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Original paper

Analysis and modeling of heaping behavior of granular mixtures within a computational mechanics framework

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Abstract—This paper presents a continuum model of the flow of granular material during filling of a silo, using a viscoplastic constitutive relation based on the Drucker–Prager plasticity yield function. The performed simulations demonstrate the ability of the model to realistically represent complex features of granular flows during filling processes, such as heap formation and non-zero inclination angle of the bulk material–air interface. In addition, micro-mechanical parametrizations which account for particle size segregation are incorporated into the model. It is found that numerical predictions of segregation phenomena during filling of a binary granular mixture agree well with experimental results. Further numerical tests indicate the capability of the model to cope successfully with complex operations involving granular mixtures.

Keywords: Granular mixtures; continuum model; viscoplastic model; heaping; segregation.

1. INTRODUCTION

When filling a silo by pouring particles from an axial jet, a conical heap is formed. The conical heap is characterized by an angle called the angle of repose, which is the maximum slope angle that unconsolidated materials can maintain. This fundamental feature of granular material behavior has only received minor attention in the simulation of industrial large-scale granular flows. However, the accurate description of the silo filling process, including the heap formation phenomenon, is a prerequisite to the development of realistic simulations of the material discharge from the silo. The segregation controlled material composition and the stresses reached after filling determine the initial conditions of the silo discharge process, which have a critical influence on the flow pattern and material behavior during

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discharging. For most of the current computational models, these initial conditions have to be obtained experimentally.

In recent years, significant effort has been put into the modeling of granular material flows, and a number of analytical and numerical models have been developed to describe them [1–6]. Discrete particle models, inspired by molecular dynamic approaches, have proven to be remarkably successful to reproduce the complex behavior of granular materials. In these models, each particle is considered separately, and the interactions between particles and the external forces acting on each particle are taken directly into account at the microscopic level [2, 6]. However, the main limitation of this approach is associated with the high computational cost of the identification of contacts between contiguous particles and the subsequent calculation of the interaction forces. Furthermore, the number of particles in a typical bulk solids handling process is very large (10^{12} or more particles in a moderately size industrial silo). It is therefore unrealistic to perform direct simulations of industrial processes at full scale.

Another important class of models, which has been the subject of extensive research, is based on continuum mechanics, where granular material is described using methods inspired by techniques employed in fluid mechanics [3]. Continuum models are suitable for the simulation of full-scale large problems. A successful continuum description requires the formulation of appropriate constitutive laws, which can account for particle interactions with neighboring particles and with their environment. Although existing models are partially successful in capturing some characteristics of the flow, there is as yet no proposed unified continuum description of granular flows capable of predicting particle flow phenomena in a variety of applications.

The aim of this work is the numerical simulation of silo filling operations, including heap formation and predictions of segregation during filling. Recently, a continuum model was presented for the simulation of discharge from hoppers and good agreement was established between numerical predictions and available experimental data [7, 8]. In the present work, this model is implemented with a more accurate description of particle interactions using a viscoplastic constitutive relation based on the Drucker–Prager plasticity yield function. Simulations of the filling of a two-dimensional (2D) silo with materials of different angles of internal friction are presented. The ability of the model to realistically predict heap formation during filling is discussed. Then, the modeling of segregation of mixtures during filling is discussed, based on the parametrization of the segregation process, as presented in Ref. [7].

2. CONTINUUM MODEL FOR GRANULAR FLOWS

In this section, the basic conservation equations of the granular flow model are first briefly outlined. Then, we describe the constitutive model, which has been adopted for the representation of particle interactions.

2.1. Continuum framework

The continuum framework is employed for the solution of the conservation equations for mass and momentum for an N-species granular mixture. For reasons of simplification, a single momentum equation for the bulk (the sum of all N-species and the air which fills the interstitial space between the solid particles) is solved and no energy equations are solved. A more detailed discussion on the consistency and validity of the various assumptions and simplifications that were employed is given in Ref. [7].

The fraction of each individual material component f_i in a control volume is calculated through the solution of the mass conservation equation for each fraction, which in the absence of source/sink terms may be written as:

$$\frac{\partial f_i}{\partial t} + \nabla \cdot (f_i \vec{u}_\mathrm{b} + J_{\mathrm{seg}\ i}) = 0, \tag{1}$$

where $\vec{u}_\mathrm{b}$ is the bulk velocity, and $J_{\mathrm{seg}\ i}$ is a 'drift' flux which represents segregation and dictates the motion of individual species in the bulk. Fraction f_i indicates the volume fraction of mixture component i, associated to a given particle size, present in the control volume. Particle size does not explicitly appear in the model equations, but is taken into consideration during the derivation of the appropriate functional forms and coefficients for the segregation 'drift' flux.

