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Mathematical Modelling of the Behaviour of Granular Material in a Computational Fluid Dynamics Framework using Micro-Mechanical Models

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Abstract

In this paper, a Computational Fluid Dynamics framework is presented for the modelling of key processes which involve granular material (i.e. segregation, degradation, caking). Appropriate physical models and sophisticated algorithms have been developed for the correct representation of the different material components in a granular mixture. The various processes, which arise from the micro-mechanical properties of the different mixture species can be obtained and parametrised in a DEM / experimental framework, thus enabling the continuum theory to correctly account for the micro-mechanical properties of a granular system. The present study establishes the link between the micro-mechanics and continuum theory and demonstrates the model capabilities in simulations of processes which are of great importance to the process engineering industry and involve granular materials in complex geometries.

1 Introduction

In recent years significant effort has been put into the modelling of granular flows using a continuum mechanics approach [1], [2]. Although these models are partially successful in capturing some characteristics of the flow, they do not incorporate essential information on material parameters, which are needed to model the various interactions between different particles or particles with their surrounding environment. Thus, they can not be used to simulate processes, which are of great importance in the process engineering industry (i.e. hopper filling/emptying, pneumatic conveying, storage in containers etc.), where these interactions lead to phenomena such as particle size segregation, degradation/breakage or aggregation/caking.
On the other hand, micro-mechanical models are able to describe successfully the flow of granular material by accounting for various types of interactions at the microscopic level [3], [4]. However, these models can only be applied to a small number of discrete particles, due to the complexity of the simulated processes. Therefore, such models are not suitable for the modeling of large-scale process, as considerable amounts of computing time would be required for the simulation of processes that involve large numbers of particles.
In the present paper a continuum framework is presented, where the micro-mechanical behaviour of different particle species in a multi-component granular mixture is parametrised and employed in the form of constitutive models. The micro-mechanical parametrisations, employed to account for particle size segregation, degradation and moisture-migration caking are outlined. As an example, the simulation of a complete process that involves granular material is presented. First, a short hopper containing a binary mixture is discharged in core flow mode. Then, a simulation of a dilute-phase pneumatic conveyor with a number of bends and straight pipes is presented. Finally, for granular material stored in a bag, its affinity to cake (arising from the interaction with its environment) is examined. Conclusions are then drawn on the capability of the numerical model to represent realistically key granular processes.

2 The Computational Framework

The full set of flow equations was solved using PHYSICA, a Computational Fluid Dynamics (CFD) unstructured-mesh, finite-volume code developed at the University of Greenwich for the simulation of coupled physical phenomena ([5]-[7]). The CFD code is utilised for the solution of conservation equations for mass and bulk momentum in the computational domain. Equations for energy were not solved because energy-linked flow parameters were accounted for in the micro-mechanical constitutive models, which explicitly link the granular temperature of the flow to bulk velocity gradients via kinetic/theoretical considerations [8]. It should also be noted that micro-mechanical criteria were employed for the prediction of the flow boundary and the existence of stagnant zones (core flow mode) during the flow of granular materials [9].
A scalar equation was solved for each of the individual fractions f_i of the mixture, representing the fractional volume of each of the material components in every computational cell. The summation of all individual fractions in a cell gave the total amount of material present in that cell at a certain time. This sum is only allowed to take values between 0 (cell empty of material) and the maximum allowed packing fraction (always less than unity). The scalar equation for each individual f_i may be written as:

$$\partial fi / \partial t + \nabla \cdot \{ fi\, (\boldsymbol{u}_b + \boldsymbol{u}_{seg}) \} = S_i \, , \tag{1}$$

where $\boldsymbol{u}_b$ is the bulk velocity (as results from the solution of the momentum equation), $\boldsymbol{u}_{seg}$ is a segregation “drift” velocity and S_i is a source/sink term representing shear-degradation/compressive-caking in the i-th particle size class (through population balance models, e.g. [10]). The approach that has been followed in this study for the representation of dilute-phase pneumatic conveying and moisture-migration caking will be outlined in the following sections.

