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Review

Discrete particle simulation of particulate systems: A review of major applications and findings

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ABSTRACT

Understanding and modelling the dynamic behaviour of particulate systems has been a major research focus worldwide for many years. Discrete particle simulation plays an important role in this area. This technique can provide dynamic information, such as the trajectories of and transient forces acting on individual particles, which is difficult to obtain by the conventional experimental techniques. Consequently, it has been increasingly used by various investigators for different particulate processes. In spite of the large bulk volume, little effort has been made to comprehensively review and summarize the progress made in the past. To overcome this gap, we have recently completed a review of the major work in this area in two separate parts. The first part has been published [Zhu, H.P., Zhou, Z.Y., Yang, R.Y., Yu, A.B., 2007. Discrete particle simulation of particulate systems: theoretical developments. Chemical Engineering Science 62, 3378–3392.], which reviews the major theoretical developments. This paper is the second one, aiming to provide a summary of the studies based on discrete particle simulation in the past two decades or so. The studies are categorized into three subject areas: particle packing, particle flow, and particle–fluid flow. The major findings are discussed, with emphasis on the microdynamics including packing/flow structure and particle–particle, particle–fluid and particle–wall interaction forces. It is concluded that discrete particle simulation is an effective method for particle scale research of particulate matter. The needs for future research are also discussed.

Contents

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1. Introduction

Particulate systems are quite common in nature and in industry. Their dynamic behaviour is very complicated due to the complex interactions between individual particles and their interactions with surrounding gas or liquid and wall. Understanding the underlying mechanisms in terms of these interactions is a key to producing results that can be generally used. This aim can be effectively achieved via particle scale research

In recent years, such research has been rapidly developing worldwide, mainly as a result of the rapid development of discrete particle simulation technique and computer technology. An important discrete model is the so-called discrete element method (DEM) originally developed by 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, which can move translationally and rotationally, is described by Newton's equations of motion. DEM simulations can provide dynamic information, such as the trajectories of and transient forces acting on individual particles, which is extremely difficult, if not impossible, to obtain by physical experimentation at this stage of development. Also, DEM has been coupled with computational fluid dynamics (CFD) to describe particle–fluid flows (Tsuji et al., 1993; Xu and Yu, 1997) which makes the study of many particulate systems in process engineering possible. Indeed, DEM-based simulation and modelling have increasingly been used in particulate research in the past two decades or so. However, the resulting information is seemingly scrappy, and the subject is lacking coherence.

To overcome this gap, we have recently completed a review of the major work in this area. It includes two parts: theoretical treatments and applications. The first part has been published (Zhu et al., 2007), which mainly considered three aspects: models for the particle–particle and particle–fluid interactions, coupling of DEM with CFD to describe particle–fluid flow, and the theories for linking discrete to continuum modelling. This article, as the second part, focuses on the applications of DEM and DEM-CFD reported in the literature, which are for convenience grouped into three areas: particle packing, particle flow and particle–fluid flow. The major findings are discussed, with emphasis on the microdynamics including packing/flow structure and particle–particle, particle–fluid and particle–wall interaction forces. An effort has been made to collect as many as possible publications in the SCI (Science Citation Index) journals and to be updated; but it is not going to be a complete literature survey because of the diversity of the applications and publications. Therefore, to be illustrative, the discussion will be focused on the most popular applications and representative studies. Its aim is to demonstrate that DEM-based simulation is an effective method for particle scale research of particulate systems and highlight some major achievements which may have impacts on the work in the future.

2. Particle packing

A packed bed is probably the simplest state for particles as all particles involved are static and in their stable positions, yet it has widely been serving as a model system to understand the structures of liquids (Bernal and Mason, 1960; Bernal, 1964; Finney, 1970a,b) and amorphous materials (Finney, 1977), and to study glassy transition (Gordon et al., 1976; Woodcock, 1976; Boudreaux and Gregor, 1977; O'Hern et al., 2001) and colloidal systems (Pusey and van Megen, 1986). Proper description of particle packing is also fundamental to many industrial processes ranging from raw material preparation to advanced material manufacturing in many industries (German, 1989). As such, extensive research has been carried out and a variety of methods have been developed to quantitatively characterize the structure of a packing (Bideau and Hansen, 1993; Mehta, 1994). The results have been directly used in the quantification of engineering properties related to particle connectivity, e.g., effective thermal conductivity (Argento and Bouvard, 1996; Cheng et al., 1999; Vargas and McCarthy, 2001, 2002a,b), or pore connectivity, e.g., permeability (Bryant et al., 1993, 1996; Thompson and Fogler, 1997; Abichou et al., 2004).

Early studies mainly focused on laboratory experiments (Scott, 1962; Finney, 1970b; Bideau and Hansen, 1993). For the packing of monosized spheres, structural properties such as coordination number (CN) and radial distribution function (RDF) have been well established for general application. However, experimental extraction of structural information is laborious and involves relatively large errors and uncertainties. To overcome this difficulty, various numerical algorithms have been developed to simulate particle packing. Most of them are Monte Carlo algorithms and based on either sequential addition or collective rearrangement. As these algorithms usually involve various assumptions about particle motion and/or stability criteria which do not always represent the reality truly, the resulting structural information may not be comparable with that measured, as pointed by Yu and his colleagues (Liu et al., 1999; Yang et al., 2000; Zhang et al., 2001; Yu et al., 2003).

Forming a packing is a dynamic process which involves various forces, and an ideal simulation method should take into account all dynamic factors related to either geometry or force. From this perspective, DEM is inherently superior to the early Monte Carlo algorithms. In the past decade or so, DEM has been increasingly used to study the packing of particles under various conditions as summarized below.

2.1. Packing of cohesionless particles

A packing can be formed in different ways related to different operations in practice. DEM simulations can be performed accordingly. Indeed, various packing methods have been used in the previous DEM studies, including, e.g. pouring or depositing particles under gravity (Yen and Chaki, 1992; Zhang et al., 2001; Latham et al., 2001; Silbert et al., 2002a,b; Bertrand et al., 2004; Latham and Munjiza, 2004; Munjiza and Latham, 2004; An et al., 2005), centripetal growth (Liu et al., 1999; Liu and Yuan, 2000), compression (Liu, 2003; Luding, 2004; Zhang and Makse, 2005; Alonso-Marroquin et al., 2005) and vibration after deposition (An et al., 2005; Yu et al., 2006). Formation of a pile, i.e., sandpiling process, is also a type of packing under unconfined geometry and has also been studied extensively in simulation (Lee and Herrmann, 1993; Luding, 1997; Baxter et al., 1997; Zhou et al., 1999, 2001, 2002, 2003b; Matuttis et al., 2000; Liffman et al., 2001; Smith et al., 2001; Smith and Tuzun, 2002a; Tuzun et al., 2004; Fazekas et al., 2005; Li et al., 2005a).

To validate simulations, extensive comparison between simulated and measured results under different conditions has been made, with reference to different aspects including macroscopic properties, microscopic structure, and force network, as discussed below.

Macroscopic properties: Packing density or porosity (1-packing density) is the simplest and most accessible macroscopic parameter for characterizing a packing. Packing densities from DEM simulations are quantitatively comparable with those measured under different conditions. For example, depending on packing methods and particle properties, packing density from DEM simulations ranges from 0.55 (Yen and Chaki, 1992) to 0.645 (Zhang and Makse, 2005). The values match the two well-known packing states for monosized spheres: random loose packing (RLP) and random close packing (RCP). Moreover, the simulated radial porosity oscillation due to the effect of wall is also in good agreement with the measurements (Yu et al., 2003). Studies have also been extended from monosized to multi-sized particles (Kong and Lannutti, 2000b; Fu and Dekelbab, 2003) or from poured to vibrated packing (Rosato and Yacoub, 2000; An et al., 2005). In particular, the transition from RLP to RCP has been reproduced by computer simulation (An et al., 2005). The validity of DEM simulation is also confirmed from the good agreement between simulated and measured angle of repose and surface profile of sandpiles (Zhou et al., 1999, 2001, 2002, 2003b), as shown in Fig. 1.

Microstructural properties: CN and RDF are two commonly used parameters describing the structure of a packing. Good agreements between measured and simulated results have been reported in the literature. For example, quantitative agreement between measured and simulated CN can be observed not only for monosized spheres but also for particle mixtures (Yu, 2004). For monosized spheres, the average cumulative number of neighbours within a radial distance, obtained from DEM simulations, is also close to the experimental one (Scott, 1962). The simulated RDF for RCP shows a clear split second peak for RCP (Liu, et al., 1999; Yang et al., 2000). Recently, An et al. (2005) demonstrated that the structural results measured by Finney through the so-called Voronoi-Delaunay tessellation (1970a, b) can be reproduced by DEM simulation (Fig. 2).

Force network: The heterogeneity of the force distribution in a packing has been observed in physical experiment (Liu et al., 1995; Morrison et al., 2007; Løvoll et al., 1999; Blair et al., 2001; Brujic et al., 2003b). The probability density function (PDF) has normally been used to characterize the force distribution and can be obtained experimentally with carbon paper (Liu et al., 1995; Mueth et al., 1998), force sensor (Løvoll et al., 1999) and confocal microscopy (Brujic et al., 2003a). It is now established that PDF shows an exponential tail at large forces. This feature has also been confirmed in DEM simulations (Fig. 3), and the simulated results are in good agreement with the experimental results (Silbert et al., 2002b; Snoeijer et al., 2003).

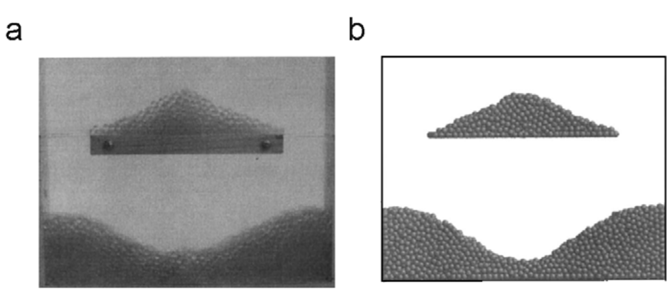

Fig. 1. Sandpiles formed by (a) physical and (b) numerical experiments (Zhou et al., 1999).

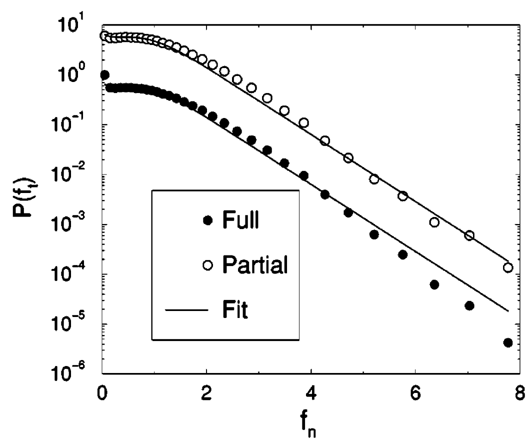

Fig. 3. Distribution of normal contact forces for packings of monosized spheres. The full distribution (solid circles) includes normal forces for all contacting particles and the partial distribution (open circles) only includes forces larger than the weight of one particle. The partial distribution is more comparable with experimental results (Silbert et al., 2002b).

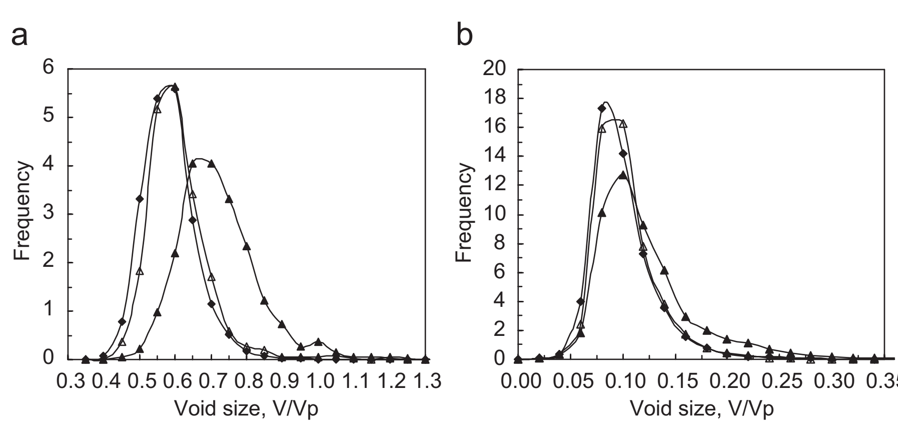

Fig. 2. Distribution of (a) Voronoi and (b) Delaunay subunits for different packings: (▲) loose packing; (⧫) dense packing; and (△) Finney's packing (Finney, 1970a). V and V_p are the volumes of a subunit and particle, respectively, (An et al., 2005).