Three mechanisms which lead to segregation were identified, i.e. strain-induced segregation, 'diffusive' processes and percolation. Functional forms for the three segregation fluxes (the components of $J_{\mathrm{seg}\ i}$), involving key flow parameters (i.e. velocities, particle concentrations) and characteristic transport coefficients of each mechanism, have been extracted using principles of kinetic theory. The procedure for calculating the transport coefficients is based on the use of discrete element method (DEM) simulations. DEM simulations, which describe bulk materials at a particle level (see Section 1), are a valuable and increasingly popular approach, as they enable us to understand the physics and capture many aspects of the behavior of group of particles, from which information can be extracted to be incorporated in a continuum model. The strategy developed in this work is to perform DEM simulations on a suitably limited number of particles (up to several thousand) for a selected set of process conditions within the 'envelope' of conditions in the process of interest. The transport coefficients are calculated from the data of each simulation by integration of the relevant time-correlation function. A more detailed description of the utilization of DEM simulations for the derivation of the individual segregation fluxes and the calculation of the appropriate transport coefficients, as well as the implementation of the segregation fluxes parametrization in the continuum model, is given in Refs [7, 9].

The summation of all individual fractions in a cell gives the total amount of material present in that cell. This sum is only allowed to take values between 0 (cell empty of material) and the maximum allowed packing fraction (always less than unity). Equation (1) is a donor–acceptor type of equation and is used for the prediction of the motion of the free surface (i.e. interface between the flowing particles and the air).

The momentum conservation equation for the bulk is written as:

$$\rho_{\mathrm{b}} \frac{\partial \vec{u}_{\mathrm{b}}}{\partial t} + \nabla \cdot (\rho_{\mathrm{b}} \vec{u}_{\mathrm{b}} \vec{u}_{\mathrm{b}}) = \nabla \cdot \sigma + \rho_{\mathrm{b}} \vec{g}, \tag{2}$$

where ρ_{b} is the density of the bulk and σ the stress tensor, which can be decomposed, in terms of the hydrostatic pressure p and the deviatoric part of the stress tensor S_{ij}, as:

$$\sigma_{ij} = -p\delta_{ij} + S_{ij}. \tag{3}$$

The constitutive relation, coupling the deviatoric part of the stress tensor with the strain tensor, is defined by analogy to that employed in fluid dynamics for incompressible flows. It reads:

$$S_{ij} = \mu_{\mathrm{b}} \left(\frac{\partial u_{\mathrm{b},i}}{\partial x_j} + \frac{\partial u_{\mathrm{b},j}}{\partial x_i} \right) - \frac{2}{3} \mu_{\mathrm{b}} \nabla \cdot \vec{u}_{\mathrm{b}} \delta_{ij}. \tag{4}$$

The parameter μ_{b} is a pseudo-viscosity coefficient (equivalent of the fluid viscosity) of the bulk mixture. The parameters ρ_{b} and μ_{b} are calculated through weighted averages of the properties of the mixture components, ρ_{gran} and μ_{gran} (solids density and pseudo-viscosity coefficient of the granular material) and the air ρ_{air} and μ_{air} (density and viscosity of air):

$$\rho_{\mathrm{b}} = \sum_i f_i \rho_{\mathrm{gran}} + \left(1 - \sum_i f_i \right) \rho_{\mathrm{air}}, \tag{5}$$

$$\mu_{\mathrm{b}} = \sum_i f_i \mu_{\mathrm{gran}} + \left(1 - \sum_i f_i \right) \mu_{\mathrm{air}}. \tag{6}$$

In the early version of the model, the pseudo-viscosity coefficient of the granular material was assigned a constant value as a first approximation, which was determined via initial calibration of the model to the material flow rate measured during hopper discharge.

2.2. Viscoplastic constitutive equation

Despite the simplifications introduced, it has been shown that the model proposed above can reasonably reproduce the flow of granular materials discharging from a silo [7, 8]. However, the model failed to describe complex features of granular materials flows, such as the heap building mechanism during filling of a silo. The main weakness of the model is the use of a constant pseudo-viscosity coefficient, which results in an ordinary Newtonian fluid-like behavior characterized by a horizontal bulk material free surface.

The issue of defining a suitable constitutive relation for the description of granular flows is complex and not completely understood at present. A number of constitutive models originating from soil mechanics or using ideas of the gas kinetic theory have been described. Nevertheless, none of them is generally applicable. Among the models proposed, the viscoplastic models based on the plasticity theory (e.g. Refs [5, 10]) and, more recently, the hypoplastic approach (e.g. Refs [11, 12]) have been widely used to model granular flows in the context of silos. Viscoplastic models require the definition of a yield or rupture surface. One of the simplest and most employed yield functions is based on the Drucker–Prager model [13], which is a simple first idealization of an elastic–perfectly plastic behavior of frictional materials [14].

