Micro-Mechanical Parameterisations for Continuum Modelling of Granular Material Using the Discrete Element Method

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Abstract

The present work uses the discrete element method (DEM) to describe assemblies of particulate bulk materials. Working numerical descriptions of entire processes using this scheme are infeasible because of the very large number of elements $(10^{12} \text{ or more in a moderately sized industrial silo})$. However it is possible to capture much of the essential bulk mechanics through selective DEM on important regions of an assembly, thereafter using the information in continuum numerical descriptions of particulate processes. The continuum numerical model uses population balances of the various components in bulk solid mixtures. It depends on constitutive relationships for the internal transfer, creation and/or destruction of components within the mixture. In this paper we show the means of generating such relationships for two important flow phenomena - segregation whereby particles differing in some important property (often size) separate into discrete phases, and *degradation*, whereby particles break into sub-elements, through impact on each other or shearing. We perform DEM simulations under a range of representative conditions, extracting the important parameters for the relevant transfer, creation and/or destruction of particles in certain classes within the assembly over time. Continuum predictions of segregation and degradation using this scheme are currently being successfully validated against bulk experimental data and are beginning to be used in schemes to improve the design and operation of bulk solids process plant.

1 Introduction

Discrete element methods (DEM) are an increasingly popular research tool for studying the behaviour of particulate solid materials such as grain, sugar or pharmaceutical powders. The term "DEM" encompasses a wide range of numerical techniques for describing discrete systems such as assemblages of particles. However, often (as here) it is associated with a technique which might be termed "granular dynamics". Such a technique is rather like the molecular dynamics approach for the calculation of thermodynamic and transport properties of fluids at the molecular level. The method is based on models for the interactions between individual grains (both elastic and inelastic / frictional interactions) and the effect of external body forces such as gravity. Over small finite time-steps the net resultant forces on each particle is calculated, and the trajectories of all particles over time are subsequently calculated by integrating Newton's second law of motion. Typical models for particle-particle interactions, and techniques for time integration of these equations, have been extensively described elsewhere in the literature [1-3] and will not be repeated here.

DEM is computationally onerous. Both the identification of contacts between contiguous particles and the subsequent calculation of the interaction forces demand a considerable computational overhead. Furthermore, the number of particles in a typical bulk solids handling process is very large (for instance, a moderately sized industrial silo may contain 10^{12} or more particles). It is therefore unrealistic to perform direct DEM simulations of industrial processes at full scale. However, there are a number of possible ways in which DEM can be usefully exploited. Depending on the phenomena and essential bulk mechanics of interest, much useful information can be obtained by simple direct down-scaling. We have done this previously for a study of air-assisted discharge of fine cohesive powders from storage vessels [3] with successful results.

"Granular dynamics" is a particularly useful approach as it allows the extraction of a wealth of information from the computer simulation. The method requires the user to calculate contact forces, velocities and positions. These in themselves can be of considerable interest. In the example mentioned above [3] we were able to learn much about the tendency of fine cohesive powders to form 'cakes' and hence become reluctant to discharge, through careful inspection of the contact force networks within the assembly. Such information is difficult (essentially impossible) to measure experimentally. It is also possible to move well beyond the "bare" data of force, velocity and position. By using standard statistical techniques (for example time series / autocorrelation analysis) one can extract extremely useful information on the behaviour of groups of particles. Such techniques are widely used in the field of molecular dynamics, to further understanding of the static and dynamic structure of molecular fluids.

In this work we employ such techniques to elicit the constitutive behaviour of groups of granular particles under a range of conditions. The basis of the approach is to perform DEM simulations on a suitably limited number of particles (up to several thousand) for several sets of process conditions within the 'envelope' of conditions within the process of interest. By extracting the important data from these simulations and then fitting suitable models to that data, we can make predictions of assembly behaviour within the entire envelope of conditions, by way of a constitutive model. This model is then applied in a continuum framework to provide predictions of bulk material behaviour.

