COMPUTER MODELLING AND SIMULATION APPLIED TO PARTICULATE AND MINERAL PROCESSING

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Abstract

Computer modeling and simulation have been extensively used to study the fundamentals of particulate and mineral processing in recent years, mainly as a result of the rapid development of simulation techniques and computer technology. This paper briefly reviews such research in the laboratory of Particulate and Multiphase Processing (PMP) at UNSW, which covers the development of computational techniques and their application to the study of various phenomena and operations related to particle packing, particle and particle-fluid flow. Focus is given to the discrete particle simulation which has been recognized as a promising technique to generate information at a particle scale. The validity and usefulness of this approach are discussed with reference to the examples relevant to operations in alumina/aluminium industry.

1 Introduction

Particulate science and technology is a rapidly developing interdisciplinary research field concerned with particle-related phenomena of different time and length scales. It is a core competency of paramount importance to many sectors of our modern economy. For example, it has been reported that an estimated minimum of 40%, or US$61 billion, of the value added by the chemical processing industry per annum is linked to particulate research in the USA (Ennis et al., 1994); it is directly related to many modern applications including pharmaceuticals and advanced material manufacturing (Davies, 2000; Muzzio et al., 2002). Particulate processing can be found in many operations in alumina and/or aluminium production, including, for example, alumina calciners, hydrate filters, pipe wear in slurry transport and so on. Understanding and modeling the packing, flow and other processing properties under different conditions in relation to various industrial processes are very helpful for property and/or process control.

Particulate materials have properties that are characteristic of each of the three primary phases, being able to withstand deformation like solids, flow like a liquid and exhibit compressibility like a gas under certain circumferences. Corresponding to the fluid- and solid-like modes, they show different flow regimes: quasi-static regime, rapid flow regime and a transitional regime that lies in between. These features give rise to another state of matter – particulate/granular matter – that is poorly understood (see, for example, Merrow, 1985; Mehta, 1993; Jaeger et al., 1996). Development of a general theory to describe the packing (statics) and flow (dynamics) of this matter has been a problem challenging the scientific community for years (see, for example, de Gennes, 1999).

The macroscopic behaviour of particulate matter is controlled by the interactions between individual particles as well as interactions with surrounding fluid and wall. Understanding the microscopic mechanisms in terms of these interaction forces is therefore key to leading to truly interdisciplinary research into particulate matter and producing results that can be generally used. This aim can be effectively achieved via particle scale study based on detailed microdynamic information such as the forces acting on and trajectories of individual particles in a considered system. It is extremely difficult to obtain microscopic, particle scale information experimentally, even with the use of newly developed advanced and expensive measuring techniques. For example, nuclear magnetic resonance (NMR) can largely measure the structure of static packing (Gladden, 2003), position emission particle tracking (PEPT) the trajectories of a few selected particles in a considered system (Parker et al. 1993), other new techniques the force structure of particles at the external surface or boundary of a particle assembly (Liu et al., 1995). However, this difficulty can be overcome by computer simulation and modelling. In recent years, such research has been rapidly developed worldwide, mainly as a result of the rapid development of discrete particle simulation technique and computer technology.

This paper presents a brief review of the work in this area in the laboratory of Particulate and Multiphase Processing (PMP) at UNSW in the past years. Various modeling and simulation techniques have been used there corresponding to different time and length scales. However, instead of discussing the traditional techniques which are often at larger scales and relatively well established, this review will be focused on the particle scale modeling and simulation. It covers the development of the simulation techniques and their application to the study of particle packing and flow, with emphasis given to the validity analysis of the simulation method developed and the usefulness of the resulting particle scale information.