In this work, a viscoplastic-like constitutive model based on the Drucker–Prager yield criterion is implemented. Assuming that the material is everywhere at yield, the Drucker–Prager plasticity yield surface equation can be written in the following form:

$$\overline{\sigma} - 3a' p - K = 0, \tag{7}$$

where

$$a' = \frac{2\sin\varphi}{\sqrt{3}(3-\sin\varphi)} \quad \text{and} \quad K = \frac{6c\cos\varphi}{\sqrt{3}(3-\sin\varphi)},$$

φ is an angle related to friction between neighboring particles and is called the internal friction angle, c is a parameter related to the cohesiveness of the material, and p is the mean normal stress (i.e. pressure). $\overline{\sigma}$ is the second invariant of the deviatoric stress tensor:

$$\overline{\sigma} = \sqrt{\frac{1}{2} S_{ij} S_{ij}}. \tag{8}$$

Substitution of the relation (4) written in terms of the pseudo-viscosity coefficient of the granular material in (8) leads to:

$$\begin{aligned}\overline{\sigma} = \mu_{\mathrm{gran}} \cdot \Bigg[2 \cdot \sum_{i=1}^{3} \left(\frac{\partial u_{\mathrm{b},i}}{\partial x_i} - \frac{1}{3} \nabla \cdot \vec{u}_{\mathrm{b}} \right)^2 + \left(\frac{\partial u_{\mathrm{b},1}}{\partial x_2} + \frac{\partial u_{\mathrm{b},2}}{\partial x_1} \right)^2 \\ + \left(\frac{\partial u_{\mathrm{b},2}}{\partial x_3} + \frac{\partial u_{\mathrm{b},3}}{\partial x_2} \right)^2 + \left(\frac{\partial u_{\mathrm{b},3}}{\partial x_1} + \frac{\partial u_{\mathrm{b},1}}{\partial x_3} \right)^2 \Bigg]^{1/2} = \mu_{\mathrm{gran}} \cdot (\mathrm{DEL}\boldsymbol{u}_{\mathrm{b}})^{1/2}.\end{aligned} \tag{9}$$

From (7) and (9), one can obtain the pseudo-viscosity coefficient of a non-cohesive granular material ($c = 0$):

$$\mu_{\mathrm{gran}} = \frac{2\sqrt{3}\sin\varphi p}{(3-\sin\varphi)(\mathrm{DEL}\boldsymbol{u}_{\mathrm{b}})^{1/2}}. \tag{10}$$

The pseudo-viscosity coefficient is now a non linear function of the pressure, the material internal friction angle and the bulk velocity gradients. As described in Section 2.1, the pseudo-viscosity of the bulk is obtained through the weighted averaging relation (6).

Two main angles are generally introduced when characterizing the behavior of a granular material. These are the angle of repose (i.e. the angle between the slope of a stable pile of unconsolidated granular matter and the horizontal base) and the angle of internal friction (i.e. the angle which relates to friction between two neighboring particles in a heap and is a unique material property). It is necessary to clarify that for the case of non-cohesive, unconsolidated granular material (which is the case described throughout this paper), the angle of repose is equal to the angle of internal friction. This can be directly derived through the Coulomb equation, which relates the shear strength to the effective normal stress for unconsolidated granular material [15]. Hence, either angle may be used to describe the angle of the slope of a granular heap.

2.3. Numerical method

The full set of equations of the mathematical model was solved numerically with the aid of a segregated solution algorithm using PHYSICA, a finite-volume code developed at the University of Greenwich [16]. The PHYSICA toolkit is a fully unstructured-mesh, 3D, computational fluid dynamics (CFD) modular suite of software for the simulation of coupled physical phenomena. The momentum conservation equation for the granular mixture was solved using a SIMPLE-based algorithm and a conjugate gradient iterative solver. A total variation diminishing-based scheme (scalar equation algorithm) proposed by Pericleous *et al.* [17] was used for the discretization of the transport equation for each individual material component. Note that for reasons of numerical stability, μ_{gran} was not allowed to vary unbounded, in order to avoid the generation of spurious oscillations of pressure and velocity values during the iterative solution procedure. A more detailed description of the numerical techniques and algorithms can be found in Ref. [7].

3. NUMERICAL RESULTS AND DISCUSSION

3.1. Simulation of the filling operation

A 2D plane flat-bottomed bin was considered for the simulations. The bin is 0.1 m in height and 0.08 m in width. The mesh of the bin is shown in Fig. 1. The bin, which is initially empty, is filled from the center with a free falling particle axial jet of 0.01 m in width. The material consists of monosized non-cohesive particles of 2 mm diameter, with a solids density of 2100 kg/m^3 and a bulk density of 950 kg/m^3. The material angle of internal friction is 30°. Calculations were performed assuming smooth walls (i.e. friction coefficient between the wall and the particles equals to 0). The values of the lower and upper bound of the pseudo-viscosity coefficient were set to 10^{-4} and 50 Pa s, respectively.

Figure 2 compares the material free surface at different times during the filling process calculated using the viscoplastic constitutive model [i.e. (10)] with that

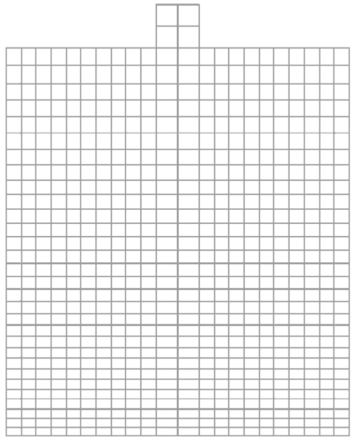

Figure 1. Computational mesh of the 2D plane bin.

obtained with a constant value of the pseudo-viscosity coefficient [i.e. (4)]. For both runs, after the filling process finished, calculations were carried on for a longer time to examine the stability of the shape of the material free surface.

