gradients of bulk velocity; and $\mathbf{v}_{\mathrm{P}i}$ is the 'drift' velocity of the ith material component due to gravity-driven spontaneous percolation of the fines in a mixture through the coarse phase. It depends primarily on the available void spaces in the coarse phase matrix through which the fines can pass.

Functional forms were extracted for the 'drift' velocities of Equation (3). This work concentrated on the study of binary mixtures consisting of fines and coarse phases of equal densities. The diffusive velocity was written as the product of a characteristic transport coefficient D_i (i.e. diffusion coefficient) and the ith phase fraction gradient:

$$\mathbf{v}_{\mathrm{D}i} = -D_i \nabla f_i \tag{4a}$$

where the negative sign indicated material motion down a fraction gradient.

The 'drift' velocity due to shear-induced segregation was taken to be a function of the bulk velocity gradient:

$$\mathbf{v}_{Si} = \frac{\eta_i}{|\boldsymbol{u}_b|} (\nabla(\boldsymbol{u}_b \cdot \mathbf{i}) + \nabla(\boldsymbol{u}_b \cdot \mathbf{j}) + \nabla(\boldsymbol{u}_b \cdot \mathbf{k})) \tag{4b}$$

where η_i is a shear-induced segregation transport coefficient for the ith mixture component, $|\boldsymbol{u}_b|$ is the magnitude of the bulk velocity vector and **i**, **j**, **k** are the unit vectors in the x-, y-, z-direction, respectively. There is no negative sign in Equation (4b), since strain-driven segregation causes material to move up a gradient of bulk strain-rate. Of the two processes, shear-induced segregation is the trigger mechanism, based on bulk velocity gradients, which causes species separation and subsequent concentration gradients, with the coarse particles concentrating in regions of high shear. Thus, diffusion is activated as a response mechanism, and causes fines to concentrate away from high-shear regions.

The percolation 'drift' velocity is different to the other two velocities, since it is driven only by a body force (i.e. gravity) and does not depend on any thermodynamic property of the mixture. The feasibility of percolation is a function of the mixture composition and size ratio. Thus, for a binary mixture, the functional form employed was

$$\mathbf{v}_{Pi} = K_i \varepsilon \left(1 - \frac{d_1}{d_2}\right) \mathbf{g} \tag{4c}$$

where K_i is the percolation coefficient, ε is the available voidage in the control-volume ($\varepsilon = 1 - f$), d_1 and d_2 are the particle diameters of the fines and coarse phases, respectively, and **g** is the gravity. This indicated that percolation acted only if two neighbouring volumes were along the line of action of gravity. It should also be noted that percolation 'drift' velocities applied only to the fines phase, i.e. K_{coarse} was zero everywhere in the computational domain.

The transport coefficients D_i, η_i and K_i of Equations (4a)–(4c) were calculated for each mixture phase in the micro-physical framework by using linear-response theory, which involved integration of the relevant time-correlation functions [3].

4. NUMERICAL SIMULATIONS AND TESTING OF THE MODEL

The numerical model was tested for its consistency in representing, realistically, binary mixture flow patterns and was then used to simulate experimental data obtained during discharge under gravity of a binary mixture from a small mass-flow cylindrical hopper. The pseudo-viscosities for the simulated mixtures were obtained as described in Section 2.1. For reasons of simplicity, and due to the observed symmetry of the flow around the central axis of the hopper for the simulated cases, a semi-3D geometry was chosen, with a hopper slice of 5° angle being simulated. An example of simulated hopper geometries and applied meshes is shown in Figure 1.

The first presented simulation was performed to test the model consistency. A 50–50 mixture was chosen (i.e. consisting of 50% fines and 50% coarse particles, uniformly distributed), of 2 : 1 particle size ratio, initial density of 950 kg m^{-3} and solids density of 2100 kg m^{-3} and was left to discharge under gravity from a hopper. The hopper's cylindrical section was 50 cm tall, its conical section was 7 cm tall and its half-angle was 30°. The inlet diameter