Our focus is two-fold. We are concerned with the prediction of two (often undesirable) phenomena in the storage and handling of particulate bulk solids. *Segregation* occurs when particles differing in some important property (often size) separate into discrete phases, either spontaneously or in response to external conditions such as the bulk flow field. *Degradation* occurs when particles break into subelements, owing to impact with each other or with confining boundaries, or in response to compression or shearing. The ultimate aim of the work is a numerical continuum model of segregation in the discharge of material from mass-flow and core-flow storage bins, and of degradation principally due to the impact of particles on pipe bends in lean-phase pneumatic conveying. This paper shows how DEM is used to parameterise these continuum models.

2 Physical Processes of Segregation and Degradation

Segregation emerges due to three physical processes. By using principles of kinetic theory we derive means of calculating the relevant transport coefficients for each process in DEM simulations. Strain-induced segregation (kinetic sieving) arises due to the preferential motion of coarser particles in the mixture across gradients of bulk velocity, towards regions where the bulk strain-rate is highest. This is the mechanism by which, for example, coarser particles in a mixture will tend to "migrate" towards high strain-rate regions such as free surfaces in a heap of material. Segregation also occurs by apparently "diffusive" processes very similar to classical molecular diffusion down a concentration gradient. This principally affects the finer particles in a multi-component mixture of granular material. Segregation may also occur through (spontaneous) percolation, which is the gravity-driven sifting of fine particles through the interstices in the matrix of coarse. For equal-density mixtures, percolation only becomes a serious issue above a certain threshold of size ratio. For the purposes of this paper we ignore percolation and thereby consider mixtures with a relatively modest particle size ratio.

We have focussed to date on segregation in the storage of granular mixtures in hoppers and bins. As bins are filled, segregation might take place owing to two mechanisms. The coarse particles in the mixture may be "attracted" to the free surfaces of the heap formed in the bin by a kinetic sieving mechanism, since the local strain-rates are highest. If so, they will also tend to roll down the free surfaces towards the edge of the bin. Furthermore, there is the possibility of fine particles percolating through the coarse whilst the material is in a quasi-static state within the bin prior to discharge. On discharge, there will tend to be lateral segregation within the bin. Strain-rate gradients will develop with the coarse particles preferentially migrating to the areas of highest strain. If there is significant development of a "core" in the centre of the bin owing to the vessel geometry, this will serve as an "attractor" for the coarser particles under a kinetic sieving mechanism. This will be compounded by the emergence of a free surface inclined inwards towards the centre, allowing preferential rolling of the coarse particles down this free surface.

3 Continuum Framework for Segregation

The continuum framework employed is PHYSICA, an unstructured-mesh finite-volume computational fluid dynamics (CFD) code for the solution of mass and momentum conservation equations in the computational domain. The basic mass continuity equation may be written as:

$$\partial \mathbf{n} / \partial \mathbf{t} + \nabla \cdot (\mathbf{n} \mathbf{v}) = 0$$
 (1)

where n is the particle concentration (bulk density) and \mathbf{v} the bulk velocity. Taking this general equation and applying it specifically to the *i*'th component of a multi-component mixture yields:

$$\partial \mathbf{n}_{i} / \partial \mathbf{t} + \nabla \cdot \left(\mathbf{n}_{i} \left[\mathbf{v} + \mathbf{v}_{i} \right] \right) = 0$$
⁽²⁾

where n_i is the concentration of i, v the bulk velocity and v_i is a "drift" velocity for species i relative to the bulk of material. Any "segregation propensity" of species *i* in the mixture will give rise to a net "drift" velocity of *i* relative to the bulk. Equation (2) is a simplified form assuming no degradation takes place. In general, the right-hand side of Equation (2) is a "source" or a "sink" term for species *i* in the mixture. A "sink" for *i* is the degradation of particles in species *i* into those in smaller size classes, and the degradation of larger particles, thereby forming particles in species *i*, provides a potential "source". In attempting to model segregation in a continuum framework, our task is to determine the drift velocities as a function of local conditions. We suppose that different mechanisms for segregation can be considered independently of each other and thus their effects can be encompassed in an expression for the drift velocity as:

$$\mathbf{v}_{\mathbf{i}} = \mathbf{v}_{\mathbf{D}\mathbf{i}} + \mathbf{v}_{\mathbf{S}\mathbf{i}} + \mathbf{v}_{\mathbf{P}\mathbf{i}} \tag{3}$$

where the three terms refer to the three mechanisms: diffusion, kinetic sieving and percolation respectively. Substituting this expression into equation (2) and re-casting in terms of segregation fluxes rather than drift velocities gives:

$$\partial \mathbf{n}_{i} / \partial t + \nabla \cdot \left(\mathbf{n}_{i} \mathbf{v} + \mathbf{J}_{Di} + \mathbf{J}_{Si} + \mathbf{J}_{Pi} \right) = 0 \tag{4}$$