The comparison of the two runs shows a clear improvement of the modeling of the flow pattern during the filling process in the case of the viscoplastic model. The top free surface of the bulk material exhibits very different shapes in the two simulations, especially after stopping the feeding particle jet. In the simulation using a constant pseudo-viscosity coefficient, the flow behaviour is as expected similar to that of a liquid, resulting in a perfectly flat final material free surface. In contrast, a clear heap-like shape of the bulk material top free surface is seen to form for the case of the viscoplastic model, which is consistent with well-known experimental observations [18]. The inclination angle of the material–air interface (defined as the slope of the free surface) reaches a final value equal to 14°. It was verified that additional mesh refinement had no significant influence on the computed inclination angle. No slow decay of the free surface to a flat state after completion of the filling operation is observed. Indeed, the shape of the free surface remains stationary between $t = 70$ s and the end of the simulation ($t = 300$ s). A similar type of flow behavior was obtained by Laux [19], who developed a two-phase fluid–particle model including a 'frictional' viscosity for the particle phase derived from the Drucker–Prager yield condition.

The formation of a heap in the case of the viscoplastic model is illustrated in Fig. 3, which shows the velocity vectors of the bulk material for the same simulation times as in Fig. 2. When filling the silo, the flowing particles are preferentially concentrated inside a region close to the material–air interface, while particles inside the heap are nearly quiescent. From $t = 70$ s onwards, the heap is stationary, as there is no flowing particles anymore. This behavior is in qualitative agreement with experimental observations of surface flows during heap formation reported in literature (see, e.g. Ref. [18]).

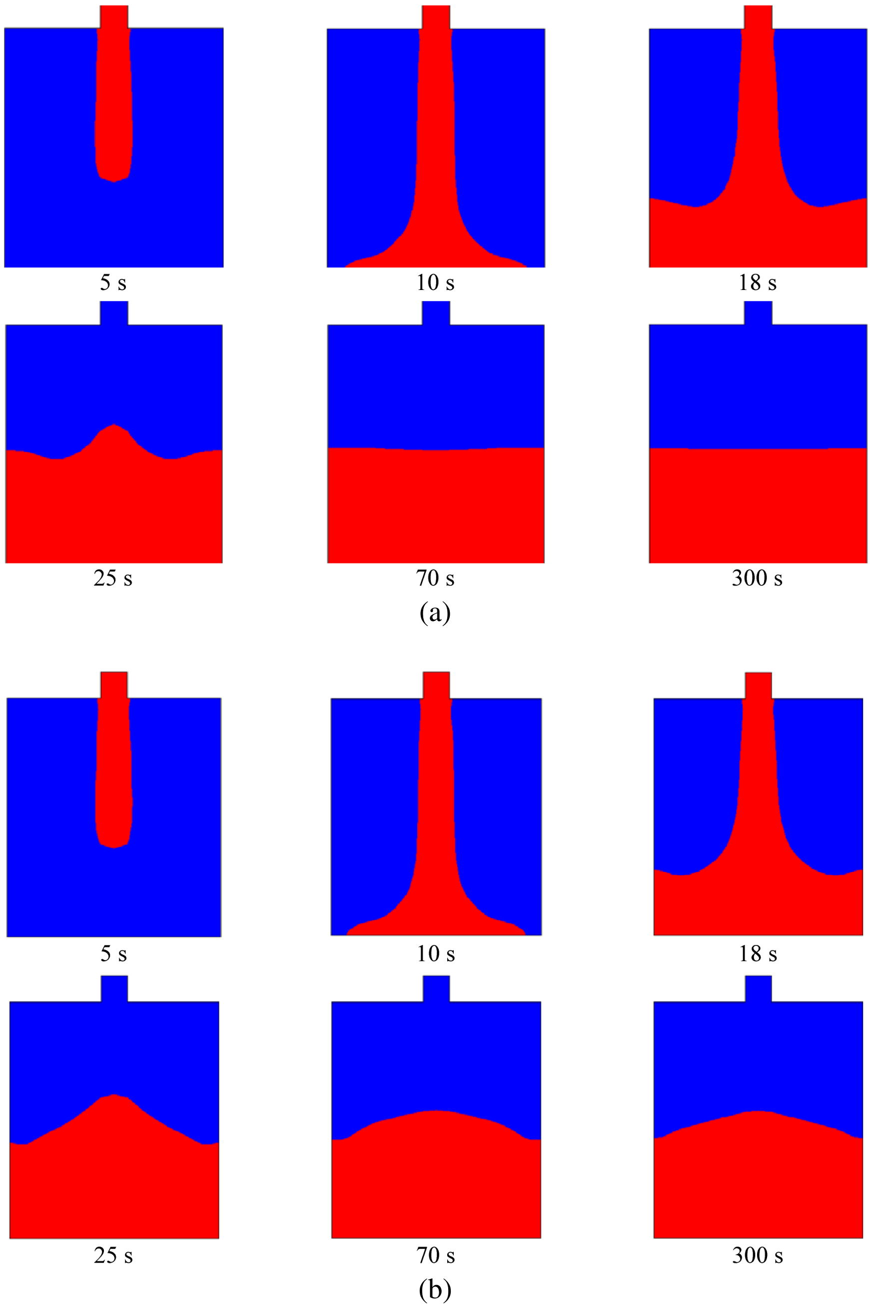

Figure 2. Predicted bulk material top free surface at different times during the filling operation (a) using a constant pseudo-viscosity coefficient and (b) using a viscoplastic constitutive model. This figure is published in colour on http://www.ingenta.com