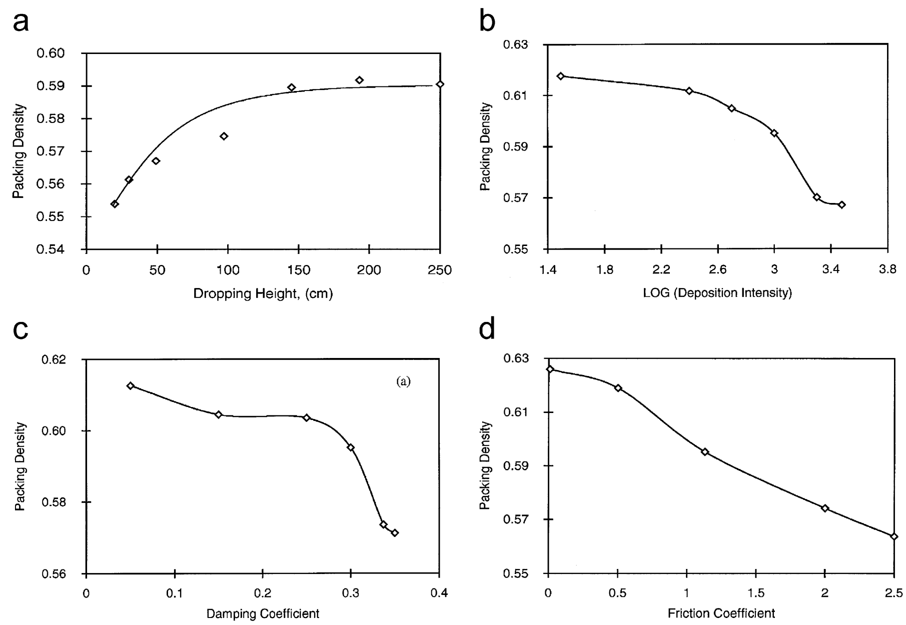

Fig. 4. Packing density as a function of (a) dropping height; (b) deposition density; (c) damping coefficient; and (d) friction coefficient (Zhang et al., 2001).

The existing experimental techniques can only measure the forces on the (external) surfaces of a packing, while DEM simulation can generate information about the internal force structure (Liffman et al., 1992; Radjai et al., 1996; Yang et al., 2000; O'Hern et al., 2002; Silbert et al., 2002b; Snoeijer et al., 2003; Agnolin and Roux 2007a,b,c). The results have shown that the PDF of the normal contact forces within a packing exhibits an exponential tail at large forces, a plateau near the mean force and a slight increase when the force towards zero. The distribution is not affected by the force law, and the slight increase in PDF at small forces is due to the presence of interparticle friction (Silbert et al., 2002b). With large particle deformation, PDF crosses over to Gaussian distribution (Zhang and Makse, 2005). Snoeijer et al. (2003) proposed the concept of "effective weight" to describe the forces acting on the container surfaces and established a link between the external force and the internal forces within a packing. Their work showed that while the internal force structure is very robust, the distribution of the normalized effective gravity is strongly affected by the contact geometry.

The effects of dynamic factors related to material properties and packing methods have been investigated by a few research groups (Zhang et al., 2001; Silbert et al., 2002a; Zhang and Makse, 2005). The effects are mainly attributed to two competitive mechanisms: externally supplied energy and energy dissipation rates (Silbert et al., 2002a). For example, a large initial energy achieved, at a large charge height in poured packing, often results in a relatively dense packing, while faster energy dissipation due to larger deposition rate, sliding friction and damping coefficients, results in a relatively loose packing (Fig. 4). Zhang and Makse (2005) observed that although packings of frictional particles are usually in a hyper-static state with a mean CN > 4, they can also reach an isostatic state with a mean CN = 4 if energy dissipation is infinitely slow. For frictionless hard spheres, the formed packing is always isostatic with packing density of around 0.64 and CN of 6, regardless the forming history. The finite hardness of spheres may increase the packing density and the CN following a power law relation (Silbert et al., 2002a; Zhang and Makse, 2005).

There are two reproducible random packing states: RLP and RCP (Scott, 1960; German, 1989; Bideau and Hansen, 1993; Mehta, 1994). Experimentally, RCP can be realized by compaction or vibration. However, the mechanisms governing the transition are difficult to experimentally study because of the lack of information about the force network and structural rearrangement. Recently, An et al. (2005) numerically reproduced the transition from RLP to RCP under one-dimensional vibration. The effects of vibration amplitude and frequency were quantified and RCP was shown to be achieved only if both parameters were properly controlled. Two densification mechanisms were identified from the analysis of the connectivity among particles: pushing filling by which the contact between spheres is maintained and jumping filling by which the contact between particles is periodically broken. In general, pushing filling occurs when the vibration intensity is low and jumping filling becomes dominant when the vibration intensity is high. Yu et al. (2006) recently extended the work from one- to three-dimensional vibration and showed that by properly controlling vibrational and charging conditions, the transition from disordered to ordered face centred cubic (FCC) packing can be obtained consistently. The method applied to both spherical and non-spherical particles. The resultant force structures are ordered but do not necessarily completely correspond to the packing structures.

DEM studies of sandpiling process focus on two properties: angle of repose and stress distribution in a sandpile (Lee and Herrmann, 1993; Luding, 1997; Zhou et al., 1999, 2001, 2002, 2003b; Matuttis et al., 2000; Liffman et al., 2001; Smith and Tuzun, 2002b; Fazekas et al., 2005). The angle of repose depends on, in addition to the way of forming a sandpile, a range of variables related to material properties such as sliding friction coefficient and density of particles, and particle characteristics such as size and shape. Zhou et al. (1999, 2001, 2002, 2003b) showed that friction is the primary reason for the formation of a stable sandpile, while particle size and container thickness also influence the angle of repose. Their findings are consistent with physical or numerical results (Lee and Herrmann, 1993; Elperin and Golshtein, 1997). It is known that the pressure distribution beneath a sandpile is affected by various factors, including base deflection, particle size distribution, and particle friction. Matuttis et al. (2000) performed two-dimensional simulations and analysed the stress distribution with both spherical and non-spherical particles. The arching or stress-chains could be observed in a resultant sandpile, which was also influenced by the history of formation. A more pronounced dip was produced in the vertical stress under the

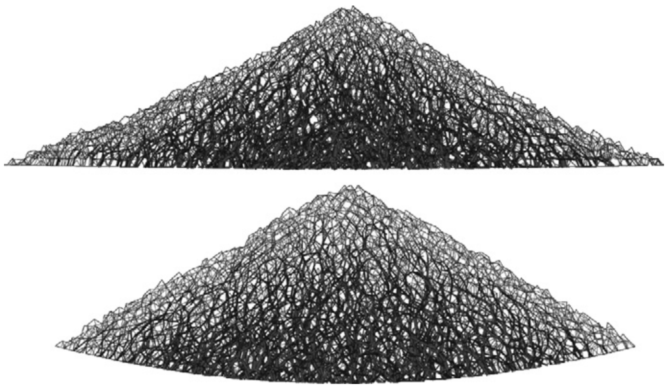

Fig. 5. Force network in sandpiles constructed with different base deflections: top, $r = 2000d$; and bottom, $r = 125d$, where d is particle diameter (Zhou et al., 2003b).

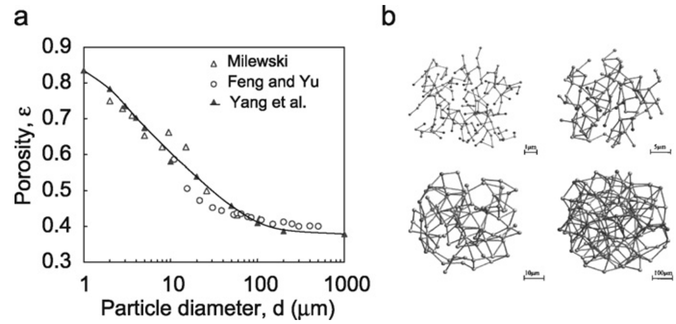

Fig. 6. (a) Porosity as a function of particle size: simulated vs. measured and (b) the contact networks in a spherical sample taken from the packing of different sized particles, where small spheres represent the centres of particles, and sticks represent the contacts between particles (Yang et al., 2000).

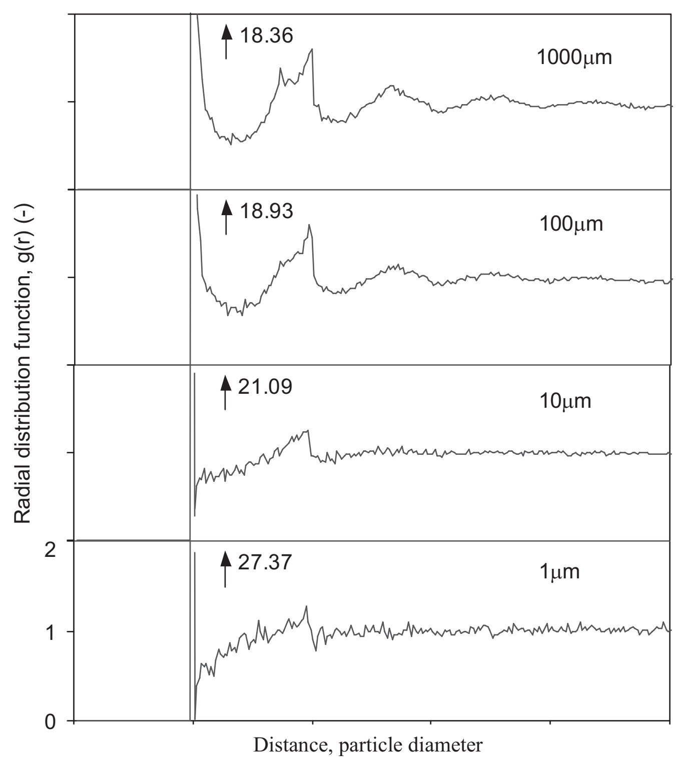

Fig. 7. Radial distribution function as a function of particle size (Yang et al., 2000).

apex of the sandpile of more eccentric polygons. On the other hand, Liffman et al. (2001) studied the force distribution at the base of a conical sandpile and found the stress dip could only be observed when the piles were composed of particles with different sizes and the particles were segregated in an ordered, symmetric and circular fashion around the central axis of the sandpile. They augured that if a pile is composed of particles with different sizes and the particles are randomly distributed throughout the pile, then no stress dip is observed. More recently, Zhou et al. (2003b) confirmed that base defection could have an effect on the normal pressure distribution (Fig. 5), particularly when a sandpile is formed with multi-sized particles and small sliding friction coefficients.

2.2. Packing of cohesive particles

Cohesive particles are associated with various non-contact forces including, for example, the van der Waals and electrostatic forces associated with fine particles and/or capillary force as a result of liquid bridge between particles. These forces affect the packing of particles significantly, as highlighted by the variation of packing density with particle size and liquid content (German, 1989; Yu et al., 1995, 1997).

Yen and Chaki (1992) first introduced the van der Waals force in DEM to simulate the packing of fine particles. While the effect of the force is demonstrated, their results could not quantitatively compare with the measured ones. Yang et al. (2000, 2002, 2003c, 2006b, 2008a,b) presented an improved DEM approach which is applicable to particles of size down to 1 μm. The results showed that packing structures become looser as particle size decreases, and the simulated relationship between porosity and particle size is comparable with the measured data (Milewski, 1987; Feng, 1998) (Fig. 6). The packing structure varies with particle size or porosity, and the CN decreases with particle size. Quantitatively, the structural variation can be identified from the RDF. As shown in Fig. 7, as particle size decreases, the first peak in RDF becomes narrower, with a sharp decrease to the first minimum. The first component of the second peak vanishes when particle size is less than 100 μm and the peaks beyond the second one gradually vanish. When particle size is less than 100 μm, the gravity is not the dominant force, and the van der Waals becomes more important. The cohesive force provides a resistant force to the relative motion between particles, leading to a relatively loose packing.

The capillary force plays a similar role with the van der Waals force. By explicitly taking into account the capillary force, the packing of wet spheres with different moisture contents can be simulated. Yang et al. (2003a) applied this approach to simulate the packing of wet glass beads, and showed that the simulated relationship between dry-based porosity and moisture content is reasonably consistent with that measured by Feng and Yu (1998) (Fig. 8). On this basis, these authors analysed the packing structures which, if expressed as a function of porosity, are qualitatively comparable to those for fine particles. This was recently further verified from experiments (Groger et al., 2003; Xu et al., 2004, 2007a). On the other hand, Nishikawa et al. (2003) studied the self-assembling of colloidal particles due to capillary immersion force. These authors showed that at low coverage, colloidal particles rapidly form small clusters that consist of several particles in the early stage; subsequently, chain-like structures with some branches are generated. At high coverage, large domains of hexagonal close-packed structures can be gradually generated.

Packing of particles in liquids is related to various operations such as sedimentation, filtration and centrifugal casting. Different from particle packing in air or vacuum, such a packing is strongly affected by liquid properties. To date, work in this area focuses largely

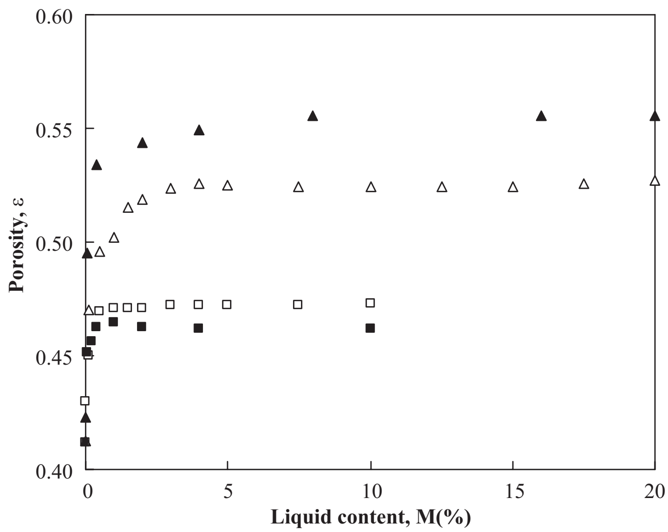

Fig. 8. Dry-based porosity as a function of moisture content for the packing of 1 and 0.25 mm particles. Blank symbols represent calculated results while solid symbols represent measured results (Yang et al., 2003a).