2 Computational methods

The existing approaches to modelling particulate matter can be generally 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 behaviour is described by balance equations, e.g., mass and momentum as used in the Two Fluid Model (TFM), closed with constitutive relations together with initial and boundary conditions (see, for example, Gidaspow, 1994). This approach, similar to the conventional Computational Fluid Dynamics (CFD), is preferred in process modelling and applied research because of its computational convenience. However, its effective use depends heavily on constitutive or closure relations and the momentum exchange between particles of different type. 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 behaviour, uniform constituency, and/or constitutive relations. Various methods have been developed in the past. A major type of discrete approach is based on the so-called Discrete Element Method (DEM) originally developed for rock mechanics (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. In principle, it is similar to molecular dynamic simulation (MDS) but the forces involved differ because of the difference in time and length scales.

Much of our work is developed on the basis of DEM. Thus, a particle in a considered system can have two types of motion: translational and rotational, determined by Newton's second law of motion. During its movement, the particle may collide with its neighbour particles or wall at the contact points and interact with the surrounding fluid, through which the momentum and energy are exchanged. The forces acting on a particle result from particle-particle and particle-fluid interactions. For particles, these interactions include the forces due to direct or non-direct contacts between particles. The direct contact forces include the contact force, viscous contact damping force and solid bonding forces. The non-direct contact forces include the forces associated with fine particles such as the van der Waals force, electrostatic force, with wet particles such as the capillary and viscous forces. Particle-fluid interactions include buoyancy, drag force, and so on. To date, the equations to determine some of the forces and torques are not fully developed. However, this does not significantly affect the use of this approach for particle scale studies for many particulate systems, particularly when only coarse, cohesionless particles are involved. The equations used in our work can be found in the literature (Xu and Yu, 1997; Zhou et al., 1999; Xu et al., 2000; Yang et al., 2000; Zhu and Yu, 2004).

Particle flow is often coupled with fluid (gas and/or liquid) flow. Various approaches have been proposed to simulate such a coupled particle-fluid flow. The time and length scales for modelling fluid flow can range from discrete (MDS, Lattice Boltzman (LB), Pseudo-particle (PP)) to continuum (Direct Numerical Simulation (DNS), Large Eddy Simulation (LES), and other conventional techniques such as the TFM) (Helland et al., 2000; Koch and Hill, 2001; Pan et al., 2002; Ge and Li, 2003). Relative to particle phase, they can also be categorized into three groups: sub-particle, pseudo-particle and computational cell. Table 1 lists a few representative combinations of different length scales for fluid and particle phases and their relative merits in different aspects.

The smaller the length scale for fluid phase, the more detailed information about the particle-fluid interaction forces. For example, the LB-DEM or DNS approach can in principle generate accurate results about the particle-fluid interaction forces to replace the empirical ones in the current combined continuum and discrete model. However, at this stage of development, the difficulty in particle-fluid flow modelling is mainly related to solid phase rather than fluid phase. For solid phase, there are only two approaches: continuum and discrete, as described above; and it is not clear if there is a need to develop approaches of different time and length scales like those for gas or liquid phase. Therefore, the so-called combined continuum and discrete model (CCDM) or CFD-DEM is attractive because of its computational convenience as compared to DNS or LB-DEM and capability to capture the particle physics as compared to TFM (Yu and Xu, 2003). In CCDM, the continuum fluid field is calculated from the continuity and the Navier-Stokes equations based on the local mean variables over a computational cell (Xu and Yu, 1997; Xu et al., 2000).

Note that the modelling of the solid flow by DEM is at the individual particle level, whilst the gas flow by CFD is at the computational cell level. Their coupling is numerically achieved as follows. At each time step, DEM will give information, such as the positions and velocities of individual particles, for the evaluation of porosity and volumetric fluid drag force in a computational cell. CFD will then use these data to determine the gas flow field which then yields the fluid drag forces acting on individual particles. Incorporating the resulting forces into DEM will produce information about the motion of individual particles for the next time step. The fluid drag force acting on individual particles will react on the fluid phase from the particles, so that Newton's third law of motion is satisfied. Such coupling has been widely accepted, although caution should be given in order to produce consistent results (Feng and Yu, 2004).