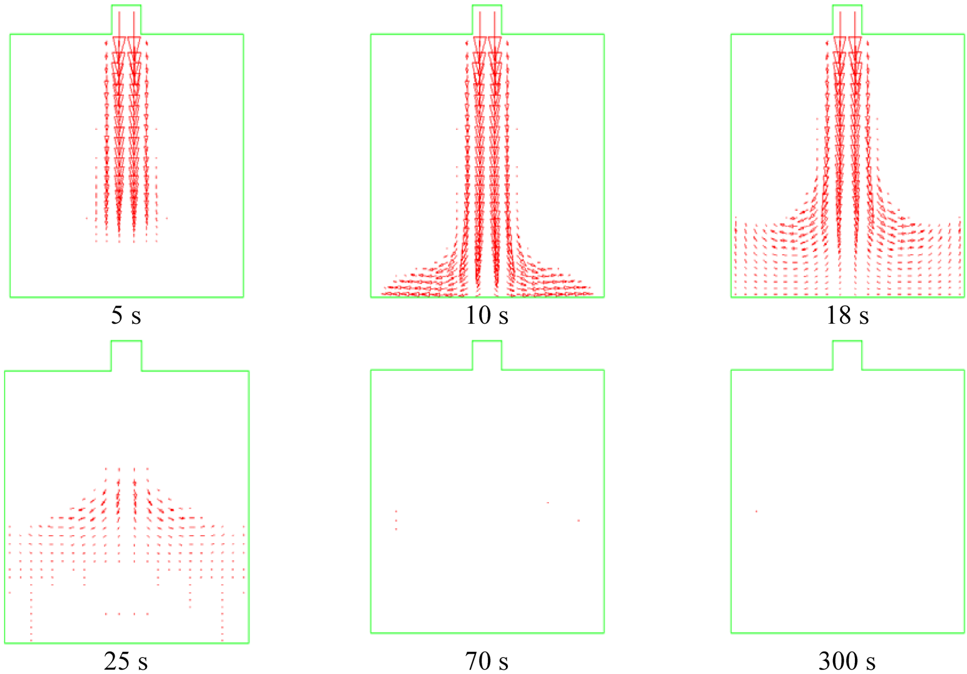

Figure 3. Calculated velocity vectors of the bulk material at different times during the filling operation. This figure is published in colour on http://www.ingenta.com

Hence, the heap building mechanism and the resulting non-horizontal shape of the material–air interface appear to be predicted by a viscoplastic constitutive model. However, it should be noted that the inclination angle of the heap does not match the material angle of repose. The predicted value differs from the internal friction angle of the material by approximately a factor of 2.

3.2. Sensitivity with respect to changes in the material angle of internal friction

Using the viscoplastic constitutive model, a parametric study for the flat-bottomed bin considered above was carried out for three different values of the material angle of internal friction: 30, 45 and 60°. Figure 4 compares the final position and shape of the material free surface in the bin predicted by the numerical model for the three different angles of internal friction. All simulations show a heap-like shape of the bulk material top free surface. An increase in the angle of internal friction of the material results in a corresponding increase of the inclination angle of the free surface.

The inclination angle obtained for each case is plotted against the angle of internal friction of the material in Fig. 5 (solid line) and compared with the theoretical relation between angle of repose–angle of internal friction (dashed line) (as stated earlier, for unconsolidated, non-cohesive granular material, the angle of repose and the angle of internal friction are identical, thus the slope of the dashed line

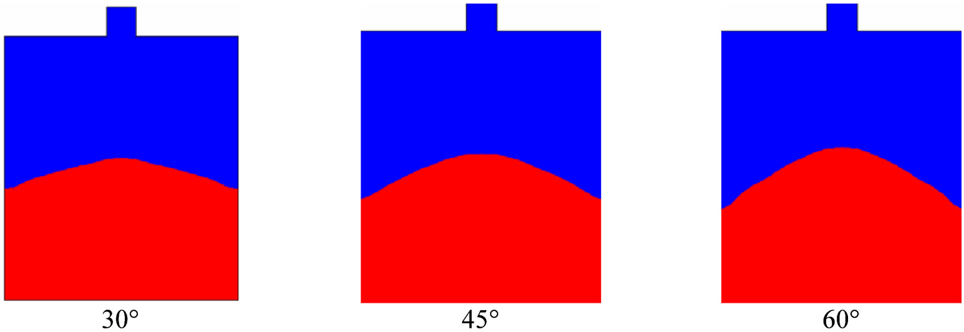

Figure 4. Final shape of the bulk material top free surface after completion of the filling operation for three different values of the material angle of internal friction (30, 45 and 60°). This figure is published in colour on http://www.ingenta.com