2.1 Parametrisation of Segregation

The segregation “drift” velocities were analysed in the micro-mechanical framework, by using principles of kinetic theory [11]. For each material component three transport processes, which lead to segregation, were identified: (a) **Shear-induced segregation** (kinetic sieving), which represents the flow of coarser particles in the mixture across gradients of bulk velocity, (b) **Diffusion**, which represents the flow of finer particles of the mixture down a concentration gradient and (c) **Percolation**, which represents the gravity-driven motion of the finer particles through the coarse phase in a mixture. Functional forms of all three “drift” components were derived and transport coefficients were calculated for each mixture phase through linear response theory and integrating the relevant time correlation functions in a Discrete Element Method (DEM) framework [3]. A full analysis of the functional forms of the derived constitutive equations for all three mechanisms and detailed validation results for mass-flow hoppers are given in [12].

2.2 Parametrisation of Degradation

The emphasis in this study was placed on dilute-phase pneumatic conveying in systems with bends of 90° only, due to their engineering importance (most pneumatic systems in bulk solids handling plants are dilute-phase pneumatic conveying systems with bends of 90°). The modeling of a pneumatic conveying system had to be performed in two discrete parts: (a) modelling of the breakage of the particles due to the collision with bend walls (it is well-established that only collisions with bend walls will give rise to significant particle damage [13]) and their subsequent deceleration due to sliding wall friction and rebound processes and (b) modelling of the re-acceleration of air and particles in the straight sections between bends. An Eulerian framework was chosen, since a combined Eulerian/Langrangian framework, although more accurate in tracking the individual particle trajectories and impacts with bend walls, is very expensive computationally. Moreover, it has been demonstrated that: (1) the distance in a straight pipe after a bend that particles have to travel for pressure drop to develop is the same for both fine and coarse particles [14], (2) the degradation occurring in a 90° bend of a pneumatic system can be represented by single particle impact degradation at an angle of 90° [15].

For the modelling of the breakage process of particles in bends, experimental data were obtained from 90° impact degradation experiments at various velocities on single particles, using a rotating disc accelerator type degradation tester [16]. These data were then utilized to construct appropriate breakage matrices, using regression analysis theory, in order to correlate the input particle size distribution to the resulting size distribution after impact and breakage. The constructed matrices account for the impact conditions (angle and velocity of impact) and are dependent on the material physical properties. Furthermore, apart from particle breakage, the effect of particle deceleration, due to wall sliding friction and the rebound processes, was also accounted for, through a simple model based upon sliding friction under centrifugal action and a coefficient of restitution. Furthermore, it was assumed that no degradation events occurred in straight sections between bends.

The particles-air re-acceleration in the straight pipe after each bend was based on momentum transfer between two distinct phases (assuming that immediately downstream of a bend particles concentrated in a strand and got gradually dispersed in the air stream) [17]. After the flow became fully dispersed, the pressure drop was modelled using a Darcy-type relation [17].

2.3 Parametrisation of Caking

The present paper concentrates on moisture-migration caking, since one of the main caking problems in the bulk solids handling industry is encountered during storage of material under conditions of sharp atmospheric temperature variations between day and night. Equations which track variations in temperature and air mixing ratio need to be considered and implemented with appropriate source terms to account for the contribution from the variations of the moisture content of the solids (see e.g. [18]). The analysis was implemented with equations for the equilibrium relative humidity and mixing ratio of the interstitial air [19] and the tensile strength of the cake was related to the radius of the solid bridges formed around the granular material particles through the Rumpf equation [20].

3 Numerical Simulations

In order to demonstrate the capabilities of the numerical model a test case was chosen, which represents a full process of handling of granular material and is an example of a process commonly met in bulk solids handling operations. It involved the discharge under core flow conditions of a binary mixture from a cylindrical flat-bottomed bin, then its pneumatic conveying through a series of bends and pipelines and, finally, its storage in a polyethylene bag in an environment where temperature varied significantly between daytime and nighttime. The core flow discharge demonstrates the effects of segregation, pneumatic conveying is associated with degradation and storage under the prescribed conditions causes the material to cake.