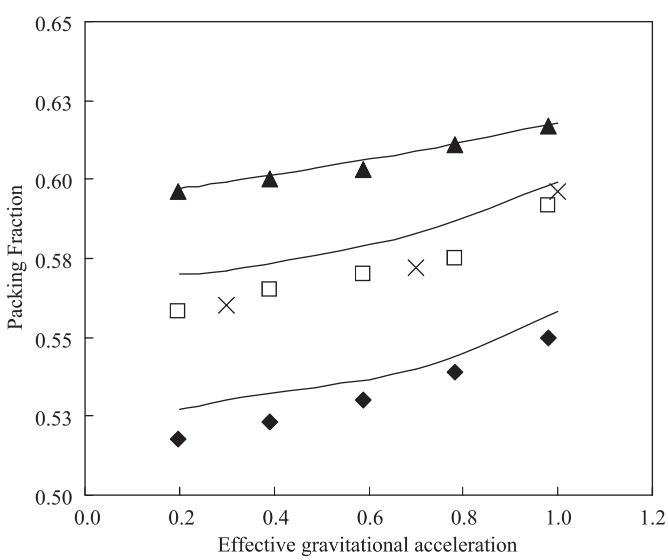

Fig. 9. Packing fraction of different sized glass beads as a function of the effective gravitational acceleration $\Delta g(=(1-\rho_f/\rho_p)g)$. Points are the measured results: (▲) $d=500\,\mu$m; (□) $d=250\,\mu$m; (♦) $d=110\,\mu$m; and (×) results of Onoda et al. (1990), and lines are the simulated results (Dong et al., 2006).

on particles at nanoscale, not electronically neutral but with strong surface charge (Fu and Dempsey, 1998; Hong, 1998; Cordelair and Greil, 2004; Li et al., 2006). To simulate such a process, attempts have been made to combine the long-range potential interactions according to the so-called DLVO theory and the JKR theory (Hong, 1996, 1997, 1998; Li et al., 2006). On the other hand, Dong et al. (2006) extended the work of Yang et al. (2000) for fine particles by incorporating some liquid related forces such as buoyancy, drag, and lift forces in the DEM. They used the approach to study the settling of uniform spheres in different liquids. Their results clearly show that packing density depends on both particle and liquid properties, and the measured results can be satisfactorily reproduced by numerical simulation (Fig. 9). The results also suggest that different packing conditions give different interparticle forces and, hence, different RLP.

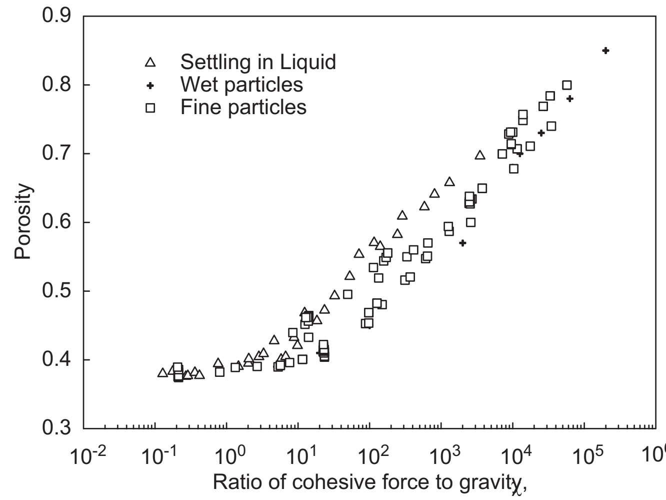

Fig. 10. Porosity as a function of interparticle force, data from various sources (i.e., packing of fine particles, packing of wet particles and packing of particles in liquid) (Yang et al., 2007).

Cohesive forces may have different forms, e.g., the van der Waals force or capillary force, but function similarly. It is therefore very helpful to formulate a general equation to describe the relationship between porosity and cohesive forces. For the packing of fine particles in air or vacuum, Yang et al. (2000) found that porosity can be related to the ratio of the van der Waals force to the gravity force on a particle. For the packing of particles in liquid, if the concept of "effective gravity" defined as the difference between the gravity and buoyancy forces is used, then their relationship is also applicable (Dong et al., 2006). It has been reported that this relationship also applies to other cohesive force such as capillary force (Yang et al., 2003a). The results further support the argument that there is a general relationship between porosity and interparticle force for commonly used particles, as illustrated in Fig. 10 (Feng and Yu, 2000; Yu et al., 2003; Yang et al., 2007). Since the relationship concerns only the final state of particle packing, it can be treated as an equation of state highlighting the importance of interparticle forces in governing the state of particle packing.

2.3. Compaction of particles

Mechanical compaction has been widely used in manufacturing near-net-shaped components with sufficient strength, such as forming greens in ceramic industry and tablets in pharmaceutical industry (StanleyWood, 1983; German, 1989). Compaction induces very complex states of stress in a packing, which in turn results in complicated anisotropic packing structure (Radjai et al., 1996; Kong and Lannutti, 2000a). The macroscopic behaviour of particles during a compaction process is the integration of the discrete interactions which are affected by material properties such as hardness, roughness and surface energy. To obtain optimal mechanical properties of a compact, better knowledge of the relationship between powder characteristics and mechanical behaviour is required. Previous experimental work and numerical models based on the continuum mechanics are largely at a bulk scale and focus on phenomenological description of a compaction process. They cannot relate the bulk response of a compact to the microscopic information such as the interactions between particles. To overcome this shortcoming, DEM simulation has been extensively used in this area (Lian and Shima, 1994; Ng, 1999; Kong and Lannutti, 2000b; Ransing et al., 2000; Gethin et al., 2001, 2003, 2006; Redanz and Fleck, 2001; Martin, 2003; Martin and Bouvard, 2003; Martin et al., 2003; Wu et al., 2003a,b; Zavaliangos,

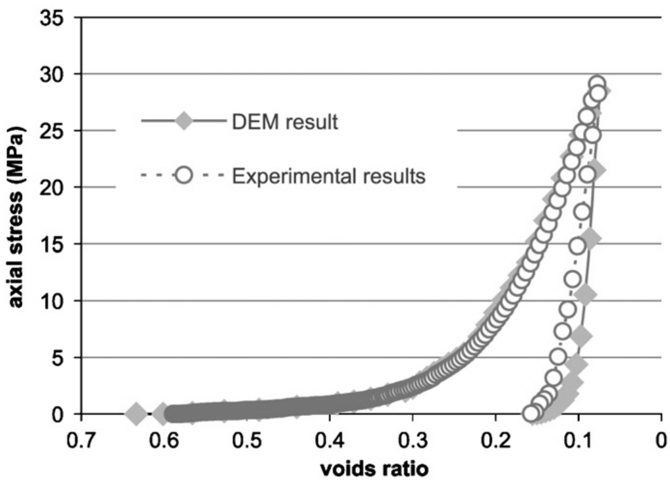

Fig. 11. Loading–unloading curve of the square die compaction tests (Sheng et al., 2004).

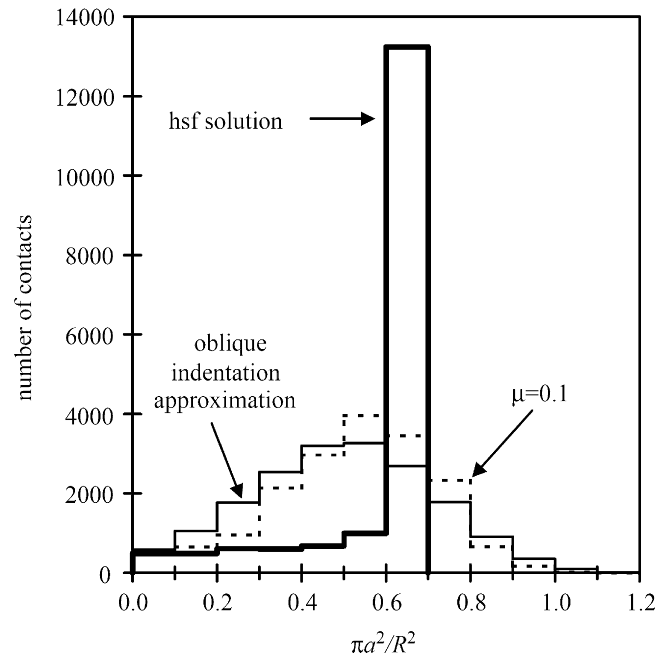

Fig. 12. Comparison of the distributions of contact areas in a packing of 4000 particles at a packing density $\rho = 0.80$, obtained by different simulation methods. hsf solution is the homogeneous strain field solution method (Martin et al., 2003).

2003; Foo et al., 2004; Hassanpour and Ghadiri, 2004; Martin and Bouvard, 2004; Nam and Lannutti, 2004; Sheng et al., 2004; Thornton et al., 2004; Skrinjar and Larsson, 2004a,b; Coube et al., 2005; Lewis et al., 2005; Procopio and Zavaliangos, 2005; Fu et al., 2006a,b; Karrech et al., 2007; Skrinjar et al., 2007; Taguchi and Kurashige, 2007; Chung and Ooi, 2008).

Particle compaction exhibits several regimes controlled by different mechanisms where the linear relationships between pressure and packing density show different slopes. At low compaction pressure (stage I), the densification is mainly achieved by the rearrangement of particles, so packing property mainly depends on particle characteristics. At high pressure (stage II), the compaction process is controlled by the large plastic deformation of particles and therefore is dependent on material properties. If particles are brittle and experience breakage, then another stage (stage III) can be observed where the densification mechanism is the rearrangement of particle fragments (or primary particles for agglomerates). Due to the difficulty in simulating particle fracture, most DEM work focuses on the first two stages, with exception of a few (Nam and Lannutti, 2004; Martin et al., 2006).

To validate DEM models, comparisons between physical and numerical experiments have been carried out. For example, Sheng et al. (2004) showed that the loading–unloading curve (average compaction pressure against voids ratio in the compact) of uniaxial compaction of alumina powders obtained in their DEM simulations were similar to the experimental results, as shown in Fig. 11. Martin et al. (2003) have studied the effect of particle rearrangement on average quantities such as the CN, the contact area and the macroscopic stress. Their results were comparable to the available experimental data and to statistical models that use a homogeneous strain field assumption. These results confirm the applicability of the DEM simulation to these tests.

From DEM simulations, detailed microscopic information of compacts can be obtained. Martin et al. (2003) observed that when particle rearrangement is introduced, the average CN and contact areas increase (Fig. 12). However, the particle rearrangement does not change the pressure response much. This is because the rearrangement induces a higher average CN together with a lower average contact area. Since the pressure is proportional to the product of these two quantities, it is not significantly affected by the rearrangement. The contact orientation, represented by the fabric tensor, also experiences more changes with particle rearrangement. On the other hand, Sheng et al. (2004) investigated the evolutions of both the CN and the plastic contact number during the loading and unloading processes. Both the CN and the plastic contact number increase with the loading, but the CN decreases significantly during unloading while the plastic contacts only have a slight drop so that the remaining contacts form the major part of the unrecoverable plastic deformation of the particle assembly.

The compaction process is significantly affected by the particle characteristics and material properties. Compaction of particles with different sizes (Skrinjar and Larsson, 2004a,b), sliding frictions (Martin et al., 2003; Sheng et al., 2004) and hardness (Kong and Lannutti, 2000b; Martin and Bouvard, 2003; Hassanpour and Ghadiri, 2004) has been investigated using DEM. Skrinjar and Larsson (2004a,b) found that the effect of size ratio is only important when the number fraction of small particles in the powder compound is high. Sheng et al. (2004) observed that when reducing the friction between particles, the final plastic contact numbers after unloading increase. This means that more plastic contacts occur with a smaller interparticle friction. Martin et al. (2003) also found that the friction has a minor effect only when rearrangement is not taken into account. When the mixtures of soft and hard particles were compacted, the friction coefficients of the hard particles play a significant role in the mechanical network of hard particles (Martin and Bouvard, 2003). The presence of hard particles has a strong effect on the compaction curve. These findings in the DEM simulations may facilitate the understanding of the mechanisms of the retardation of compaction observed in experiments.