The diffusive flux J_{Di} is given as the product of a characteristic diffusion coefficient and a concentration gradient:

$$\mathbf{J}_{\mathrm{D}i} = -\mathbf{D}_{\mathrm{i}} \, \nabla \mathbf{n}_{\mathrm{i}} \tag{5}$$

and similarly for kinetic sieving, except that the gradient is in bulk velocity:

$$\mathbf{J}_{\mathrm{Si}} = \boldsymbol{\eta}_{\mathrm{i}} \, \nabla \big(\ln \mathbf{v} \big) = \big(\boldsymbol{\eta}_{\mathrm{i}} \,/\, \mathbf{v} \big) \ln \mathbf{v} \tag{6}$$

where η_i is a characteristic transport coefficient for the kinetic sieving of species *i*. The procedure for implementing this continuum framework is as follows:

- perform DEM simulations under a selected number of conditions, and calculate the transport coefficients
- fit constitutive models to the calculated data to give a prediction of the transport coefficients over the full range of conditions in the silo
- use the transport coefficient models in the continuum simulation to give a prediction of "segregation propensity" of the granular material at all points in space and in time
- derive an overall prediction of segregation in the material bulk from the continuum simulation.

4 Calculation of Transport Coefficients

4.1 Mapping DEM conditions onto conditions in the continuum framework

The transport coefficients must be calculated for conditions representative of local regions of the continuum domain (i.e., the hopper vessel), and the constitutive models emerging from the calculations must cover the full range of conditions encountered in the vessel. The "conditions" essentially encompass three parameters: the overall solids fraction in the local region, the local mixture composition, and some measure of the "activity" within the region, i.e., local velocity. The method for calculating transport coefficients in DEM is similar to that employed in molecular dynamics. An assemblage of particles (typically several thousand) is placed in a computational domain held under controlled conditions. The domain is a periodic cell - where particles leaving one side of the domain instantly re-enter the domain on the opposite side. The periodic cell is taken to be a statistically representative sample region of a larger domain under the representative conditions. In molecular dynamics, a key state variable for the calculations is the thermodynamic temperature. This gives rise, from the kinetic theory, to a mean "fluctuating velocity" of molecules about the mean bulk velocity which for most molecular dynamics simulations is held at zero. Much work in recent years [4-8] has focussed on the use of a kinetic-theory type approach for granular materials. The concept of "granular temperature" derived from a mean fluctuating velocity of particles about the bulk velocity, has been widely employed.

In the present work we perform DEM simulations in periodic cells over a range of overall solids fractions, mixture compositions and granular temperatures. However, the granular temperature (fluctuating velocity) is not readily measurable for granular materials in the same way as the thermodynamic temperature for molecular fluids. We must relate our DEM conditions to those in the continuum domain in order to implement our transport coefficient models in PHYSICA. To this end we invoke the Savage-Jeffrey parameter, R [7] which is calculated readily from simple material parameters and process conditions, and relates the granular temperature, T and the bulk velocity (actually the bulk strain-rate, $\dot{\gamma}$) in the following way:

$$T = 3 \left(\frac{d\dot{\gamma}}{R} \right)^2 \tag{7}$$

where d is the (average) particle diameter. In the continuum model we calculate the bulk strain-rate for each cell of the domain and also the Savage-Jeffrey parameter. Knowing the composition of the material in the domain, we can compute the local average particle diameter and hence an estimate for the local granular temperature. We can therefore implement transport coefficient models based on the granular temperature.