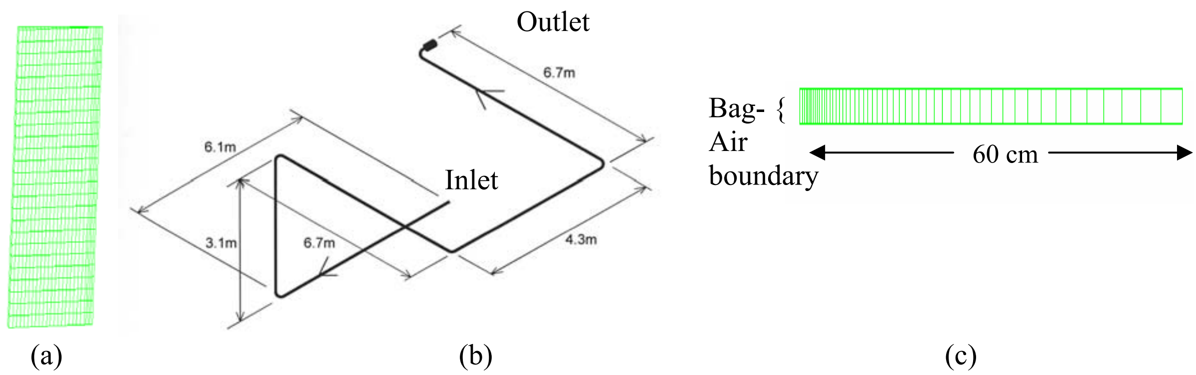


Figure 1: (a) Applied geometry and mesh for the core flow flat-bottomed bin (segregation), (b) The pneumatic conveying system (degradation), (c) Applied mesh for simulated bag strip (caking).

3.1 Segregation during discharge from a flat-bottomed bin in core flow mode

The initial mixture consisted of coarse and fine particles of bulk density of 1000 kg m^{-3} and of 2:1 size ratio (particle diameters of 5.2 and 2.6 mm). A moderate size ratio was chosen in order to exclude the effects of random percolation from the system. The material angle of repose was 32º. The initial composition by weight was 60% fines and 40% coarse and the bin initial segregated state at fill was fitted according to theoretical predictions and experimental data [21], with the finer particles concentrating around the central axis of the bin (62% fines, 38% coarse at the centre) and the coarser particles concentrating closer to the walls (32% fines, 68% coarse at the wall region). The cylindrical flat-bottomed bin was of 55 cm diameter, 77 cm height and had a 7.5 cm orifice at the bottom, around its central axis. Because of the material properties and the vessel geometry, it was predicted through the micro-mechanical flow criteria [9] that the discharge of the mixture was going to occur in core flow mode (where stagnant material regions exist). Due to the axisymmetric nature of this case, a semi-3D geometry was chosen, with a slice of 5º angle being simulated. The simulated bin geometry and applied mesh are shown in Figure 1a. Material exited from the bin at a prescribed volumetric flow rate, 2.8×10^{-3} m^3 s^{-1}, as determined through the Beverloo correlation [9].

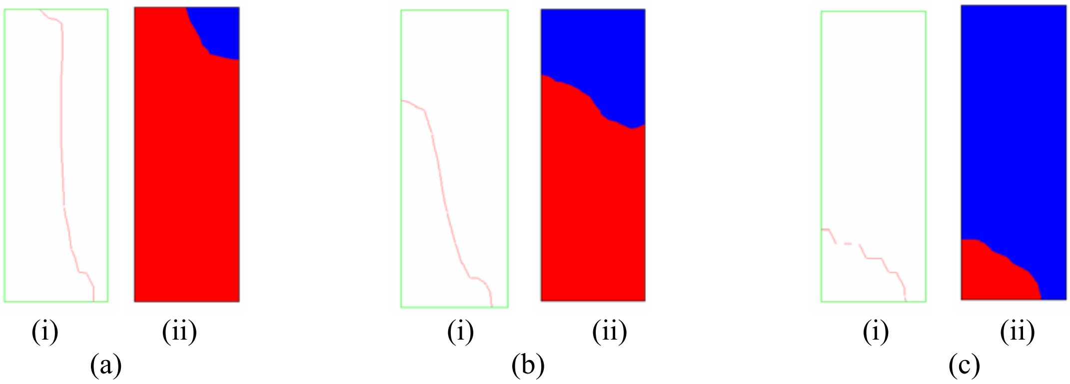


Figure 2: Development of (i) flow / no-flow boundary, (ii) interface between material (red) and air (blue) at times (a) 2s, (b) 30 s and (c) 60 s. The channel above the orifice is maintained filled until the creation of the final stagnant region at the material angle of repose.