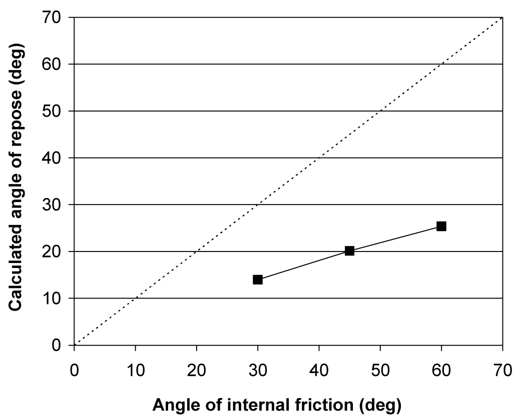

Figure 5. Comparison of the theoretical relation between angle of repose and angle of internal friction (dashed line), and the predicted relation between heap inclination angle and angle of internal friction (solid line).

is 1). There is an approximate linear relation between the predicted heap inclination angle and the actual angle of internal friction. However, the inclination angle is significantly underpredicted, with respect to the material angle of repose, with the discrepancy becoming greater for larger angles of internal friction.

3.3. Study of segregation of a binary mixture

The viscoplastic model is then applied to study the scenario of filling of the bin with a binary mixture of 2:1 size ratio and the resulting segregation of the mixture. The mixture consisted of 50% coarse particles (of 5.2 mm diameter) and of 50% finer particles (of 2.6 mm diameter). The initial bulk density was taken as 950 kg/m^3 and the solids density as 2100 kg/m^3. The material angle of internal friction was 30°. The segregation transport coefficients were calculated for the two mixture phases in the micro-physical framework and were directly imported in the continuum framework [7]. The values of the diffusion and shear-induced segregation transport coefficients were found to be 6.5×10^{-8} and 2.1×10^{-7} m^2/s, respectively, for the fines fraction. The values of the diffusion and shear-induced segregation transport coefficients for the coarse fraction were found to be 2.8×10^{-7} and 2.5×10^{-6} m^2/s, respectively. A discussion on the importance and the derivation of these coefficients is given in Ref. [7].

The material interface profile is as shown in Fig. 2b. Figure 6 presents the predicted interfaces of each of the two material components. Segregation is evident, with the coarser particles rolling along the interface and concentrating further away from the axis of filling, while the finer particles seem to concentrate around the axis of filling. This behavior is expected and is consistent with experimental observations of granular mixtures in bins of these dimensions [20].

There were experimental data available for the final concentration at the end of the fill for each of the two components of this particular mixture. The concentration was measured 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 patterns [20]. The segregation tester consists of a rotating transparent mixer and a parallelepiped section underneath the mixer, which is adjusted to an inclination in order to represent the material angle of repose (Fig 7). The parallelepiped section is divided into five compartments, which can be separated after the end of the filling process by inserting vertical steel plates between them, so that material may be analysed from each compartment separately.

In the numerical simulations, after filling stopped and the heap had reached its final shape, data were collected at various heights from five equally spaced strips between the axis of filling and the bin wall, average concentrations were obtained for each of the two mixture components and were compared to the experimental data. This comparison is presented in Fig. 8 for the fines fraction, with the x-axis representing the proportion of heap length between axis of filling (point 0) and bin wall (point 1). The y-axis shows the total percentage of fines in the mixture composition after the end of the filling process and the creation of the heap. As becomes clear from this graph, there is reasonable agreement between experiment and simulation (the difference between them ranging from 3.5 to 9.5%). Note that there is a 4% error in the experimentally obtained values. It can be concluded that the numerical model is capable of not only representing realistically the creation of the heap, but also of giving a good indication of the observed segregation pattern during filling of the bin.

3.4. Numerical study of double-heap creation and segregation during a complex filling process

In this case, a numerical study was undertaken in order to demonstrate the capabilities of the numerical model to represent complex processes and scenaria,