4.2 Kinetic sieving coefficients from DEM

Shear-induced particle migrations (kinetic sieving) arise in a mixture under shear due to inhomogeneities in the concentration, hence gradients in the shear stress. Analysis of a possible form of the single-species momentum equation [8] lead us to a simplified expression for shear-induced migration velocities of the form of equation (6), the kinetic sieving coefficient being calculated from the integral of the stress autocorrelation function:

$$\eta_{\alpha\beta} = \int_{0}^{\infty} \left\langle J_{\alpha\beta}(0) J_{\alpha\beta}(t) \right\rangle dt$$
(8)

where α and β are different coordinate directions, and $J_{\alpha\beta}$ is hence an off-diagonal (shear) component of the microscopic stress tensor, which is defined by:

$$J_{\alpha\beta} = \sum_{i=1}^{N} m_i v_{i\alpha} v_{i\beta} + \frac{1}{2} \sum_{j=1}^{N} \sum_{i=1}^{N} r_{ij\beta} F_{ij\alpha}$$
⁽⁹⁾

where m_i is the mass of particle *i*, $v_{i\alpha}$ is the α -component of the velocity of particle *i*, $r_{ij\beta}$ is the β component of the vector joining particles i and j, $F_{ij\alpha}$ is the α -component of the interaction force between *i* and *j*, and N is the total number of particles in the system. The stress tensor has two terms (a kinetic part corresponding to the dilute limit, and a configurational part owing to solid-solid interactions). Hence the autocorrelation function has three terms (one corresponding to each part of the stress tensor, and a cross term). If there is more than one component in the system, then the overall stress tensor for the mixture is itself made up of a number of parts. The key in determining the kinetic sieving coefficients for each species is to determine which parts of the overall stress tensor are attributable to the individual species. One part of the stress tensor clearly relates entirely to the particles in species 1 of a binary mixture:

$$J^{1}_{\alpha\beta} = \sum_{i=1}^{N1} m_{i} v_{i\alpha} v_{i\beta} + \frac{1}{2} \sum_{j=1}^{N1} \sum_{i=1}^{N1} r_{ij\beta} F_{ij\alpha}$$
(10)

where N1 is the number of particles in species 1. This part contains the momentum carried by particles in species 1 and the interactions between particles in species 1. Note that the superscript refers to the species. A second part relates entirely to the particles in species 2 (which are labelled from N1+1 to N inclusive, the latter being the total number of particles in the system):

$$J^{2}{}_{\alpha\beta} = \sum_{i=N1+1}^{N} m_{i} v_{i\alpha} v_{i\beta} + \frac{1}{2} \sum_{j=N1+1}^{N} \sum_{i=N1+1}^{N} r_{ij\beta} F_{ij\alpha}$$
(11)

There is also a cross term, which gives the contribution to the overall mixture stress tensor as a result of interactions between particles of different species:

$$J^{12}_{\ \alpha\beta} = \sum_{j=1}^{N1} \sum_{i=N1+1}^{N} r_{ij\beta} F_{ij\alpha}$$
(12)

Note that there is no momentum contribution to the cross term, since only the configurational term depends on interactions between particles in different species. Also note that since there is no "double counting", the factor of $\frac{1}{2}$ present in the potential terms of equations (9-11), which takes into account Newton's third law, does not appear. The overall stress tensor given by (9) is the sum of these three terms:

$$J_{\alpha\beta} = J^{1}_{\alpha\beta} + J^{2}_{\alpha\beta} + J^{12}_{\alpha\beta}$$
(13)

It can be seen that the shear stress autocorrelation function for a mixture (the product of the stress tensor at two different times, averaged over the whole simulation) contains nine terms in all; three "product" terms and six "cross" terms. Our aim was to calculate the contributions to the mixture stress autocorrelation function from each species, and hence to ascribe kinetic sieving coefficients for each species. We calculated the shear stress autocorrelation function term-by-term for a number of conditions, finding the contribution of the six cross terms to be negligible compared to that of the three product terms. We thereafter made the following assumptions regarding the calculation of individual species' contributions within the mixture:

- the cross terms were neglected
- the $J^{1}_{\alpha\beta} J^{1}_{\alpha\beta}$ and $J^{2}_{\alpha\beta} J^{2}_{\alpha\beta}$ products contributed solely to the autocorrelation function for the individual species (1 and 2 respectively)
- the cross product $J^{12}_{\alpha\beta} J^{12}_{\alpha\beta}$ was deemed to contribute to both individual species' autocorrelation functions, according to the mixture composition

It emerged that for all the cases we considered, the kinetic sieving coefficients for the coarse particles in a mixture greatly exceeded those for the fines (by an order of magnitude or more, even for very modest size ratios). We thus made the further simplifying assumption that kinetic sieving was deemed to apply only to the coarser particles in a mixture.