To simulate stage III where the fracture of particles occurs, Martin et al. (2006) investigated the compaction of aggregates which are formed by bonding primary particles together. The bonds between the primary particles have a possibility to break when their strength is exceeded in order to simulate the breakage of aggregates in compaction, as shown in Fig. 13. They observed that the densification of the powders is mostly due to aggregate attrition and crushability, coupled with rearrangement. They also discussed the effects of bond size, aggregate strength and morphology, a topic which has attracted attention from various investigators

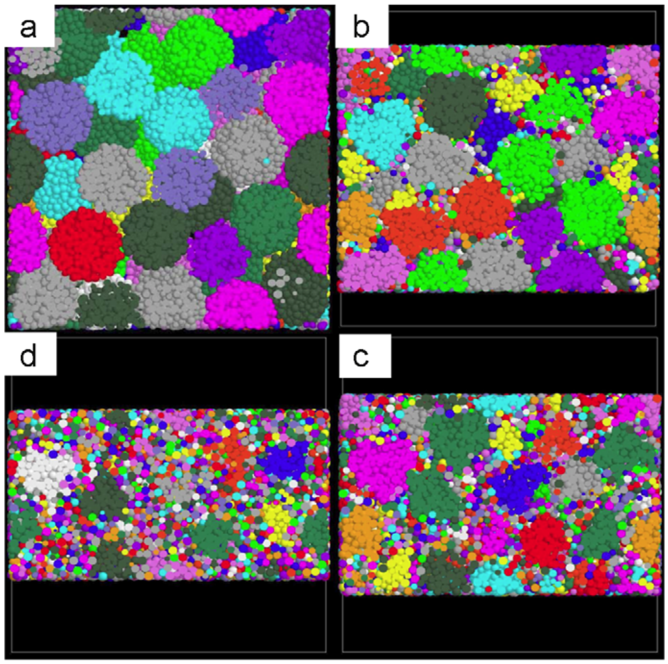

Fig. 13. Packing evolution during uniaxial compaction of 100 breakable aggregates. The colour indicates particles that are still bonded into an aggregate (Martin et al., 2006).

(Thornton et al., 1996; Ning et al., 1997; Subero et al., 1999; Kafui and Thornton, 2000; Mishra and Thornton, 2001).

2.4. Summary and discussion

Particle packing has been studied for many years. Although often regarded macroscopically homogenous, a packing is heterogeneous at the microscopic, particle level and the interactions between two complementary phases—particle and pore—play a crucial role in determining its transport and mechanical properties. Therefore, quantification of packing structures is critical in order to understand the behaviour at a particle or pore level. Forming a packing is a dynamic process involving various forces in addition to gravity, including the contact forces due to the collision and friction among particles, the van der Waals and/or electrostatic forces associated with fine particles, and the capillary force with wet particles. These forces may effect individually or cooperatively, depending on the packing conditions involved. By incorporating these forces, DEM has been used to study the packing of particles under various conditions related to various operations.

For cohesionless particles, DEM models have successfully reproduced the two well-known packing states, RCP and RLP, with the packing structures quite comparable to those measured. Notably, the interparticle forces, which are very difficult to obtain by the conventional experimental techniques, have been analysed and the results show that the distribution of the contact forces exhibits an exponential tail at large forces, a plateau near the mean force and a slight increase when the force towards zero which is believed due to particle frictions. Packing methods and material properties have significant effects and these effects can be generally explained by two competing mechanisms: external energy supply and energy dissipation rate. Moreover, two densification mechanisms have been identified in the transition from RLP to RCP by vibration. By properly controlling vibrational and deposition conditions, the transition from disordered to ordered packings can also be obtained. DEM has also been successfully used to study the packing of particles in unconfined conditions, e.g., the sandpiling process.

When the cohesive forces become dominant over gravity, packing structures change significantly. The cohesive forces may have different forms, e.g., the van der Waals force or capillary force, but function similarly. The role of the cohesive forces can be characterized in terms of the ratio of the cohesive force to the gravity, or the so-called bond number. There is a general relationship between packing density and bond number for commonly used particles.

Slow mechanical compaction can be regarded as quasi-static process which induces very complex states of stress inside a compact. The macroscopic behaviour of particles during a compaction process is the integration of the discrete interactions which are affected by particle material properties, such as hardness, roughness and surface energy. DEM simulations can produce detailed microscopic information of particle assemblies. The simulation results are comparable to available experimental data that are mainly at a bulk scale and have been used to test the commonly used statistical models based on the homogeneous strain field assumption. By establishing the relationship between powder characteristics and mechanical behaviour, optimal mechanical properties of a compact can be acquired.

While DEM has been successfully applied to simulating particle packing, there are still many unsolved problems in this area which requires further improvement to DEM simulations. For example, how to model more complicated particulate systems from monosized to multi-sized, from coarse to fine, from dry to wet, from small deformation to large deformation; how to link the microscopic structure (particle-to-particle or pore-to-pore) obtained from DEM simulations with the macroscopic mechanisms governing transport phenomena, such as fluid flow, heat transfer and mass transfer in porous media; and how to develop more robust and efficient models and algorithms so that the capability of particle scale simulation can be extended to industrial applications. In this connection, one challenge is to extend the present simulation from packing to sintering process (Luding et al., 2005). Some of the problems are related to the theoretical developments as discussed by Zhu et al. (2007). Some are more directly related to the application of the simulation technique to packing research. Their studies may therefore represent an opportunity to develop a common and powerful tool for investigating not only particle packing but also other particle problems.

3. Particle flow

DEM has been extensively used to study various particle flows. Here, we only consider the most common ones, which are for convenience clarified into two categories: fundamental and applied. In the so-called applied research, the systems considered are more related to operations in practice, whereas the fundamental research mainly concerns simplified systems for understanding or characterization.

3.1. Fundamental research

Fundamental research on particle flow by DEM is mainly to acquire information that can be used generally. The flows selected for this study are often geometrically simple but representative, including confined and non-confined flows depending on the geometry used.

3.1.1. Confined flow

Confined flow is referred to as a flow whose boundaries are confined, and is related to the flows in direct shear test, annular cell, vertical pipe, biaxial and triaxial compressions in this review. These flows have been extensively investigated experimentally and numerically to understand the quasi-static rheological behaviour of granular materials. Direct shear testers are usually used to measure the bulk strength of materials. There are several shear testers available so far, including Jenike, Peschl, Schulze, and uniaxial testers (Svarovsky, 1987). The Jenike cell is the oldest direct shear tester used to measure the yield properties of granular materials, and the most popular one in the DEM simulation. The annular (or torsion) cell developed by Hvorslev (1936) is another important shear test to measure the shear strength of soils, and has been used for particle flow measurements by, e.g., Howell et al. (1999). Slow vertical flow is often encountered in industrial processes such as hoppers, silos or moving bed reactors. Because of its simplicity, such vertical flow is also of great fundamental interest, particularly for understanding the basic features of quasi-static granular flows (Nedderman and Laohakul, 1980; Pouliquen and Gutfraind, 1996). On the other hand, the nature, origins and evolution of localization in granular materials are often investigated by means of biaxial and triaxial tests (Ng and Dobry, 1992; Cheng et al., 2003; Powrie et al., 2005). In these experiments, a certain stress state is imposed on a sample by means of mobile plates. In the triaxial test, for example, a flexible membrane maintains the sample together while imposing a hydrostatic pressure on the lateral direction, whereas two hard plates at the top and the bottom impose a certain axial stress. In the biaxial test, the experimental device generally consists of four hard walls perpendicular to a fixed base imposing a two-dimensional stress state.

Earlier studies in this area were mainly focused on laboratory experiments. The results are macroscopic, and often used to validate continuum theories or support continuum modelling. However, the experiments are usually incapable of providing insight into the microscopic characteristics of granular materials, and the lack of such information limit the fundamental understanding and the application of the resultant findings. DEM simulation can overcome this shortcoming. It can provide information directly linked to the mechanisms governing the dynamic behaviour of particles, and the intrinsic characteristics of granular matter for general application. For this reason, DEM simulation has been extensively used to study the quasi-static behaviour of granular matter for different shearing flows, including:

- direct shear (Masson and Martinez, 2001; Thornton and Zhang, 2003, 2006; Liu and Matsuoka, 2003; Bilgili et al., 2004; Lobo-Guerrero and Vallejo, 2005; Liu et al., 2005; Liu, 2006; Cui and O'Sullivan, 2006; Zhang and Thornton, 2007; Wang et al., 2007b; Härtl and Ooi, 2008);
- annular shear (Lätzel et al., 2000, 2003; Luding et al., 2001; Hassanpour et al., 2004; MiDi, 2004; Baran and Kondic, 2006; Ning and Ghadiri, 2006; Lobo-Guerrero and Vallejo, 2006; Luding, 2008);
- vertical flow (Gutfraind and Pouliquen, 1996; Zhu and Yu, 2003; Zhu et al., 2004);
- biaxial compression (Antonellini and Pollard, 1995; Williams and Rege, 1997a,b; Iwashita and Oda, 1998, 2000; Kuhn, 1999; Masson and Martinez, 2000b; Oda and Iwashita, 2000; O'Sullivan et al., 2002; Fakhimi et al., 2002; Liu and Sun, 2002; Mirghasemi et al., 2002; Nouguier-Lehon et al., 2003; Luding et al., 2003; Tordesillas et al., 2004; Hu and Molinari, 2004; Potyondy and Cundall, 2004; Delenne et al., 2004; Rothenburg and Kruyt, 2004; Emeriault and Claquin, 2004; Antony et al., 2004; Jiang et al., 2005, 2006; Taboada et al., 2005; Powrie et al., 2005; Luding, 2005a,b; Asaf et al., 2006; Kadau et al., 2006; Hosseininia and Mirghasemi, 2006; Kruyt and Rothenburg, 2006; Tordesillas, 2007; Tykhoniuk et al., 2007; David et al., 2007; Rock et al., 2008);
- triaxial compression (Ng and Dobry, 1992; Malan and Napier, 1995; Sitharam et al., 2002; Sitharam and Dinesi, 2003; Cheng et al., 2003; Washington and Meegoda, 2003; Ishibashi and Capar, 2003; Ng, 2004a,b,c, 2005; Dinesh et al., 2004; O'Sullivan et al., 2004; Klerck et al., 2004; McDowell et al., 2006; Collop et al., 2006; Fazekas et al., 2006; El Shourbagy et al., 2006 Cui et al., 2007; David et al., 2007).

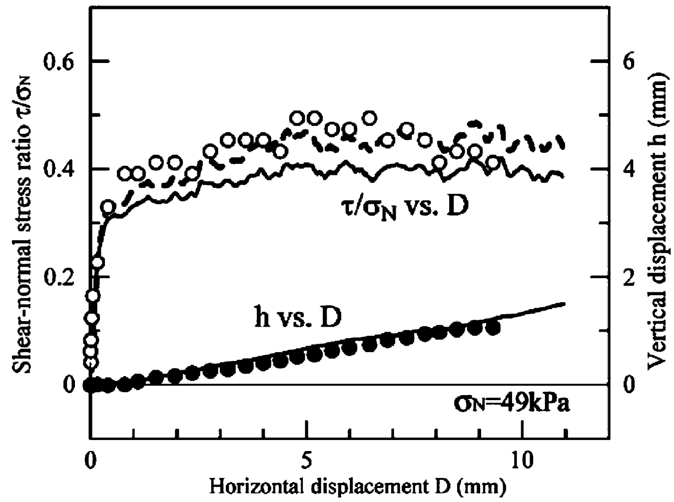

Fig. 14. Numerically simulated evolution of shear–normal stress ratio and volume change for the conventional direct shear tests where the upper shear box is fixed: circles represent measured results, while solid and dashed lines show simulated results (Liu et al., 2005).

In these studies, extensive comparison between physical and numerical experiments has been made in order to verify the applicability of the DEM simulation to these tests. For example, Ng and Dobry (1992) and Cheng et al. (2003) showed that the macroscopic behaviours of triaxial tests obtained in their DEM simulations are similar to laboratory results on sands/silica. Liu et al. (2005) calculated the stress ratio of a conventional direct shear test. The result is qualitatively in good agreement with the experimental one on the aluminum rods, as shown in Fig. 14. Powrie et al. (2005) investigated a biaxial test. Their results on effective angles of friction at peak strength and critical state are similar to those determined for real sands.

In addition, DEM results have also been used to test the conventional theoretical approaches based on some assumptions. It has been illustrated that the stress-force–fabric expression is in agreement with the measured shear resistance in the biaxial test simulations (Mirghasemi et al., 2002). On the other hand, shortcomings of some theories have also been shown in the comparison with DEM simulations. For example, it has been suggested from a biaxial simulation that the assumption used in the double-shearing model is not in agreement with the DEM data, and the energy dissipation requirements in the double-sliding free-rotating model is unduly restrictive as a constitutive assumption (Jiang et al., 2005). A direct shear simulation suggests that the conventional interpretation of the location of the Mohr stress circle at the steady state may result in an overprediction of the major principal stress, and the corresponding flow function may underpredict the unconfined yield stress for a given value of the major principal stress (Thornton and Zhang, 2003).