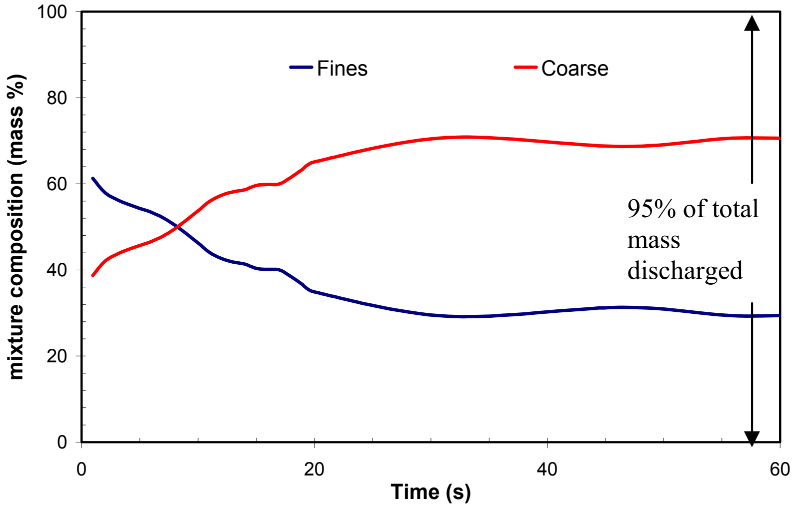


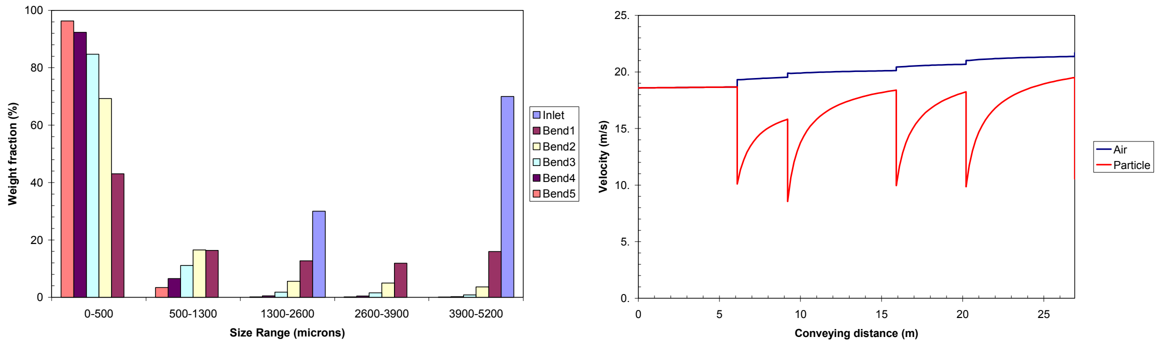
Figure 3: Temporal segregation profile of the individual mixture components during core flow discharge.

The total time for discharge was about 60 s, which is in good agreement with experimentally observed discharge times of hoppers of similar dimensions [9]. During the initial stages of discharge, the central part was observed to collapse, thus creating a channel. Once the channel reached the top surface (in less than 10% of the total emptying time), this began to descend and steepen until it reached the material angle of repose. Thereafter, the material emptied from the bin very slowly through

avalanching into the central channel from the surface region of the bulk, with the angle of repose always being maintained at the interface between material and air. Eventually, a stagnant region was left in the domain, with no more material exiting the bin. The final stagnant material was also maintained at the angle of repose. The evolution of the interface between air and material and the corresponding flow / no-flow boundary at various points in time is depicted in Figure 2.
Figure 3 presents the temporal segregation profile of the mixture (plotted as mass percentage of the individual fractions), averaged over the outlet. As can be observed, the amount of fines exiting the domain dropped very quickly due to the kinetic-sieving / diffusion process, which drove the coarser particles towards regions of high shear (close to the centre of the hopper). This behaviour was expected, according to theoretical and experimental predictions (see e.g. [21]).