3 Particle packing

Particle packing can be found in many industries, the material and mineral industries in particular. For example, the densification of a powder mass is important in the shaping of solids in ceramics, powder metallurgy or composite synthesis; proper description of particle packings at either microscopic or macroscopic level is also fundamental to many mineral processes such as solid-liquid separation (sedimentation, thickening and filtration), raw material handling (stockpiling, blending, drying, storage and transportation), and primary extractive processes (agglomeration, coke making, ore sintering, blast furnace ironmaking and new ironmaking processes). Therefore, it has been identified as one of the few core research areas in particulate science and technology, even in the classical description by Dallavalle (1943). There are two fundamental concerns here: (i) an assessment of the variables which govern the packing of particles at a macroscopic level, and subsequently, the development of methods for its control; and (ii) an examination of the structure of a packing of particles with particular reference to the pore and/or particle connectivity. In connection with our macroscopic modelling (Yu and Zou, 1998), DEM has been used to simulate the packing of particles under various conditions, in order to generate microscopic information for structural analysis. Representative work includes the packing of cohesionless (Liu et al., 1999; Zhang et al., 2001) or cohesive (fine or wet) particles (Yang et al., 2000, 2003a, 2003b), the formation of sandpiles (Zhou et al., 1999, 2002) and the settling of particles in liquids related to sedimentation and filtration (Dong et al., 2003).

These studies clearly show that forming a packing is a dynamic process involving various interparticle forces in addition to the gravity

Table 1 Typical models for particle-fluid flow and their relative merits

Model type	Length scale for fluid phase	sub-particle (discrete or continuum)	pseudo-particle (discrete)	computational cell (continuum)	computational cell (continuum)
	Length scale for particle phase	particle (discrete)	particle (discrete)	particle (discrete)	computational cell (continuum)
	Nature of coupling	continuum + discrete or discrete + discrete	discrete + discrete	continuum + discrete	continuum + continuum
	Example	LB-DEM or DNS	PP-DEM	CCDM or CFD-DEM	TFM
Closure of equations		Yes (but may experience numerical difficulty for systems with strong particle-particle interactions)	No (difficulty to determine physical properties of a pseudo-particle)	Yes	No (constitutive relation for solid phase and phase interactions not generally available)
Incorporation of distribution effects of dispersed, solid phase		Yes	Yes	Yes	No
Computational effort		Extremely demanding	Very demanding	Demanding	Acceptable
Suitability for engineering application in relation to process modelling and control		Extremely difficult	Very difficult	Difficult	Easy
Suitability for fundamental research in relation to fluid physics		Most acceptable (can be used to determine particle-fluid interaction for CCDM)	Acceptable (but only valid for well defined PP system)	acceptable	No

force, for example, the van der Waals force for fine particles and the capillary force for wet particles. A successful simulation method must take into account all dynamic factors related to both geometry and force. Most of the previous methods only consider the former and ignore the latter, and hence fail to generate realistic packing structure, particularly when forces rather than the gravity are dominant. The results presented in the above papers clearly confirm that DEM can overcome this problem. This is evident from the following facts representing different aspects:

- The relationship between porosity and particle size can be reproduced, confirming macroscopically the validity of DEM and the important role of the van der Waals force in governing the behaviour of fine spheres ranging from 1 to 100 μm (Yang et al., 2000).
- The split second peak in the radial distribution function for monosized coarse spheres can be simulated by the DEM (Liu et al., 1999; Yang et al., 2000) and the simulated coordination number distributions for particle mixtures are quantitatively comparable with those measured, confirming the validity of the DEM approach from the viewpoint of microstructure (Pinson et al., 1998; Zou et al., 2003).
- There is a good agreement between the simulated and measured distributions of normal contact forces between particles for a packing formed under the gravity, confirming the capability of the DEM in generating quantitative force information which, like the coordination number, is difficult to obtain with the current experimental technique (Yu, 2004).
- With the incorporation of a rolling model, DEM can naturally simulate the formation of a sandpile, as evident from the good agreement between the simulated and measured results in forming sandpiles (Zhou et al., 1999, 2002).