New insights about the microscopic origins of the macroscopic properties of granular materials have been obtained from the analysis of the microstructures such as displacement fields and force transmission (e.g., Williams and Rege, 1997b; Iwashita and Oda, 2000; Taboada et al., 2005), which are hard to obtain from physical experimentation and other numerical simulations. In particular, it has been shown that DEM simulation has particular advantages in the study of the formation of shear band, which is a key characteristic in the quasi-static rheology of materials. For example, Williams and Rege (1997b) revealed that the velocity vectors in a simple deformation test appeared to be quite dramatic, allowing visual identification

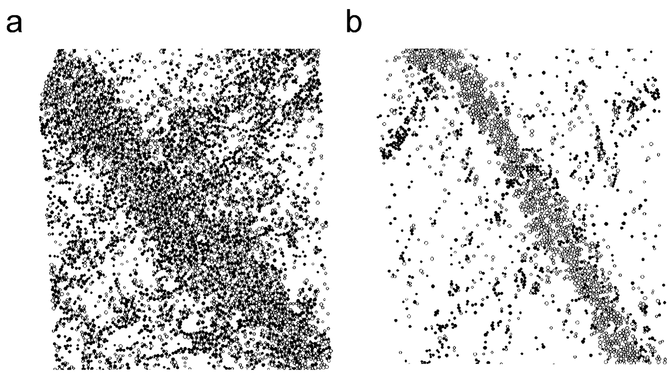

Fig. 15. Distributions of highly rotated particles in (a) free rolling test and (b) rolling resistance test: (•) the particles rotating counterclockwise by more than 15°; (◦) the particles rotating clockwise by more than 15° (Iwashita and Oda, 2000).

of the coherent circulation cell structures where particles instantaneously translated and rotated as a rigid body about a common centre. The circulation cells play an important role in the formation of shear bands. Iwashita and Oda (1998, 2000) and Oda and Iwashita (2000) investigated the microstructure of the formation process of shear bands in a biaxial test. It is found that DEM can be a powerful tool for simulating not only the generation of large voids inside a shear band but also the high gradient of particle rotation along the shear band boundaries, in a quite similar manner to those observed in natural granular soils. Rolling resistance is demonstrated to play an important role in the development of the shear bands (Fig. 15). Their results also suggest that the basic micro-deformation mechanism ending up with the formation of shear bands is in the generation of a column-like structure during the hardening process and its collapse in the softening process. Besides, microbands (thin obliquely trending bands of void cells within which slip deformation is most intense) have been observed under biaxial loading (Kuhn, 1999). These microbands appeared spontaneously throughout the test, even at the start of loading, ranging in thickness between one and four particle diameters.

The behaviour of granular materials is affected by particle characteristics such as particle size, shape and angularity or roughness, and material properties such as friction and damping coefficients. These parameters are difficult to control in physical experiments. But this difficulty can be overcome readily in numerical experiments. The influence of these properties on the mechanical behaviour of granular materials of the confined flows has been quantified by DEM simulations, as highlighted below:

Particle characteristics: Compared with spherical particles, angular ones have a higher angle of internal friction (Nouguier-Lehon et al., 2003), and greater maximum volume change level (Mirghasemi et al., 2002). The maximum values of shear stress ratio for the circular and oval particulate systems are fairly identical. However, the nature of the variation of shear stress ratio for both the assemblies during compression is significantly different (Antony et al., 2004). As the angularity of particles increases, the density and shear strength increase (Mirghasemi et al., 2002). For dense sands, the peak effective angle of friction increases by 258 (or 66%) as the shape factor ($=1+r/R$, where R and r are respectively the radii of the larger and smaller spheres considered) is increased from 1 to 2, and by 198 (or 43%) as the shape factor is increased from 1.3 to 2.0. The corresponding increases in the dilation angle at peak strength are 208 and 158, respectively (Powrie et al., 2005).

Material properties: It has been shown that the peak friction angle decreases as the standard deviation of the distribution of particle surface friction increases (O'Sullivan et al., 2002). For dense samples (sands) having a shape factor of 1.5, increasing the interparticle friction angle from 178 to 358 increases the peak angle of shearing resistance by 198 (48%), with comparable changes in dilation rates (Powrie et al., 2005). The width of shear band does not change conclusively with the friction, rolling resistance parameters. However, cohesive strength significantly increases the width of shear band (Hu and Molinari, 2004).

3.1.2. Unconfined flow

In contrast with confined flow, unconfined flow is referred to as a flow as long as one of its sides is unconfined. Here, we focus on plane shear flow, surface flow (flow on inclined plane or pile), and vibrating flow. Compared with confined flows, these flows are more complicated, as both solid-like and fluid-like behaviours may occur simultaneously. The study of these flows can help understand the fundamentals governing the related complex phenomena, e.g., transition between flow regimes. Plane shear flow, i.e., the granular flow bounded between two parallel plates, has been extensively used due to its geometrical simplicity. It is related to the kinetic regime (Lun et al., 1984; Johnson and Jackson, 1987; Babic, 1997), frictional regime (Mei et al., 2000; MiDi, 2004; Iordanoff et al., 2005) and their transition (Zhang and Campbell, 1992). Similar problems have been considered by investigating granular flow down a plane-inclined chute. The studies in this aspect generally emphasize the bulk flow behaviour (Roberts, 1969), the mechanics of local flow behaviour (Savage, 1979; Drake, 1991), or both of them (Johnson et al., 1990). Vibrating flows under various conditions have also been studied, where the main concern is the fluid-like behaviour, such as convection (Gallas et al., 1992b; Yang and Hsiau, 2000), segregation (Brone and Muzzio, 1997; Knight et al., 1993; Poschel and Herrmann, 1995; Rosato et al., 1997), heaping (Clement et al., 1992; Behringer et al., 2002), and surface waves and pattern formation (Melo et al., 1994; Goldman et al., 2002).

These unconfined flows have been extensively investigated by DEM to gain insights into the underlying mechanisms, including:

- *plane shear flow* (Yi and Campbell, 1992; Campbell, 1994; Babic, 1997; Schwarz et al., 1998; Higashitani and Iimura, 1998; Karion and Hunt, 1999, 2000; Mei et al., 2000; Dahl et al., 2003; Iordanoff et al., 2005; Aarons and Sundaresan, 2006; Saitoh and Hayakawa, 2007);
- *flow on inclined plane or pile* (Chang, 1992; Poschel, 1993; Zheng and Hill, 1996, 1998; Hanes and Walton, 2000; Zhang and Vu-Quoc, 2000; Mustoe and Miyata, 2001; Mitarai and Nakanishi, 2001; Silbert et al., 2001, 2002c, 2003; Urabe, 2005; Brewster et al., 2005);
- *vibrating flow* in vertical direction (Gallas et al., 1992a,b, 1993; Herrmann, 1992; Tamura et al., 1993; Taguchi, 1994, 1995; Yoshida, 1996b; Lee, 1997; Lan and Rosato, 1997; Rapaport, 1998; Yang and Hsiau, 2000, 2001a,b; Matchett et al., 2000; Shishodia and Wassgren, 2001; Levanon and Rapaport, 2001; Asmar et al., 2002a,b, 2003, 2006; Wassgren et al., 2002; Hsiau and Yang, 2003; Fernando and Wassgren, 2003; Katayama et al., 2004; Zhang and Rosato, 2004; Lu and Hsiau, 2005; Hu et al., 2005; Catherall et al., 2005; Shi and Ma, 2005; Baran and Kondic, 2006; van Zeebroeck et al., 2006; Ramaioli et al., 2007; Fang and Tang, 2007; Rosato et al., 2008; Zeilstra et al., 2008), horizontal axial direction (Saeki et al., 1998; Saeki, 2005; Ciamarra et al., 2005), both vertical and horizontal directions (Gallas et al., 1992c, 1993), vertically rotational direction (Malik et al., 2003), and both vertical and horizontally rotational directions (Gotzendorfer et al., 2005).

To examine the applicability of DEM to these flows, various comparisons of DEM results with experimental data have been conducted. It has been reported that the flow patterns and velocity distributions from DEM simulations are in good agreement with the experimental results in the cases of inclined flow (Zhang and Vu-Quoc, 2000; Hanes

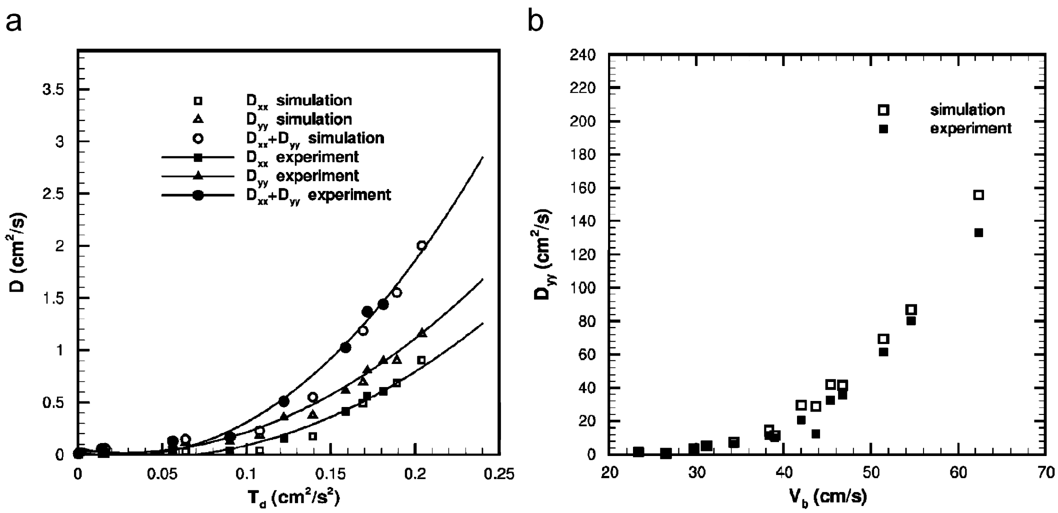

Fig. 16. (a) Diffusion coefficient as a function of the granular temperature in a vibrated granular bed and (b) vertical diffusion coefficient as a function of vibrated bed velocity. D, T_d,fD_{yy} and V_b represent the diffusion coefficient, granular temperature, vertical diffusion coefficient and vibrated bed velocity, respectively. The granular temperature is associated with the fluctuation velocity by averaging the deviations between the mean velocity and particle velocities in a strip or a cell (Yang and Hsiau, 2001b).

and Walton, 2000) and vibrating flow (Matchett et al., 2000; Yang and Hsiau, 2000, 2001b; Gotzendorfer et al., 2005; Saeki, 2005). In particular, Matchett et al. (2000) performed experiments and simulations on a range of materials including glass spheres, bronze spheres, acrylic beads and NBR rubber granules, in a cell subjected to single frequency, vibrational excitation over a range of acceleration magnitudes, and showed that the DEM was able to qualitatively reproduce the major features found in the experiments. Yang and Hsiau (2001b) conducted the diffusive analysis in a vibrated granular bed based on DEM simulations. Their results are close to the experimental ones, showing that the diffusive coefficients increase with the granular temperature, and the self-diffusion also has a strong dependence on vibration bed velocity which is not dependent on the vibration amplitude and vibration frequency (Fig. 16). Saeki (2005) illustrated that the DEM was effective for estimating the damping effect of multi-unit particle dampers. His calculated results match the experimental ones well in terms of the root mean square value of the primary system amplitude. DEM results have also been shown to agree with those by some conventional continuum theories, for example, the kinetic theories of Jenkins and Richman (1985) and Lun et al. (1984) for two- and three-dimensional vibrating flows, respectively (Dahl et al., 2003).

Convection and segregation are two important characteristics of granular flow. Various unconfined flows have been studied to elucidate the mechanisms governing the two phenomena. Compared with the traditional studies, the advantage of DEM simulation in this aspect is obvious, as the flow pattern, velocity field, solid fraction, granular temperatures and the influence of particle properties can be readily obtained. Gallas et al. (1992a) and Yang and Hsiau (2000, 2001b) investigated the convection of vibrated granular materials. Their results show that for dry granular materials, the frictional force dominates the strength of the convection cell, while for wet granular materials, both frictional force and liquid bridge force that result from surface tension and viscosity of interstitial fluid dominate the convection cell. Moreover, Fernando and Wassgren (2003) studied the mechanism leading to segregation in terms of the rising rate of a large impurity in an otherwise homogeneous granular bed subject to discrete and continuous vertical oscillations. The rising rate is shown to depend upon the oscillation method when side-wall convection effects are negligible. When side-wall convection effects are present, the rising rate of the impurity increases linearly

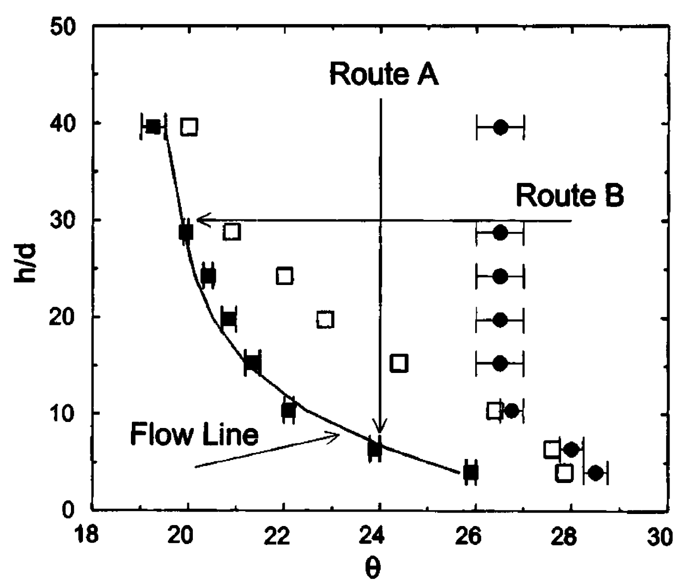

Fig. 17. The h–θ phase diagram for granular flow down a rough inclined plane, where h is the height of the pile while θ is the inclination angle. The filled squares and solid circles divide the plane into three regions: no flow, stable flow and unstable flow, and the open squares are the inclination required to initiate flow. Route A corresponds to a path taken by keeping the angle fixed and reducing the system size N, whereas Route B has N fixed and decreasing inclination (Silbert et al., 2003).

with the oscillation velocity amplitude regardless of the vibration method.