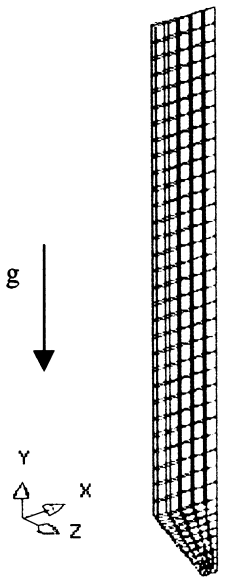

Figure 1. Example of simulated hopper slice geometry and the applied mesh.

was 10.5 cm, while the outlet diameter was 2.5 cm. A sharp discontinuity in the mixture composition was assumed for a small slice of material around the centre of the hopper. At this region, the material composition was assumed to consist of 95% fines and only 5% coarse particles. All transport coefficients were set to zero for all material phases. This was done in order to test the applicability of the TVD scheme in the absence of transport processes, i.e. whether it did not allow numerical diffusion to corrupt the results. Figure 2 presents snapshots of the fines phase fraction at various stages during the mixture discharge. It can be seen that the slice of the mixture, which was depleted from coarse particles, came out of the hopper domain in its entity following the motion of the bulk, with a sharp interface being maintained between the two separate regions of the fines phase. This result was anticipated and is in agreement with experimental observations for material under mass-flow conditions, where material components that come first into the domain are expected to come out first [15].

Simulations were then performed to model a hopper with a short cylindrical section, for which experimental data were available. Two types of hopper discharge experiments were performed for this study. In the first set of experiments ('segregation in time' discharge experiments), a proportion of the hopper contents were removed at a time to investigate the amount of segregation attained during flow; this should then give some understanding to the level of segregation in time. In the second set of experiments, 'segregation in space' tests were used to assess the segregation across the outlet. These tests were performed by sub-dividing the orifice area into a number of smaller areas, capturing the material discharging through these areas at certain points in time and measuring the composition for each area. Moreover, the free surface profile during the discharge was monitored and its drop with respect to a fixed point was recorded.

The hopper geometry and dimensions were as above; the only difference being that the cylindrical section was only 6.3 cm tall. A binary mixture was examined, of 2 : 1 particle size

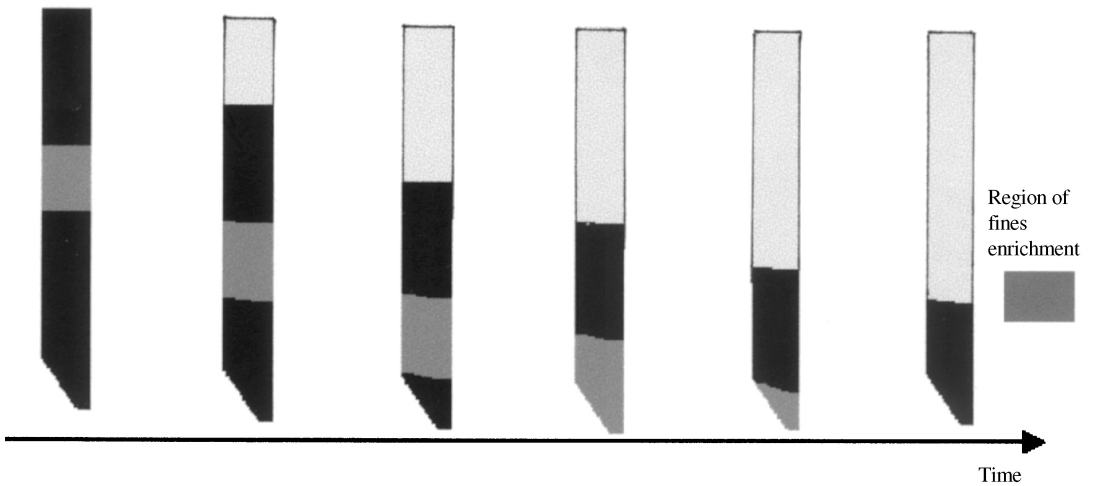

Figure 2. Variation of fines phase fraction with time during hopper discharge. 50–50 binary mixture of 2 : 1 size ratio, with a sharp discontinuity at its centre, consisting of 95% fines and 5% coarse particles. All transport coefficients are set to 0.

ratio, initial density of $950\,\mathrm{kg\,m^{-3}}$ and solids density of $2100\,\mathrm{kg\,m^{-3}}$. It consisted of 60% fines and 40% coarse particles, i.e. a 60–40 mixture (initial uniform distribution assumed).