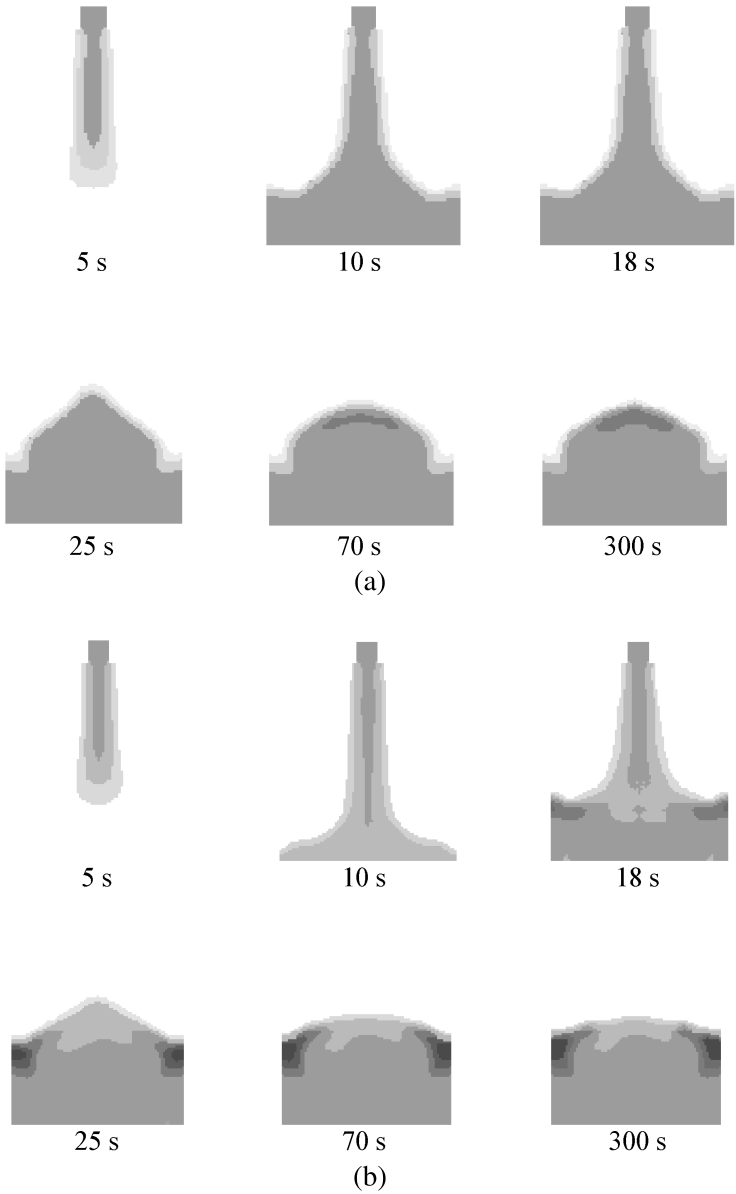

Figure 6. Predicted profiles of (a) fines and (b) coarse fractions of a 50–50, 2:1 binary granular mixture at various times during filling of a flat-bottomed bin. Clear evidence of segregation with non-uniform concentration of each of the two material components can be seen. The grey scale represents the material concentration in a computational cell (i.e. lighter greys signify less material and darker greys signify more material).

which are commonly met during operations involving granular mixtures. The problem represents the filling of a 2D plane flat-bottomed bin with two orifices. The bin was 0.1 m in height and 0.15 m in width, with two filling orifices of 0.01 m

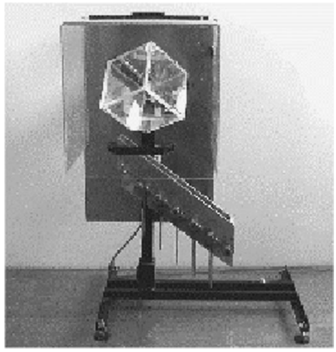

Figure 7. Segregation tester. Experimental device to assess material radial segregation during the filling operation of a silo.

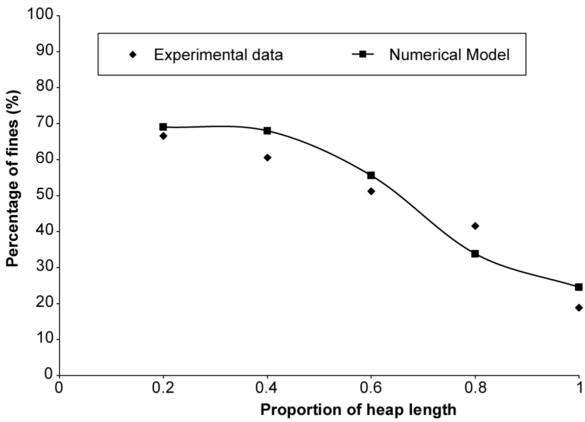

Figure 8. Comparison between experimental and numerical data for the percentage of fines in the final mixture composition after the filling had ended and the heap had obtained its final shape. The x-axis represents the proportion of heap length from the axis of filling (0) to the bin wall (1).

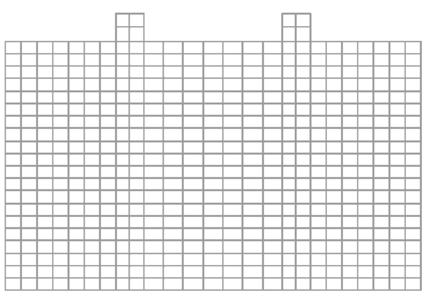

Figure 9. Computational mesh of the 2D plane bin with the two orifices.

width, each situated at 0.04 m distance from the bin walls. The mesh of the bin is shown in Fig. 9. The granular mixture properties are as given in the previous section.