Solid-like and fluid-like behaviours are two key features of granular materials. Development of a general theory to describe these features has been a challenging task for many years. DEM simulations of various unconfined flows have been conducted to study the two behaviours and the corresponding phase transition, and demonstrated to be capable of providing useful information for such development. For examples, Silbert et al. (2003) studied the rheology of granular particles in an inclined plane, and obtained the flow–no flow boundary for piles of varying heights over a range of inclination angles (Fig. 17). Three angles are found to determine the phase diagram: the angle of repose (the angle at which a flowing system

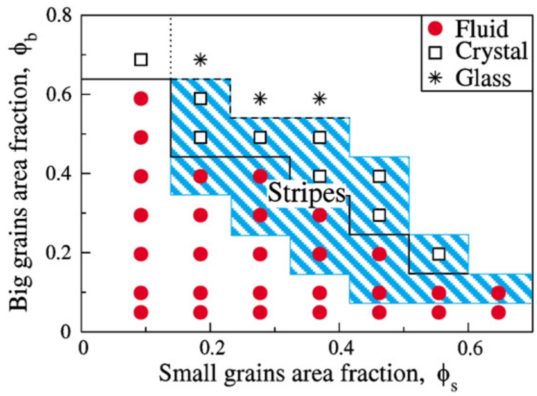

Fig. 18. Ordering properties of the late stage configurations of a granular mixture under oscillating horizontal shear as a function of the area fractions of the two components. The shaded area covers the region where segregation via stripes formation occurs. Circles represents that the large grains are in a fluid state. Squares represents that the large grains form a crystal. Stars represents that the system appears blocked in a glassy disordered configuration (Ciamarra et al., 2005).

comes to rest), the maximum angle of stability (the inclination required to induce flow in a static system), and the maximum angle for which stable, steady state flow is observed. In the stable flow region, three flow regimes can be distinguished: Bagnold rheology, slow flow, and avalanche flow.

Recently, Ciamarra et al. (2005) conducted simulations of a binary mixture of particles under horizontal vibrations, and revealed the existence of a new dynamic instability and shed light on the process of size segregation under oscillatory shear and its connections to pattern formation in granular flows. Within such a unifying framework, a "phase diagram" of the mixing or segregation states of the mixture and its corresponding transitions has been derived, as shown in Fig. 18. On the other hand, Gotzendorfer et al. (2005) showed that a solid-like and a fluid-like domain coexisted in the fluidization of a monolayer of glass beads in a horizontally and vertically vibrated annular container. The sharp boundaries between the two regions travel around the channel faster than the particles are transported. The number density in the solid phase is several times that in the gas, while the temperature is orders of magnitude lower.

The behaviour of granular materials depends on material/particle properties and operational conditions. This has been shown in the DEM simulations of some unconfined flows. Asmar et al. (2002a) simulated the behaviour of particle mixtures under vertical vibration conditions, and showed that the behaviour of particles was affected by particle size and density, friction, vibration conditions and fluid drag mixing index. Furthermore, Zhang and Rosato (2004) showed that the structure before vibrations were applied played an important role in determining the depth profiles of granular temperature and the phase pattern only at low accelerations. Large accelerations can break up the poured packing structure quickly so that the initial state does not play a major role in computed profiles and hence the phase pattern.

3.2. Applied research

In applied research, the systems considered are more related to operations in practice. In these systems, particle movements are driven by gravity or external mechanical forces as a result of interaction between particles and device. For example, for flow in a hopper, the driving force is the gravity; for flow in a rotating drum, the driving force is the sliding friction between particles and drum surface. Other more complicated equipments include various types of blenders or mixers and mills. Particle flow in these devices exhibits a range of complex phenomena which are important to both scientific research and industrial application (see, for example, Poschel and Buchholtz, 1995; Shoichi, 1998; Taberlet et al., 2006b).

Research at an individual particle level would improve our knowledge of the flow behaviour as the bulk behaviour of flow depends on the collected outcome of the interactions among particles and between particles and device. Earlier work was mainly conducted by photographic experiments through a transparent wall, or by freezing bed to reveal the inner flow patterns, which were laborious and suffered a great deal of uncertainty (Bridgwater and Bagster, 1968; Malhotra et al., 1988). Recently, some non-invasive experimental techniques have been developed, such as positron emission particle tracking (PEPT) (Broadbent et al., 1995; Parker et al., 1997; Stewart et al., 2001) and magnetic resonance imaging (MRI) (Nakagawa et al., 1993; Sederman et al., 2007). While these experiment techniques are useful, they all have their limitations and particularly in information generation. As an illustration, Table 1 shows the advantages and disadvantages of PEPT relative to DEM, or vice versa.

One rapidly growing avenue for the study of these systems is numerical simulation. Several modelling techniques have been developed, including Monte Carlo, molecular dynamics and DEM. DEM provides information that would be very difficult to extract with the current experimental techniques but useful for better fundamental understanding as discussed above. Many operations have been studied by DEM. Here, we only focus on particle flow in four commonly used devices: hopper, mixer, drum and mill.

3.2.1. Flow in hoppers

Hoppers are widely applied in engineering practice mainly due to their capacity to enhance flow conditions for granular materials. They must be properly designed for reliable control. Therefore, a comprehensive understanding of the dynamic behaviour of granular flow in a hopper is essential. In addition, theoretical treatment of granular flow in hoppers provides a class of benchmark boundary-value problems for analysing and predicting the behaviour of granular materials under external mechanical excitations. The relatively simple geometry, well-defined flow patterns but complicated flow characteristics have made hopper flow an attractive case to study new research technique for granular flow. For these reasons, particle flow in hoppers has been an important topic of research worldwide for several decades (for example, see Jenike et al., 1973; Nguyen et al., 1979; Haussler and Eibl, 1984; Seville et al., 1997). Especially, in recent years, the dynamics of the flow has been studied extensively by means of both experimental technique and numerical simulation at a microscopic or particle scale (Langston et al., 1994; Seville et al., 1995; Faderani et al., 1998; Zhu and Yu, 2004). Such studies take into account the discrete nature of granular materials without requiring any global assumption needed in the previous macroscopic approaches and thus allows a better understanding of the underlying mechanisms. DEM is again the most important simulation approach for this connection. Particle flows in hoppers with various geometries have been studied, including:

- *two-dimensional model* (Langston et al., 1994, 1995a,b, 1997, 2004; Ristow and Herrmann, 1995; Kohring et al., 1995; Rong, 1995a,b; Potapov and Campbell, 1996; Ristow, 1997; Rotter et al., 1998; Holst et al., 1999b; Masson and Martinez, 2000a,b; Favier et al., 2001; Sanad et al., 2001; Cleary and Sawley, 2002; Wassgren et al., 2002; Fraige and Langston, 2004; Parisi et al., 2004);
- *three-dimensional model* (Sakaguchi et al., 1993; Hidaka et al., 1994; Yuu and Umekage, 1995; Yuu et al., 1995; Langston et al., 1995a,b, 1996, 1997, 2004; Lu et al., 1997; Negi et al., 1997; Kano et al., 1998; Gutfraind and Savage, 1998; Umekage et al., 1998; Baxter et al., 2000; Joseph et al., 2000; Hirshfeld and Rapaport, 2001; Xu et al., 2002b; Zhu and Yu, 2001, 2004, 2005a,b; Theuerkauf

Table 1
PEPT vs DEM for particle scale research (Zhou et al., 2004d)

Technique	PEPT	DEM
Feature	• An experimental technique for tracing the motion of a radioactively labelled particle within a particle system	• A numerical technique for simulating the dynamics of a particle system
Information generated	• Trajectory of a labelled particle from which flow field can be derived	• Trajectories and velocities of all particles • Particle/particle and particle/device interactions
Advantages	• Real physical measurement • Tracing for a long time	• Low cost • Full dynamic information
Disadvantages	• Expensive • No force information and hence incomplete dynamic information • Indirect link between behaviours of a single particle and particles in a system	• Limited by computing capability (relatively small number of particles and short time simulation) • Only applied to situations where equations for calculating interparticle forces are well established

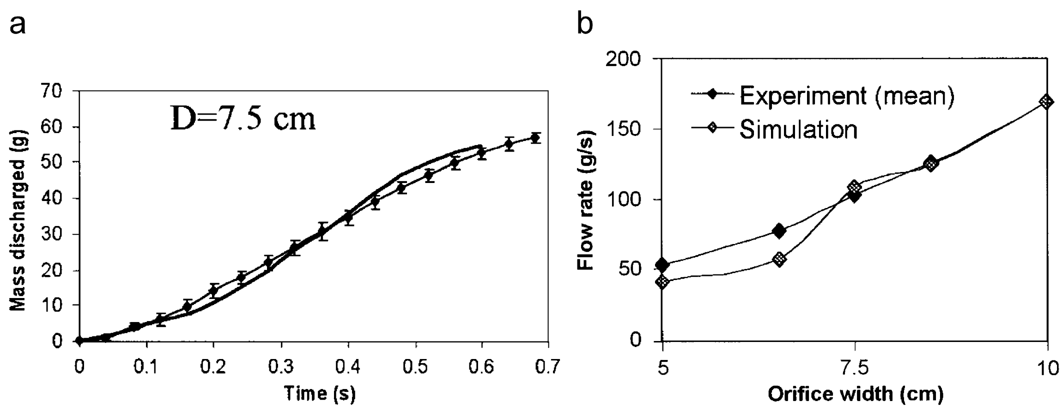

Fig. 19. (a) Discharged mass of particles from hopper through orifices of diameter in experiments (•) and simulations; and (b) rate of discharge during steady state flow from hopper at different orifice widths. *D* represents the orifice diameter (Favier et al., 2001).

et al., 2003; Tuzun et al., 2004; Li et al., 2004b; Lia et al., 2004; Abou-Chakra et al., 2004; Goda and Ebert, 2005; Zhu et al., 2005, 2006; Balevicius et al., 2006, 2007, 2008; Kruggel-Emden et al., 2006; Ketterhagen et al., 2007, 2008; Datta et al., 2008).

These studies are mainly focused on three aspects: wall stress/pressure, discharge rate and internal properties. The study of the bulk material pressure on the walls of a hopper is very important for hopper design. It has extensively been investigated by means of analytical, experimental and numerical approaches. However, the fundamentals about the pressure are not comprehensively understood due to its dependence on many parameters such as the geometry of hopper, material properties of hopper and particles, and flow conditions. DEM studies can enhance the understanding. The comparison of wall pressures along the silo height, obtained by discrete element and finite element simulations, analytical approaches or experiments, shows a good global agreement between the two methods (Langston et al., 1995a; Negi et al., 1997; Holst et al., 1999a,b; Rotter et al., 1998; Masson and Martinez, 2000a,b; Goda and Ebert, 2005). Furthermore, it has also been reported that the wall pressure is affected by particle shape (Cleary and Sawley, 2002), air-assisted flow which leads to increased wall stresses (Langston et al., 1996), and inserts whose presence influences the force transmission patterns within a silo, producing strong and localized loads on the walls and the inserts (Parisi et al., 2004).

The prediction of the discharge rate is of importance for the effective operation and control of a transport system, and is difficult due to the complexity associated with granular flow such as inhomogeneous solid distribution, irregular velocity profile and diverse particle size and shape (Seville et al., 1997). Various empirical formulations have been proposed. Despite widespread study, there remains an incomplete description of discharge rate due to its complexity. DEM simulations have been conducted to address this problem. It has been reported that the hopper discharge rate by DEM is qualitatively in good agreement with that by experiments (Favier et al., 2001), and the empirical predictions (Langston et al., 1994, 1995a; Kano et al., 1998; Zhu and Yu, 2004). This can be seen in Fig. 19, as an example. The discharge rate is affected by particle characteristics and material properties. DEM simulations can quantify these effects. It has been shown that compared with spherical particles, disc flow is about 20–30% faster (Li et al., 2004b); the discs of aspect ratio 5 are discharged 40% faster than the circles (Langston et al., 2004); and elongated particles produce flow rates up to 30% lower than for circular particles (Cleary and Sawley, 2002). DEM simulations also show that the discharge rate is not so sensitive to the stiffness of particles, wall roughness and damping coefficient, but is affected by particle friction (Langston et al., 1994, 1995a; Kano et al., 1998; Zhu and Yu, 2004). As an example, Fig. 20 shows the effects of the orifice size, friction and damping coefficients between particles and wall roughness on discharge rate of particles from a cylindrical hopper with flat bottom. Other properties such as hopper geometry and operation also affect the discharge rate. For example, the discharge rate largely depends on the hopper orifice and half-angle (Langston et al., 1994, 1995a; Kano et al., 1998; Zhu and Yu, 2004). The ratio of the discharge rates from a vibrating hopper to a non-vibrating hopper decreases with vibration except at the highest frequencies (Wassgren et al., 2002).