3.2 Degradation during dilute-phase pneumatic conveying

A dilute-phase pneumatic conveyor was then employed to convey the mixture through a series of bends and straight pipes. All bends were at 90° and the pipe / bend diameter was 5.3 cm. The system configuration / straight pipe lengths are shown in Figure 1b. At the inlet, the volumetric flow rate of air was taken to be 0.041 $m^3 s^{-1}$ and the mass flow rate of solids was 0.61 kg s^{-1}. The initial binary mixture was split into 5 discrete size classes (5.2-3.9 mm, 3.9-2.6 mm, 2.6-1.3 mm, 1.3-0.5 mm and, finally, particles below 0.5 mm or "fine dust"), thus allowing particles to degrade into sizes smaller than the 2.6 mm size range of fine particles used for the core-flow discharge. It is of great importance to the bulk solids handling industry to know the tendency of a given material to degrade during pneumatic conveying (i.e. amount of "fine dust" produced), in order to be able to maintain a consistent product quality for a particular material. As seen from Figure 3, the bin outlet mixture composition during discharge varied; however, during the latter stages of discharge, the composition at the outlet was observed to be approximately 70% coarse and 30% fine particles. This profile was chosen to be the inlet particle size distribution for the pneumatic conveyor (with the 70% coarser particles placed in the 5.2-3.9 mm size range and the 30% finer particles placed in the 2.6-1.3 mm size range).



(a) (b)

Figure 4: Dilute-phase pneumatic conveying of material through the system described in Figure 1b, (a) Particle size distribution after each degradation event, (b) Air-material velocity profiles during the conveying process.

Figure 4 shows the particle size distribution after each bend and the velocities of the air and the particles at every stage of the conveying process. The sharp deceleration during the material conveying through the bends can be seen in Figure 1b. After each bend the particles re-accelerated but did not reach the velocity of the air, since the straight pipe lengths were smaller than the required ones for the flow to become fully suspended. As can be deduced from Figure 1a, almost all particles have degraded during the conveying process to sizes below 0.5 mm (more than 90% of the total mass at the outlet of the pneumatic conveyor is made up of particles in the "fine dust" region). Hence, it can be concluded that this specific material was very prone to degradation under the given pneumatic conveying conditions and if particles larger than 0.5 mm were required, alternative conveying conditions / pneumatic system configuration had to be considered.

3.3 Moisture-migration caking during storage

It was assumed that downstream of the pneumatic conveyor the granular material was packed in a polyethylene bag of 1.2 m diameter and stored for 24 hours in an environment where temperature varied between 40° C during daytime and 10° C during nighttime. The bag was assumed to be impermeable to environmental humidity (hence, no humidity was allowed to enter / leave the system) and the only interaction between material and environment allowed was through the bag layer (of 5 mm thickness) and occurred through the temperature variations between daytime and nighttime. Thus, the total water content of the system was constant and the moisture content of the solids was allowed to change only due to the evaporation/condensation process and diffusion (moisture migration) between bag-material interface and bag centre. Due to the symmetry of the problem (no detectable changes in the temperature and moisture content of the system towards the centre of the bag and assumption of totally impermeable boundaries at top and bottom), only a thin strip across the bag (from polyethylene lining to bag centre) of 0.6 m length was modelled. The simulated strip geometry is shown in Figure 1c.