4.3 Diffusion coefficients from DEM and an example constitutive model

The diffusion coefficient for each species of a multi-component system is given by the integral of the velocity autocorrelation function for the particles in that species:

$$\mathbf{D}_{i} = \int_{0}^{\infty} \langle \mathbf{v}_{i}(0) \mathbf{v}_{i}(t) \rangle \, \mathrm{d}t \tag{14}$$

Note that there are no "cross" terms and hence diffusion coefficients for each phase of a multicomponent mixture can be calculated readily. The diffusion coefficient gives the segregation propensity of each phase under the local conditions.

Simulations for a given simple mixture (a binary mixture of spheres with size ratio 2:1) have been performed over a range of solids fractions, mixture compositions and granular temperatures. Results for a number of conditions are given in Figures 1 and 2.



Figure 1: Diffusion coefficients of fines in a binary 2:1 size ratio mixture, 20% coarse

The Figures also show fitted constitutive models for the diffusion coefficients as a function of overall solid fraction, mixture composition and granular temperature. The constitutive model was found to be a reasonable fit to the DEM simulation data over a wide range of conditions.



Figure 2: Diffusion coefficients of fines in a binary 2:1 size ratio mixture, 40% coarse

The constitutive model for the diffusion coefficient of fines took the following form:

$$\mathbf{D} = 6\left(1 + \mathbf{x}\right)\mathbf{T}\phi^{-1.5} \tag{15}$$

where D is the diffusion coefficient (m^2/s), x the proportion of coarse particles in the mixture, T the granular temperature and ϕ the overall solids fraction. The -1.5 power dependence of the diffusion coefficient on the overall solids fraction appears to make physical sense in that the diffusion coefficient is somehow related to the mean free path of the particles in the mixture. Increasing the overall solids fraction will reduce the mean free path and hence the "segregation propensity" of the (fine) material in the mixture. Combining the above with equation (7) gives us the final expression for the diffusion coefficient of the fines in terms of measurable parameters:

$$D = 18 (1 + x) (d\dot{\gamma} / R)^2 \phi^{-1.5}$$
(16)

where the parameters are as defined for equations (7) and (15). Extensive validation studies of the continuum numerical models for segregation based on the transport coefficient calculations presented in this study have been performed, and the results are presented in the literature [9].

5 Conclusions

This paper outlines the framework for parameterising continuum numerical simulations of segregation and degradation processes by using the discrete element method. It is demonstrated how DEM simulations fit into an overall research strategy which is complemented by selective experimentation and continuum numerical modelling. Specifically, the link between discrete and continuum methods is made explicit. The results of the continuum modelling studies are very encouraging - extensive validation against experimental data has been completed. This suggests that the strategy for parameterising such simulations using DEM is sound, and the DEM simulations give rise to very useful results. Ongoing work is concentrating on a number of areas - widening the "envelope" of conditions for which constitutive models for segregation (kinetic sieving and diffusion) can be applied, and investigating the effect of particle properties (notably those of particle shape). It is likely that the final forms of the constitutive models will be considerably more complicated than is suggested by the above once the effects of additional parameters are taken into account. However, ongoing sensitivity studies are aiming to eliminate as many parameters as possible from the equation set, if it emerges that bulk constitutive behaviour is not especially sensitive to those parameters. Full parameterisation of existing constitutive models for degradation is also ongoing. The envisaged outcome is a useful tool for engineers, whereby through selective limited experimentation and simulation using DEM to characterise particles and processes, they can gain useful predictive information on the phenomena of segregation and degradation for the smart design and efficient operation of bulk solids process plant.

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