It is important to understand the microscopic structure and its relations to the mechanisms governing hopper flow. DEM simulation takes into account the discrete nature of granular materials, and therefore is very effective for this purpose. In the past, particle velocity or kinetic energy, flow structure and force structure of granular materials in hoppers have been investigated. These studies are mainly focused on two aspects of these properties:

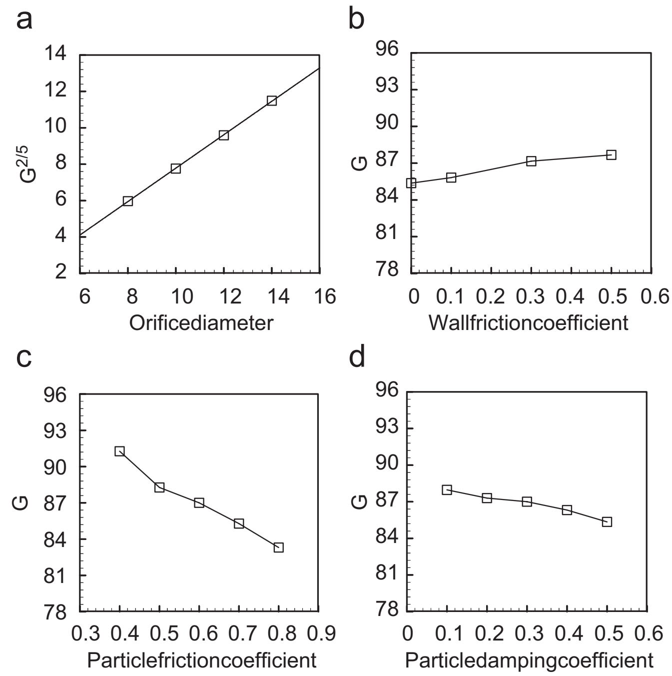

Fig. 20. Dependence of discharge rate (units for discharge rate are $d^2\sqrt{gd}$) on (a) Orifice diameter; (b) Wall friction coefficient; (c) Particle friction coefficient; and (d) Particle damping coefficient (Zhu and Yu, 2004).

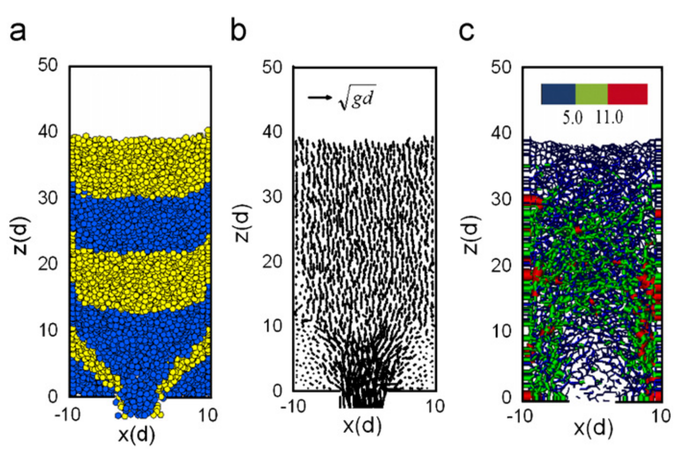

Fig. 21. Snapshots of (a) flow pattern; (b) velocity field; and (c) force structure of the unsteady state granular flow in a cylindrical hopper with flat bottom (Zhu and Yu, 2005a).

Spacial distributions: DEM simulations confirm that there are several different flow zones in a hopper flow (Langston et al., 1994, 1995b, 1996; Rong et al., 1995a,b; Rotter et al., 1998; Parisi et al., 2004). For example, there are generally four flow zones for the granular flow in a cylindrical hopper with flat bottom: stagnant, plug flow, converging flow, and transitional zones (Zhu and Yu, 2004). In different zones, the flow pattern, flow structure (Langston et al., 1997; Zhu and Yu, 2004) and force structures (Langston et al., 1995b; Gutfraind and Savage, 1998; Parisi et al., 2004; Zhu and Yu, 2004, 2005a) are different as, for example, shown in Fig. 21. These studies indicate that hopper flow can be qualitatively described in terms of these spacial distributions.

Statistical distributions: DEM simulation results show that the statistical distributions of the properties such as velocity, CN, porosity and force can be used to describe the hopper flow quantitatively. It is suggested that variables such as porosity and force vary in a large range, and force distributions decay approximately in an exponential manner, as shown in Fig. 22. Further comparison between the force distributions for unsteady and steady state flows in a hopper indicates that the steady state flows have less particles with large interaction forces, which can be attributed to macroscopically smaller resistance when particles transforming from plug flow to converging flow for a steady state flow (Zhu et al., 2006). In addition, the effect of hopper geometry and particle properties on the flow has also been quantified by these statistical distributions (Zhu and Yu, 2004).

As discussed by Zhu et al. (2007), through a proper averaging method, macroscopic quantities such as density, velocity, stress and couple stress can be obtained based on DEM results. For hopper flow, the velocity, density, stress and couple stress distributions have been extensively investigated. These distributions are shown largely related to the corresponding microscopic structures. In particular, the results about velocity and mass density are qualitatively in agreement with the experimental results and the microdynamic analysis (Potapov and Campbell, 1996; Zhu and Yu, 2002, 2005b). As an example, Figs. 23(a) and (b) show the velocity and mass density of the granular flow in a cylindrical hopper with flat bottom. The consistency between the micro- and macroscopic variables confirms the applicability of the average method to the granular flow in hoppers. Moreover, the results indicate that the distributions of the stresses are related to the force structures, controlled by the magnitude and direction of the interaction forces and the contact direction between particles (Langston et al., 1995b; Potapov and Campbell, 1996; Gutfraind and Savage, 1998; Masson and Martinez, 2000a,b; Zhu and Yu, 2002, 2005b). Only near the walls of hopper, couple stress is significant; when far from the walls, it can be ignored, as shown in Fig. 23 (Zhu and Yu, 2005b). The results also suggest that the treatments that employ plasticity models under the assumption that the material is always yielding are not valid, and hopper flows cannot be modelled as rapid granular material (Potapov and Campbell, 1996). These studies also indicate that the combined approach of discrete approach and averaging method offers a convenient way to link fundamental understanding generated from DEM-based simulations to engineering application often achieved by continuum modelling.

3.2.2. Flow in mixers

The mixing of particulate materials is a vital operation in various industries such as pharmaceutical, chemical, food, ceramic and metallurgical ones. It is of paramount importance to understand and control mixing behaviour. For example, in the pharmaceutical industry, product homogeneity is an extremely important factor (Muzzio et al., 1997). Inadequate mixing may result in rejection of the finished product because of poor quality. However, compared with fluid mixing, there is not much knowledge about the mixing of granular materials due to the complex dynamic behaviour involved. As a result, to date, reliable design and control of mixing processes are largely ad hoc. This has generated considerable interest leading to extensive research on the subject in the past. Simulation on a particle scale has been recognized as a promising approach in this field (see, for example, Stewart et al., 2001; Zhou et al., 2003c; Bertrand et al., 2005). Mixers studied by DEM include:

- *rotational mixers* such as V-blender (Moakher et al., 2000; Kuo et al., 2002; Lemieux et al., 2007, 2008), tote blender (Sudah et al., 2005; Arratia et al., 2006), and double–cone blender (Moakher et al., 2000);

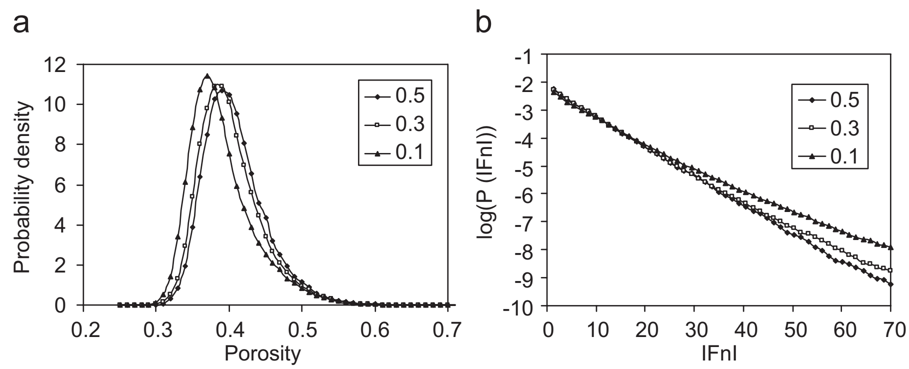

Fig. 22. Statistical distributions of porosity and normal forces of the steady state granular flow in a cylindrical hopper with flat bottom for different wall roughness (Zhu and Yu, 2004).

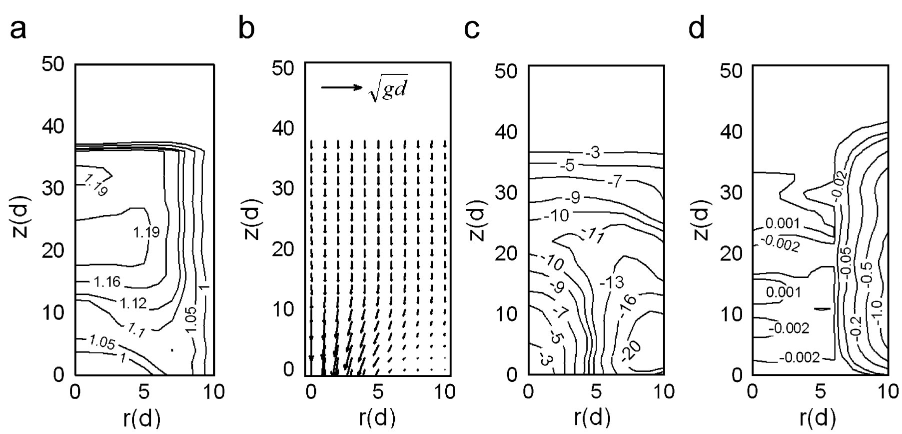

Fig. 23. Distributions of (a) mass density; (b) velocity; (c) stress; and (d) couple stress of the unsteady state granular flow in a cylindrical hopper with flat bottom (Zhu and Yu, 2005a).

- *external surface driven mixers* such as rotor-type mixer (Endoh et al., 2000; Iwasaki et al., 2001; Hotta et al., 2001; Kano et al., 2001), and rotating drum which will be discussed in Section 3.2.3;
- *internal blade driven mixers* such as helical mixer (Gyenis et al., 1999; Kaneko et al., 2000; Schutyser et al., 2003), vertical axis bladed mixer (Stewart et al., 2001; Terashita et al., 2002; Zhou et al., 2003c, 2004d; Kuo et al., 2004; Spillmann et al., 2005; Bertrand et al. 2005; Sato et al., 2008), rotating mixer with baffles (Muguruma et al., 1997; Chaudhuri et al., 2006), and mechanofusion device (Chen et al., 2004).

In these studies, the validity of DEM approach has been examined in various ways, including:

Qualitative, visual comparison of flow pattern: Moakher et al. (2000) considered double-cone and V-blenders, while Iwasaki et al. (2001) studied a high-speed elliptical-rotor-type powder mixer rotor. Their calculated flow patterns are shown to agree with the experimental observations. Fig. 24 gives an illustrating example of the agreement between the numerical and experimental results.

Quantitative particle scale comparison: There is a good agreement between the simulated and measured flow fields of particles under comparable experimental conditions, including the flow of particles in vertical bladed mixer (Stewart et al., 2001), conical helical-blade mixer (Schutyser et al., 2003), V-blender (Kuo et al., 2002), as, for example, shown in Fig. 25. The experimental results are obtained by PEPT.

Other comparisons: Kaneko et al. (2000) used a coloured particle to measure the circulation time in a vessel provided with a helical ribbon impeller, and showed that the computed circulation time agreed well with that of the experiments. Sudah et al. (2005) and Iwasaki et al. (2001), respectively, showed that the calculated values agreed fairly with the experimental data in mixing and segregation rates for different fill levels and loading conditions of tote blender, and in peak height of torque on the rotor shaft and periodicity of a high-speed elliptical-rotor-type powder mixer.