The transport coefficients were calculated for the two mixture phases in the micro-physical framework and were directly imported in the continuum framework. The calculated values of the diffusion and shear-induced segregation transport coefficients showed that it was essentially the coarse fraction that dictated what happened in the mixture during the discharge. The diffusion coefficients were found to be $6.5 \times 10^{-8}\,\mathrm{m^2\,s^{-1}}$ for the fines fraction and $2.8 \times 10^{-7}\,\mathrm{m^2\,s^{-1}}$ for the coarse fraction. As seen, the coefficient for the coarse exceeded the fines coefficient by almost a factor of 4. For the shear-induced segregation coefficients, the results were clearer; the coefficient for the fines fraction was found to be $2.1 \times 10^{-7}\,\mathrm{m^2\,s^{-1}}$ and for the coarse fraction $2.5 \times 10^{-6}\,\mathrm{m^2\,s^{-1}}$, exceeding the fines coefficient by an order of magnitude. It should be noted that the shear-induced segregation mechanism appeared to be the dominant of the two. This result was anticipated for the relatively high solids fraction employed in these experiment simulations and is in accordance with molecular dynamics theory [16]. The percolation mechanism was calculated to be much weaker than the diffusion and shear-induced segregation mechanisms and a percolation coefficient of the order of 10^{-10} was used for the fines fraction in the simulations.

The model predictions were then compared to the available experimental data. Figure 3 presents the material interface profile at various stages during discharge. The interface profile was seen to dip towards the centre as the material head approached the conical section. This result was in qualitative agreement with the experimentally determined material interface behaviour during discharge, which is shown in Figure 4. It should be noted that in the experimental data presented in Figure 4, the heights of the interface were measured from the switch point between cylindrical and converging sections. Distances above ‘point-zero’ at the switch point are given as positive numbers and distances below this point are given as negative numbers. Figure 5 shows the predicted averaged fines weight fraction across the outlet

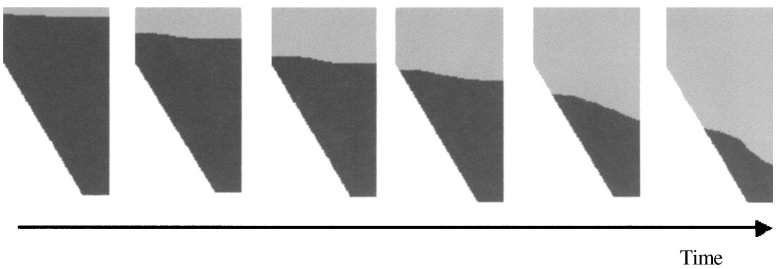

Figure 3. Material interface profile during hopper discharge. 60–40 binary mixture of 2 : 1 size ratio. Transport coefficients calculated in micro-physical framework.

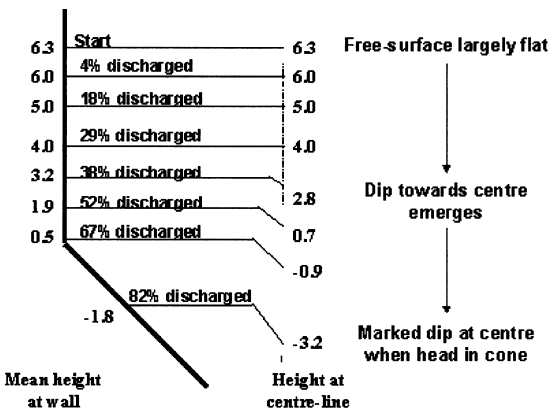

Figure 4. Experimentally determined interface profiles during hopper discharge. Height is given from the switch point between cylindrical and converging sections. Note that distances above 'point zero' are positive and below are negative.

with respect to the proportion of the total inventory discharged ('segregation in time' curve) and how it compares with the available experimental data. The numerical simulations are in general agreement with the experimental data and confirm the experimental observation that the critical point of the discharge was when the material head reached the cone. At the initial stages of the discharge some limited percolation was predicted (the model under-predicted the initial observed fines fraction, probably caused by non-uniform hopper filling effects). Once the material head reached the cone, the fines fraction was seen to decrease quite rapidly, a depletion which the model predicted to have continued right to the end of the discharge.