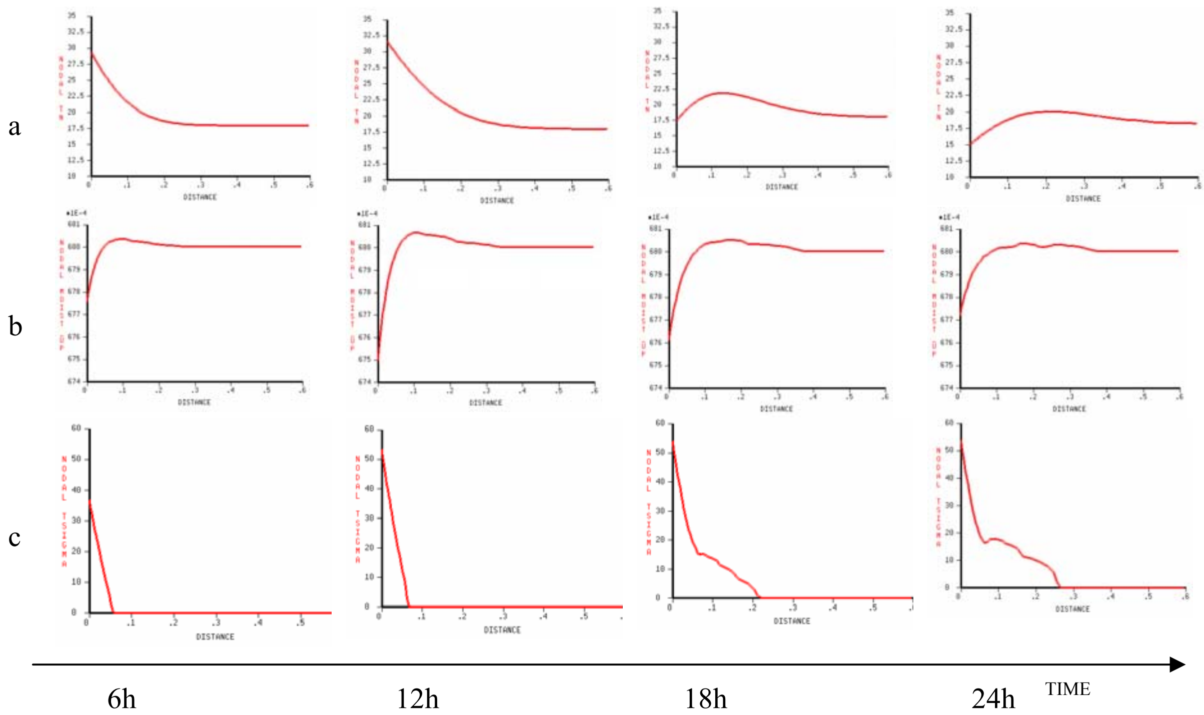


Figure 5: Variation along the simulated strip (bag-air interface at 0 m, bag centre at 0.6 m) of (a) temperature (in ° C), (b) solids moisture content (in %), (c) caking strength (in Pa) at various times during a 24-hour cycle.

The system was assumed initially at equilibrium at 18° C with the solids moisture content being 0.068%. The voidage was taken to be 0.44. Figure 5 depicts the changes along the simulated strip of temperature, solids moisture content and caking strength at various times during a 24-hour cycle where the environmental temperature was first raised to 40° C and then lowered to 10° C. The transition between 40° C and 10° C in the environmental temperature was assumed to occur instantaneously. As can be observed, the variations in temperature caused the moisture to migrate between the bag-material interface and bag centre. Where the moisture was migrating into, liquid/solid bridges were formed around the granular material particles. Where the moisture was migrating out of, this caused the hardening of the created solid bridges, which led to the increase in the caking strength of the material at these areas (see Figure 5c). The repetition of this cyclic process (i.e. further storage for a number of days) will increase the caking strength and will lead to the creation of "hard cake" close to the bag-material interface and the creation of "soft cake" further in, towards the centre. As becomes obvious, the hardest cake will occur in the material adjacent to the bag lining (the region that will experience the steepest gradients in temperature and solids moisture content). These results are in agreement with experimental and theoretical predictions (see e.g. [19]).

4 Conclusions

In this paper, a computational framework was presented for the modelling of granular flows, based on Computational Fluid Dynamics and implemented with micro-mechanical constitutive models for the effective representation of the interactions between particles at the microscopic level. The presented simulations demonstrated the potential capability of the model to realistically represent key granular processes (segregation-degradation-caking), which are of great importance to the process engineering industry. The developed model represented realistically the discharge in core flow mode of material from a flat-bottomed bin, dilute-phase pneumatic conveying of the material downstream of the bin and, after conveying, its storage in a bag for 24 hours. The associated problems that may occur during this process (namely, segregation, degradation, caking) were described realistically by the model and good agreement was found for the trends of segregation-degradation-caking between the numerical model and theoretical / experimental observations. It is believed that this description of a full granular process under a continuum mechanics framework with the aid of micro-mechanical / experimental parametrisations is unique in its kind. The completed numerical model will constitute a powerful computational tool for engineers, which will aid them in the characterisation of granular materials and processes that these are involved in.

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