The validated DEM model offers a convenient way to carry out controlled numerical experiments to study the packing of particles under various conditions. For example, it has been used to quantify the effects of dynamic variables such as deposition intensity and dropping height, material properties such as the sliding and rolling friction coefficients related to the surface forces, the Hamaker constant and the particle density related to the body forces acting on a particle (Zhang et al., 2001; Yang et al., 2003a). Similar work has been carried out on the formation of sandpiles where focus is on the dependence of the angle of repose and bottom stress distribution on key variables related to particle characteristics and material properties, in addition to the method of formation (Zhou et al., 2002). Importantly, the particle scale results produced by means of DEM can significantly enhance the structural analysis and modelling of the packing of particles, help quantify the governing mechanisms and generate reliable predictive methods for engineering application. This can be seen from the following examples:

- They have been used in the quantification of the packing structure of fine particles and in the establishment of the link between macroscopic and microscopic properties, for example, the correlations between porosity, radial distribution function, coordination number, and interparticle forces (Yang et al., 2000, 2002). The relationship between porosity and interparticle force, as an equation of state, can be generalised in terms of cohesive force relative to effective gravity force, although further work is necessary to understand its dependence on variables related to surface forces (Yu et al., 2003; Yang et al., 2003a, 2003b; Dong et al., 2003).
- They can be directly used to study the structural properties of porous media, including, for example, permeability related to pore-to-pore connectivity and effective thermal conductivity related to particle-to-particle connectivity. In fact, based on such structural information and simple analytical formulation for heat transfer, the effective thermal conductivity of a packed bed and the underlying heat transfer mechanisms can be quantified (Cheng et al., 1999; 2002), which should be useful to the development of a reliable predictive mathematical model.
- They have been used to study the three-dimensional packing structure and force network of a sandpile in relation to a range of variables related to particle characteristics, material properties and method of formation (Zhou et al., 2002). The resulting information could be useful to understand the origin of the stress dip which is considered as a key characteristic of particulate matter (see, for example, de Gennes, 1999).

In line with the microscopic simulation described above, macroscopic models have been developed to predict porosity and other packing properties as a function of particle size and shape distributions under different conditions (Yu and Standish, 1988, 1991; Yu et al., 1996, 1997). Such modelling has been successfully applied to alumina properties such as bulk density and flowability (Zou et al., 2004). It has also been applied to fine Bayer mud slurries to understand the differences in rheological behaviour of such muds from different bauxites (Roach et al., 2001). This development enables improved predictions related to solids density to be made based on the physical properties and particle size distribution of the muds.

4 Particle and particle-fluid flow

Particle flow, coupled with fluid (gas and/or liquid) flow, is a very common feature in almost all types of particulate processes. Understanding the fundamentals governing the flow and formulating suitable governing equations and constitutive relationships are of paramount importance to the development of better strategies for process control. The phenomena dealt with often happen simultaneously at different length and time scales, which necessitates a multiscale approach as recognised for years (see, for example, Villermaux, 1996). Previous studies are largely at a macroscopic or global scale, the resulting information being helpful in developing a broad understanding and design of a process of particular interest. However, the lack of quantitative fundamental understanding makes it difficult to generate a general method for reliable scale-up, design and control/optimisation of processes of different types. The bulk behaviour of a particle system depends on the collective interactions of individual particles, and hence research on a particle scale has been recognised as a promising approach to overcome this difficulty. In other words, particle scale modelling should be key to a successful multi-scale approach to a particulate process. With this realisation, DEM and CCDM have been developed and extensively used at UNSW to study dynamic particulate systems on the particle scale under various conditions, including particle flow in bladed mixers (Stewart et al., 2001, Zhou et al., 2003, 2004), in granulation or grinding mills (Yang et al., 2003c, 2004) and in hoppers (Zhu and Yu, 2002, 2004, 2005), gas fluidisation of cohesionless (Xu and Yu, 1997; Feng et al., 2004; Feng and Yu, 2004) and cohesive (Xu et al., 1999; Yu and Xu, 2003) particles, and particle-fluid flow in blast furnace (Xu et al., 2000; Nouchi et al., 2003; Feng et al., 2003; Zhou and Pinson et al., 2003).