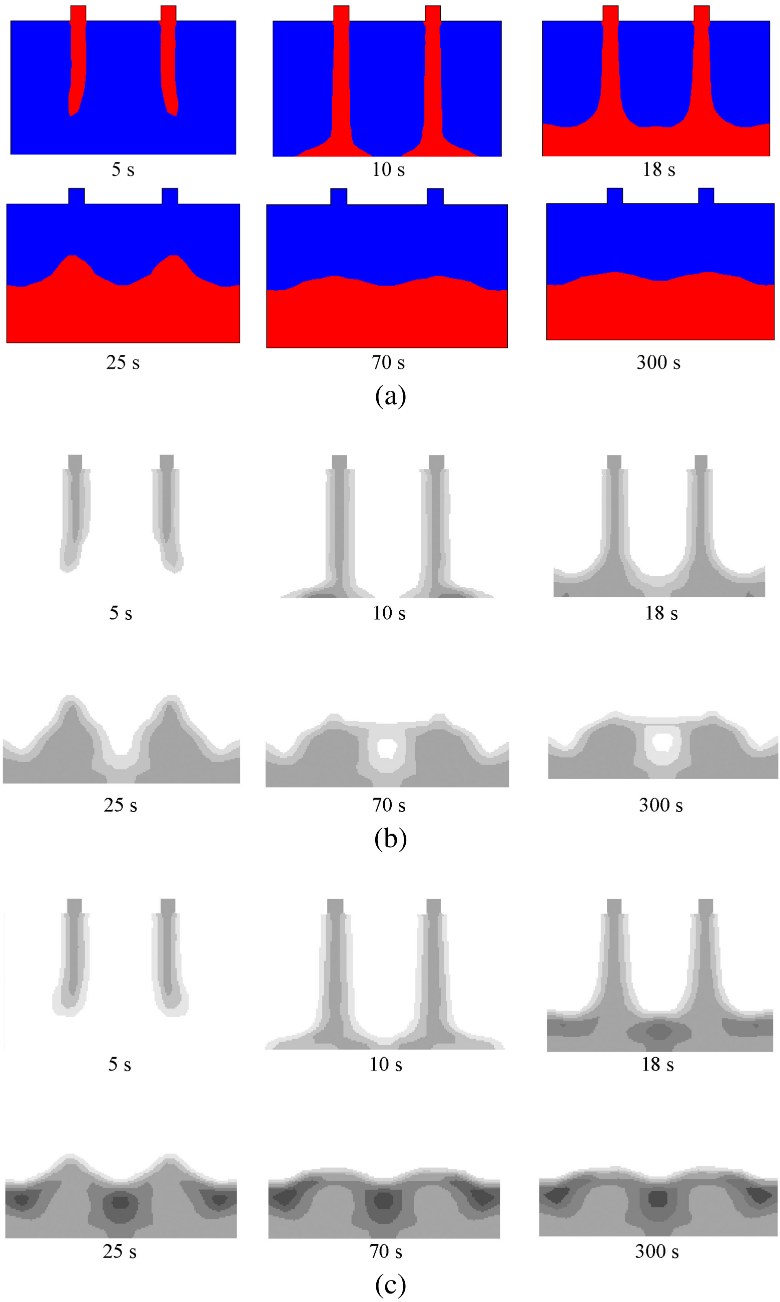

Figure 10. Predicted profiles of (a) material interface, (b) fines and (c) coarse fractions of a 50–50, 2:1 binary granular mixture at various times during filling of a flat-bottomed bin with two orifices. Clear evidence of segregation with non-uniform concentration of each of the two mixture components can be seen. The grey scale represents the material concentration in a computational cell (i.e. lighter greys signify less material and darker greys signify more material). This figure is published in colour on http://www.ingenta.com

This scenario was chosen because of the simultaneous creation of two heaps, which also interact with each other. The ability of the model to represent realistically the segregation of the mixture components was tested, particularly around the center of the bin where the two heaps merge. Figure 10 presents the material interface profile, as well as each of the individual fines and coarse fractions profiles at various times during the filling process. It is observed that two symmetrical heaps are created, which maintain their inclination. Again, as expected from theoretical and experimental predictions (see, e.g. Refs [20, 21]), coarser particles are seen to concentrate further away from the axis of filling of each heap, whereas finer particles concentrate around the axis of filling. The model has been able to reproduce realistically the behavior of this complex filling scenario, with the correct representation of the mixture segregation behavior. Unfortunately, no experimental data were available for this case to compare to the predicted material behavior. However, the exhibited symmetry between the two heaps may be regarded as proof of the consistency of the model with the theoretically expected behavior.

4. CONCLUSIONS

A viscoplastic constitutive model based on the Drucker–Prager criterion has been implemented in a granular flow continuum model for simulating the filling of silos. Numerical results have shown the capabilities of the model to represent reasonably the heap formation mechanism and the corresponding non-zero inclination angle of the air–material interface during bin filling operations, as well as the segregation behavior of a binary granular mixture. The prediction of bin filling with the representation of heap formation and the simultaneous prediction of segregation behavior of granular mixtures in a computational mechanics framework is believed to be unique. Further work is underway in order to achieve better agreement between the material angle of repose and the predicted inclination angle of the heap. Further validation tests are necessary in order to establish the applicability of this model to a wide range of materials. Despite its limitations, the presented framework appears to be a promising route for the description of complex features of flows of granular mixtures in important engineering problems.

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