When comparing the behaviour of individual parts of the outlet ('segregation in space'), it was seen that for regions between the centre of the hopper and the hopper wall (i.e. intermediate cells) there was little variation in the fines fraction throughout the discharge. For regions though, close to the centre of the hopper (i.e. central cells), there was a significant fines depletion (and subsequent coarse enrichment) at the later stages of the discharge. This result indicated that there were free-surface effects once the material head reached the cone, with the coarser particles rolling down the interface. The fines weight fractions from the model–experiment comparisons for individual regions of the outlet during the discharge are

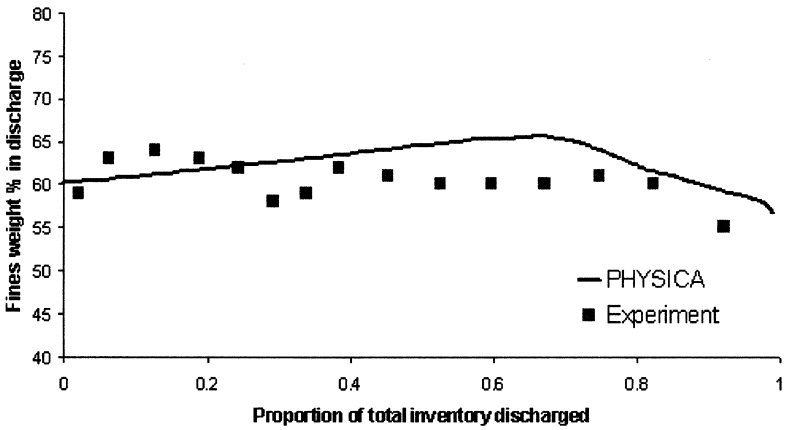

Figure 5. Temporal variation in fines weight fraction (averaged across outlet) during hopper discharge ('segregation in time'). 60–40 binary mixture of 2 : 1 size ratio. Transport coefficients calculated in micro-physical framework.

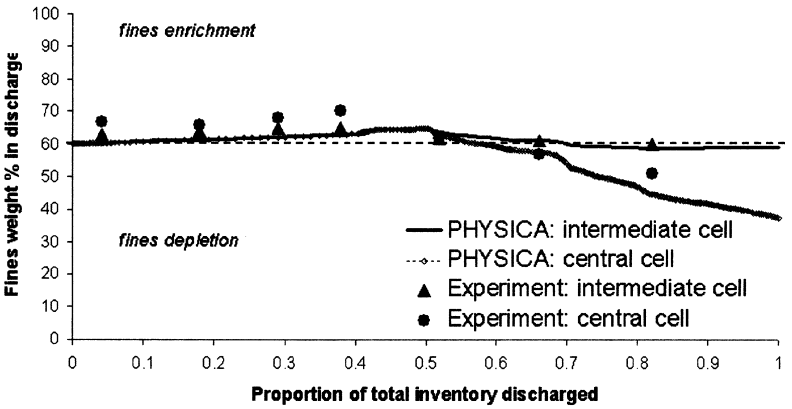

Figure 6. variation in fines weight fraction at various parts of outlet during hopper discharge ('segregation in space'). 60–40 binary mixture of 2 : 1 size ratio. Transport coefficients calculated in micro-physical framework.

presented in Figure 6. The observed behaviour of the mixture was correctly represented by the numerical model and there was general agreement between experiment and model on the onset and ultimate extent of the fines depletion at the central regions of the hopper.

It should be noted that the performed experiments are time consuming, requiring significant amounts of time to perform (i.e. initial hopper filling, calibration, collection and analysis of data) for these short hopper geometries. Unfortunately, there are no data readily available from large-scale hoppers used in industrial bulk-solids handing operations, because of the practical difficulties which arise during data collection. The experimental data which were presented are representative of the type of data required by the industry to monitor segregation during mass-flow, large-scale hopper discharges. The presented continuum model and its coupling

with micro-physics set the framework for the prediction of granular material behaviour during flow and its propensity for segregation. The model's potential capability has been demonstrated through this initial simulations and comparisons with the available experimental data. Once completed, the model will constitute a useful tool for practising engineers in order to assess granular material behaviour and trends of segregation during mass-flow. Further development will enable the model to account for other important granular processes, such as degradation and aggregation.

