Third International Conference on CFD in the Minerals and Process Industries
CSIRO, Melbourne, Australia
10-12 December 2003

DISCRETE PARTICLE SIMULATION OF GRANULAR FLOW

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(EXTENDED ABSTRACT)

Granular materials, which can be either wet or dry and range from nanometers to centimetres in size, are widely encountered in industries and in nature. As with solids, they can withstand deformation and form heaps; as with liquids, they can flow; as with gases, they exhibit compressibility. These features give rise to another state of matter that is poorly understood (Ennis *et al.,* 1994; Jaeger, *et al*., 1996; de Gennes, 1999). This can be highlighted from the study of granular flow which, corresponding to the fluid- and solid-like modes, has different flow regimes such as quasi-static regime, rapid flow regime and a transitional regime that lies in between. Development of a general theory to describe granular flow has been a challenging problem in the scientific community for years (see, for example, Edwards and Grinev, 2001; Kishino, 2001).

Essentially, the existing approaches to granular flow can be classified into two categories: the continuum approach at a macroscopic level and the discrete approach at a microscopic level. In the continuum approach, the macroscopic behavior of granular flow is described by the balance equations facilitated with constitutive relations and boundary conditions. The most difficult problem in implementing this approach lies in the determination of suitable constitutive relations. In the past, different theories have been devised for different materials and for different flow regimes. For example, models have been proposed to derive the constitutive equations for the rate-independent deformation of granular materials based on either the plasticity theory or the double shearing theory (see, for example, Spencer, 1964; Oda and Iwashita, 1999; Spencer and Hill, 2001); rapid flow of granular materials has been described by extending the kinetic theory of dense gases (see, for example, Lun *et al*., 1984; Campbell, 1990; Savage, 1998); the transitional regime that involves both collisional and frictional mechanisms is studied by use of the kinetic theory combined with the Mohr-Coulomb quasi-static theory (Johnson and Jackson, 1987). However, to date, there is no accepted continuum theory applicable to all flow conditions. As a result, in engineering application, phenomenological assumptions have to be made to obtain the constitutive relations and boundary conditions which have very limited application (see, for example, Zhang *et al.*, 1998; Feise and Daiβ, 2001).

The discrete approach is based on the analysis of the motion of individual particles and has the advantage that there is no need for global assumptions on the solids such as steady-state behavior, uniform constituency, and/or constitutive relations. A major type of discrete approach is based on the so-called Discrete Element Method (DEM) originally developed by Cundall (1971) for rock mechanics or its extended version applied to granular materials (Cundall and Strack, 1979). The method considers a finite number of discrete particles interacting by means of contact and non-contact forces, and every particle in a considered system is described by Newton's equations of motion related to translational and rotational motions. DEM-based simulation has been recognized as an effective method to study the fundamentals of granular materials (see, for example, Thornton, 2000; Kishino, 2001; Yu, 2003). However, it is difficult to adapt this approach to process modelling because of the limited particle numbers that can be handled with the present computing capacity. Therefore, it is very useful to develop an average theory to link the continuum approach to the discrete approach so that the constitutive relations and boundary conditions can be derived from DEM results to support the continuum-based process modelling.

This presentation will discuss the above issues via illustrative case studies of a few typical particulate systems: solid flow in grinding/granulation operations, gas-solid flow in fluidisation, and solid flow in hopper.

Case study I - Drum dynamics: Rotating drums are widely used in engineering processes for various purposes such as mixing, drying, milling, coating and agglomeration. A comprehensive understanding of the flow of particles in a drum under different conditions or drum dynamics as a whole is essential in order to optimize such processes. The flow of particles in a horizontal rotating drum has been studied based on the results generated by DEM (Yang *et al*., 2003). Simulation conditions are similar to those used in the experimental study of Parker *et al*. which involves the use of the so-called Positron Emission Particle Tracking (PEPT) (Parker *et al*., 1997). The simulation method is validated from its good agreement with the PEPT measurement in terms of the dynamic angle of repose and spatial velocity fields. The dependence of flow behaviour on rotation speed is then analysed based on the DEM results. This has led to the establishment of the spatial and statistical distributions of microdynamic variables related to flow structure such as porosity and coordination number, and force structure such as particle interaction forces, relative collision velocity and collision frequency. The results, which are not possible to obtain with the current experimental techniques, are found to be useful to understand the effect of rotation speed on agglomeration. The recent development in simulating the flow of particles under Isamill conditions is also discussed.

Case study II - Gas fluidisation: It has been reported that an expanded bed exists for particles of sufficiently small size and low density, when gas velocity exceeds that required for minimum fluidization (Davies and Richardson, 1966). Such a bed becomes unstable at a so-called minimum bubbling velocity above which characteristic bubbles appear in the bed and fluidization results. In his well-known classification of powders, Geldart (1973) refers to this type of particles as aeratable or type A powder based on particle size and density difference between particle and fluidizing gas. This classification is purely phenomenological and leaves the fundamentals underpinning the bed expansion and stability unanswered. Understanding these fundamentals has not only practical importance in process design and operation but also has scientific significance in elucidating the transition of a granular system from solid-like to fluid-like behavior under various forces. The key issue is to identify the role of these forces in bed expansion and stability of gas fluidization.

Recently, we have conducted a microdynamic analysis of bed expansion and stability of gas fluidization using a combined continuum and discrete model in which the motion of discrete particles is obtained by solving Newton's equations of motion and the flow of continuum gas by the Navier-Stokes equations (Xu and Yu, 1997 & 2001; Yu and Xu, 2003). The existence of an expanded bed between the minimum fluidization velocity and minimum bubbling velocity, unique to this type of powder, is predicted from this first principle approach. The results show that the presence of macropores of different size and orientation is the main feature of such a bed. It is the formation of macropores that results in bed expansion and the collapse of macropores that initiates fluidization. Numerical experiments are carried out to clarify the long-standing dispute about the role of interparticle forces. It is found that while the fluid drag force balances the weight of particles, both the van der Waals and frictional forces are critical to forming and stabilizing an expanded bed where the two forces balances each other not only at a bulk solid scale but also at an individual particle scale. On this basis, a phase diagram is developed to describe the transition between fixed, expanded and fluidized beds under gas flow in terms of the particle-particle and particle-fluid interactions.

Case study III - Hopper flow: In the past, extensive research has been carried out to develop an averaging theory to link the microscopic variables in the discrete approach to the macroscopic variables in the continuum approach, including, for example, the efforts of Drescher and de Josselin de Jong (1972), Kanatani (1981), Walton and Braun (1986), Campbell (1993), Babic (1997), and Lätzel *et al.* (2001). We have recently developed an averaging method to link discrete to continuum variables of granular materials (Zhu and Yu, 2001 & 2002). Compared to the other methods proposed in the literature, it has advantages of being applicable to all flow regimes, and to granular flows with or without the effect of physical boundaries. Its application is here demonstrated in the determination of the macroscopic properties such as mass density, velocity, stress and couple stress distributions of a hopper flow, where the discrete results are generated by means of DEM simulation. It clearly demonstrates that discrete and continuum approaches are related and the constitutive relations and boundary conditions can be derived from DEM results to support the continuum-based process modelling.

ACKNOWLEDGMENT

The author is grateful to the ARC, BHP Steel and UNSW for the financial support of the work, and the contribution of Drs. Yang, Zou, Xu and Zhu to the case studies used.

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