In these studies, extensive comparison between physical and numerical experiments has been made at various time and length scales in order to validate the proposed DEM or CCDM. Representative examples include

- There is a good agreement between the simulated and measured flow fields of particles under comparable experimental conditions, this including the flow of particles in a rotating drum (Yang et al., 2003c) and bladed mixer (Stewart et al., 2001). Notably, the experimental results are obtained by means of PEPT that is non-invasive and also at a particle scale.
- Coupled with CFD for the flow of continuum fluid, DEM can also reliably simulate the particle-fluid two-phase flow as, for example, for gas-solid flow under raceway conditions obtained by Xu et al. (2001). Such good agreements can also be observed for size segregation in gas fluidisation (Feng et al., 2004; Feng and Yu, 2004) and liquid-solid flow simulating the conditions relevant to blast furnace hearth (Nouchi et al., 2003).

The dynamics of particle flow includes at least three aspects: velocity, structure and force. Previous studies have to be largely limited to velocity field because of the difficulty in obtaining information for the other two. Consequently, there have been problems in probing the underlying mechanics and solving practical problems reliably. Our above studies show that DEM or CCDM simulation is an effective technique that can overcome this problem, although like many techniques for physical or numerical experimentation, it may not be perfect at this stage of development. Microdynamic analysis can lead to a better understanding of the underpinning physics of particle flow. The capability and usefulness of such particle scale study can be highlighted by:

- the successful simulation of complicated phenomena associated with the transition between fluid-like and solid-like behaviors in raceway formation and bed expansion in gas-solid flow, leading to a better understanding of the roles of various particle-particle and particle-fluid interaction forces (Xu et al., 2000; Yu and Xu, 2003)
- the establishment of a comprehensive picture about particle flow and segregation in bladed mixer (Zhou et al., 2004), rotating drum (Yang et al., 2003c), gas fluidisation (Feng et al., 2004), and hopper (Zhu and Yu, 2004), achieved by detailed analysis of the spatial and statistical distributions of microdynamic variables related to flow and force structures.
- the determination of the macroscopic variables used in the continuum approach from the microscopic variables in the discrete approach by a proper local average method, which is an important step to make use of the particle scale results in the continuum-based modelling in terms of constitutive relations and boundary conditions, and is helpful to the development of a general continuum theory to describe granular flow (Zhu and Yu, 2002, 2005).

Finally, we would like to point out that discrete particle simulation is computationally very demanding, and its application thus far is largely limited to phenomenon rather than process simulation. However, with the rapid development of computer technology, more and more efforts have been made to apply this technique to process simulation. In fact, DEM or CCDM has been directly used in our modelling of a number of industrial processes although such work is not covered in this review. On the other hand, for particulate systems which require continuum-based process models and are relatively well defined by such governing equations and constitutive relations, conventional CFD models can be used. This approach has also been used in our work, for example, in the modelling of the gas-powder-liquid-solid four-fluid flow in a blast furnace (Wang et al., 1997, 2000; Zhang et al., 1998; Dong et al., 2004), gas fluidisation (Zhang and Yu, 2002) and particle-fluid flow in cyclones (Wang et al., 2004, 2005).

5 Concluding remarks

The bulk behaviour of particulate materials depends on the collective interactions among individual particles. Particle scale modelling and analysis is therefore key to elucidating the underlying physics and linking fundamental to applied research, particularly in developing from know-how to know-why knowledge. Our work clearly demonstrates that discrete particle simulation, although not perfect at this stage of development, does capture the main features and is an effective way to achieve this goal. With the rapid development of the computer technology, it offers a cost-effective way to meet the challenge of understanding the ever-changing particle science and technology resulting from the continuing development of new processes and products. It should be useful to the alumina/aluminium industry where particulates can be widely found and processed.

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