5. CONCLUSIONS

In this paper, a continuum framework was presented, which employs micro-physical parametrizations to model the effects of segregation in granular mixtures. The model was then used to simulate discharge of binary mixtures from mass-flow hoppers and general agreement was established between the model and experimental investigations, representing successfully all the main characteristics of the flow. This demonstrates the potential capability of the model to simulate large-scale industrial processes with granular material. The presented work is unique in its use of parametrizations of the micro-physical properties of granular material in a continuum framework. Development and testing of the model continues and inclusion of sink/source terms in Equation (2) will enable the modelling of other important processes such as degradation/aggregation. Further work is also under way in order to construct a robust VOF-type multi-material interface tracking algorithm, suitable for application in fully unstructured meshes.

REFERENCES

1. Tardos GI. A fluid mechanistic approach to slow, frictional flow of powders. *Powder Technology* 1997; **92**:61–74.
2. Karlsson T, Klisinski M, Runesson K. Finite element simulation of granular material flow in plane soils with complicated geometry. *Powder Technology* 1999; **99**:29–39.
3. Baxter J, Tüzün U, Burnell J, Heyes DM. Granular dynamics simulations of two-dimensional heap formation. *Physical Review E* 1997; **55**:3546–3554.
4. Cross M. Computational issues in the modelling of materials based manufacturing processes. *Journal of Computer Aided Materials Design* 1996; **3**:100–116.
5. Rhie CM, Chow WL. Numerical study of the turbulent flow past an aerofoil with trailing edge separation. *AIAA Journal* 1983; **21**:1525–1532.
6. Versteeg HK, Malalasekera W. *An Introduction to Computational Fluid Dynamics*, *The Finite Volume Method* (1st edn). Longman: Harlow, 1995.
7. Bailey C, Taylor GA, Bounds SM, Moran GJ, Cross M. PHYSICA: a multi-physics framework and its application to casting simulation. In *Computational Fluid Dynamics in Mineral & Metal Processing and Power Generation*, Schwarz MP *et al.* (Eds) CSIRO: Sydney, Australia; 1997; 419–425.
8. Cross M, Bailey C, Pericleous KA, Bounds SM, Moran GJ, Taylor GA, McManus K. Computational modelling of interacting phenomena in the shape casting process. In *Modeling of Casting*, *Welding*, *and Advanced Solidification Processes—VIII*, Thomas BJ, Beckermann C (Eds). The minerals, Metals & Materials Society: Warrendale, PA; 1998; 787–794.
9. Nikitidis MS, Tüzün U, Spyrou NM. Measurements of size segregation by self-diffusion in slow-shearing binary mixture flows using dual photon gamma-ray tomography. *Chemical Engineering Science* 1998; **53**:2335–2351.
10. Brown RL, Richards JC. *Principles of Powder Mechanics* (1st edn). Pergamon Press: Oxford, 1970.
11. Arteaga P, Tüzün U. Flow of binary mixtures of equal-density granules in hoppers-size segregation, flowing density and discharge rates. *Chemical Engineering Science* 1990; **45**:205–223.
12. Hirt CW, Nichols BD. Volume of fluid (VOF) method for the dynamics of free boundaries. *Journal of Computational Physics* 1981; **39**:201–225.

13. Pericleous KA, Moran GJ, Bounds S, Chow P, Cross M. Three dimensional free surface flows modelling in an unstructured environment for metals processing applications. *Applied Mathematical Modelling* 1998; **22**: 895–906.
14. Zamankhan P. Kinetic theory of multicomponent dense mixtures of slightly inelastic spherical particles. *Physical Review E* 1995; **52**:4877–4891.
15. Arnold PC, Maclean AG, Roberts AW. *Bulk Solids*: *Storage*, *Flow and Handling*. TUNRA Bulk Solids Handling Research Associates, University of Newcastle: NSW, Australia, 1982.
16. Haile JM. *Molecular Dynamics Simulation*: *Elementary Methods* (1st edn). Wiley: New York, U.S.A., 1997.