Driven by internal blade or external surface, particles in a mixer often move in a very complicated pattern, although angular rotation is dominant for most considered cases. DEM simulations show that the flow features of particles in different devices are quite different. For a helical mixer, the flow can be divided into three main zones: a small region near the wall where particles are rapidly transported upward, a larger region near the central axis where particles move downward, and top surface region where particles migrate toward the central axis (Schutyser et al., 2003). For a vertical axis bladed mixer, particles rise to form a heap in front of a blade and then either flow downward on the bed surface over the blade or to the base of the heap to rejoin the flow toward the blade, and there is a recirculating zone in front of the blade (Zhou et al., 2003c, 2004d). For a tote blender, the flow is composed of two regions: a high velocity layer cascading atop and a nearly "solid body" rotation region (Arratia et al., 2006). In addition, Moakher et al. (2000) compared the flows in a double-cone blender and a V-blender, and found that the flow in a double-cone blender was nearly continuous and steady, while

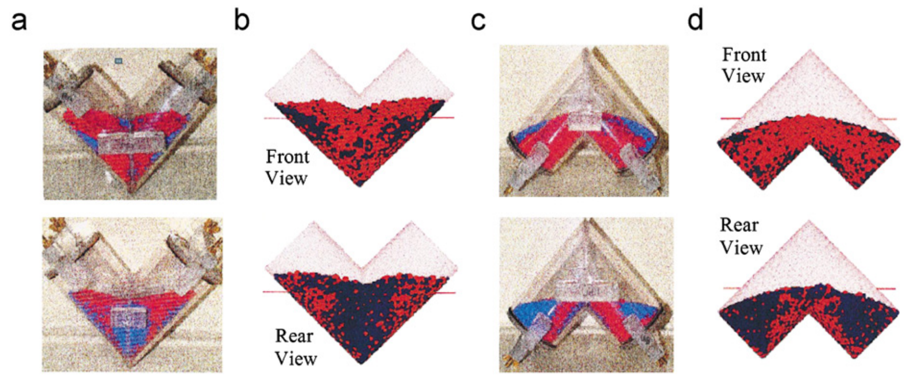

Fig. 24. Patterns from (a) experiment with different size particles in upright transparent V-blender; (b) corresponding simulation after two revolutions; (c) experiment in inverted orientation; and (d) simulation in inverted orientation (Moakher et al., 2000).

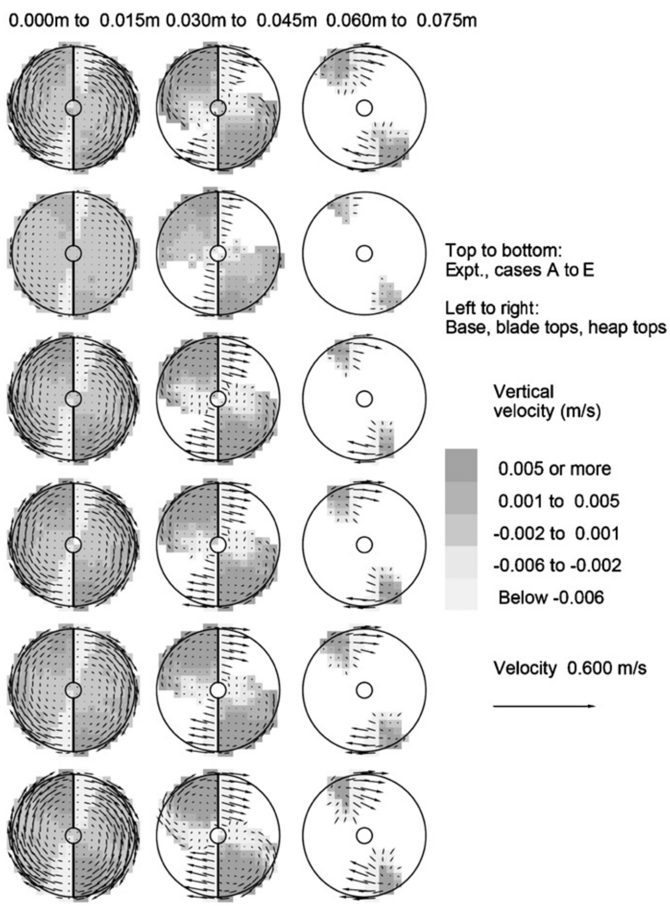

Fig. 25. Velocity fields of a bladed mixer at different heights from PEPT experiment and DEM simulations. The top layer represents the experimental results, while others are the simulated results for five cases with different sliding and rolling friction coefficients: case A, 0.2 and 0.025 mm; case B, 0.3 and 0.0 mm; case C, 0.3 and 0.025 mm; case D, 0.3 and 0.05 mm; case E, 0.5 and 0.025 mm. The cell shade indicates the vertical velocity while the vectors show horizontal velocity (Stewart et al., 2001).

the flow in a V-blender was intermittent and consisted of two very distinct processes. On the other hand, their results also show that the flows in the two blenders may share commonalities: both have the same mixing bottleneck dispersing across a plane of symmetry and asymptotic segregated patterns established quite rapidly and persisting indefinitely.

Optimization of the performance of a mixer is an issue of great significance in industry. Therefore, the study of mixing performance under various conditions is important. DEM simulation has advantage in such studies because mixing behaviour can be readily quantified, even under dynamic states. As discussed above, DEM can predict the degree of mixing and segregation for most of the experiments performed. In addition, through the analysis of the mixing behaviour, useful results, largely for engineering application, have been obtained. Muguruma et al. (1997) predicted that the mixing rate in a rotating mixer could be improved by use of baffles and there was an optimal baffle length/height ratio for particle mixing in the mixer. Terashita et al. (2002) showed that an optimal fill level was around 50% in a high-shear mixer. This optimal fill level provided particles with free space in the agitating vessel, allowing most of the particles to maintain adequate particle velocity and to conduct particle motion. Zhou et al. (2003c) suggested that decreasing the difference in particle size or density considerably improved the mixing performance. Sudah et al. (2005) revealed that the presence of a hopper and bin section in a tote blender, as well as axial offset introduced greater axial mixing rates that would be expected from pure dispersion. Furthermore, Arratia et al. (2006) pointed out that blender suffered from hindered transport across the plane of symmetry. This lack of axial particle dispersion was in part due to the geometrical symmetry of the blender, which constrained particles pathlines. One way to improve mixing in this blender was to break spatial symmetry by designing non-symmetric blenders.

Dynamic information such as transient forces acting on individual particles, which is extremely difficult to obtain by physical experimentation, is very important to understanding the underlying physics in particle flow in mixers. Zhou et al. (2003c) showed that large/light particles in a binary size/density mixing system received a relatively larger upward force than small/heavy ones at an initial mixing stage, generating a driving force for segregation. At the dynamic equilibrium stage, there is a large force fluctuation resulting in chaotic motion of particles to maintain a constant mixing index. Furthermore, Zhou et al. (2004d) suggested that in a vertical bladed mixer, contact forces propagated mainly in the angular direction, starting from the particles in front of the blades where they were driven by the blades and confined by the wall, and then forced to move in the system. This is the reason why particles at the lower part mainly flow in an angular direction. Moreover, the wall generates strong forces to restrict particles flowing outside of the mixer, which causes the particles in front of the blade and those at the top part in particular to move towards to the centre of the mixer. Therefore, the flow and force structures are related. Fig. 26 gives an illustrative example of the force networks of particles in the mixer (Zhou et al., 2004d). On the other hand, Kuo et al. (2002) considered

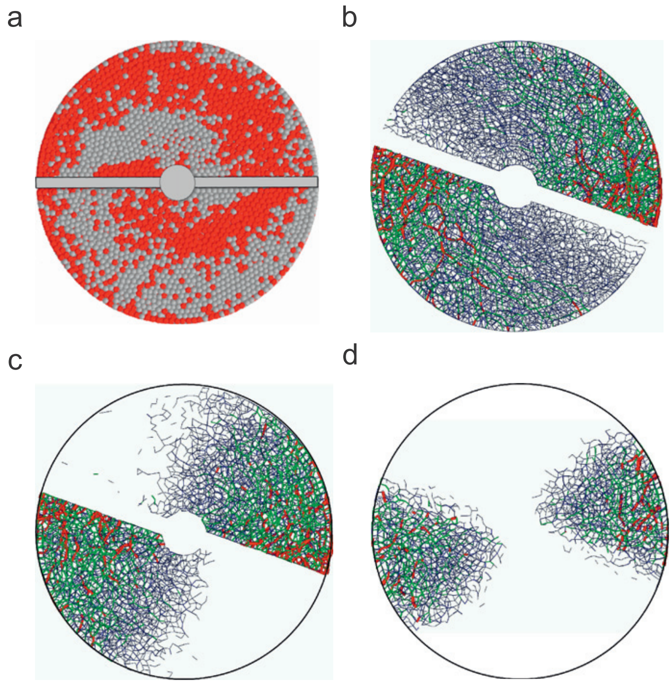

Fig. 26. Flow pattern and normal force network in different horizontal sections at different heights of a bladed mixer: (a) flow pattern; (b) between 0 and 20 mm; (c) between 20 and 40 mm; and (d) between 40 and 60 mm (Zhou et al., 2004d).

the influence of particle properties related to interparticle force on particle motion in a V-mixer, and showed that the friction affected the particle transition from the static to the dynamic state more significantly and the restitution coefficient had a greater influence on the behaviour of moving particles.

3.2.3. Flow in drums and mills

Particle flow in rotating drums and mills exhibits a range of complex phenomena, such as avalanche, segregation and convection. This has generated considerable interests among physicists in the recent years (Ottino and Khakhar, 2000). On the other hand, drum and mill are common devices in industry for mixing, drying, milling, coating or granulation/agglomeration. Therefore, knowledge of the dynamics of particles in a drum or mill is also of high interest in engineering. Over the past few decades, many experimental efforts, mainly at a macroscopic scale, have been done in this area. However, to date, it is still difficult to generate a reliable method for process design and control without substantial empirical input. To overcome this problem, some non-invasive experimental techniques have been developed to investigate the flow dynamics at a microscopic or particle level, such as PEPT (Broadbent et al., 1995; Parker et al., 1997) and MRI (Nakagawa et al., 1993). While these experiment techniques have been useful, they all have their limitations as discussed earlier.

DEM has been applied to this area since 1990s in order to develop a better understanding of the particle dynamics. These studies include:

- *Drum* mainly the horizontally rotating drums (Buchholtz et al., 1995; Poschel and Buchholtz, 1995; Shoichi, 1998; Wightman et al., 1998; Dury et al., 1998a,b; Dury and Ristow, 1999a,b; Yamane et al., 1998; Schutyser et al., 2001; Yamane, 2001, 2004; Olivi-Tran et al., 2002, 2004; Rapaport, 2002; Yang et al., 2003b, 2008c; Taberlet et al., 2004, 2006a,b; Finnie et al., 2005; Pandey et al., 2006; Kwapinska et al., 2006; Taberlet and Richard, 2006; Faqih et al., 2006; Sakai et al., 2006; Portillo et al., 2007).
- *Mill* including tumbling ball mill (Mishra and Rajamani, 1990, 1992, 1994; Inoue and Okaya, 1996; Agrawala et al., 1997; Cleary, 1998, 2000, 2001a; Datta et al., 1999; Misra and Cheung, 1999; van Nierop et al., 1999; Buchholtz et al., 2000; Rajamani et al., 2000a,b; AbdEl-Rahman et al., 2001; Mishra and Thornton, 2002; Venugopal and Rajamani, 2001; Datta and Rajamani, 2002; Monama and Moys, 2002; Hlungwani et al., 2003; Mishra, 2003a,b; Kalala and Moys, 2004; Mori et al., 2004; Powell and McBride, 2004; Kwan et al., 2005; Djordjevic, 2005; Kalala et al., 2005a,b; Cleary et al., 2006a; Gudin et al., 2006, 2007; Makokha et al., 2007; Morrison et al., 2007), planetary ball mill (Dallimore and McCormick, 1997; Rajamani et al., 2000a,b; van Nierop et al., 2001; Dong and Moys, 2002; Feng et al., 2004a), centrifugal mill (Hoyer, 1999; Inoue et al., 1999; Cleary, 2000, 2001b; Cleary and Hoyer, 2000; Cleary and Sawley, 2002), AG/SAG mill (Bwalya et al., 2001; Cleary, 2001a,b, 2004, 2006; Cleary et al., 2003; Djordjevic et al., 2004, 2006; Morrison and Cleary, 2004),rod mill (Cleary, 2004), jet mill (Han et al., 2002), stirred mill (Yang et al., 2006a; Jayasundara et al., 2006, 2008; Sinnott et al., 2006; Cleary et al., 2006b), and granulator (Mishra et al., 2002).

Flow pattern of particles in a rotating drum varies. Six flow regimes have been observed in the transverse direction over a range of rotational speeds (Henein et al., 1983). Some of these regimes have been reproduced by DEM simulations (Poschel and Buchholtz, 1995; Dury and Ristow, 1999a,b; Monama and Moys, 2002; Olivi-Tran et al., 2002, 2004; Cleary et al., 2003; Pandey et al., 2006; Yang et al., 2008c). It has been observed that at a low speed with particles moving in a stick-slip mode, there are avalanches of different size at the surface of the granular material, and there are unstable convection cells at a very low but constant angular velocity. These observations are important to understanding the dynamics of the flow (Poschel and Buchholtz, 1995). In the rolling regime, the flow in a rotating drum has an even surface. The dynamic angle of repose of granular material depends on the angular velocity, and is significantly higher at the end caps than in the middle of three-dimensional rotating drum (Dury et al., 1998b). By varying parameters such as drum diameter and length, particle size and density, gravitational acceleration and rotation speed, Dury et al. (1998b) proposed a characteristic length zeta which scales with the drum size but does not depend on either the density or the gravitational constant. For larger rotating speeds, the surface profile is not close to an even plane but reveals typical S-shape (Poschel and Buchholtz, 1995). Taberlet et al. (2006b) suggested that the S-shape was caused by the friction on the drum end. They also proposed a theoretical model which accounts for the effect of the end plates and the equation of the shape of the free surface. The model reveals a dimensionless number which quantifies the influence of the end plates on the shape of the pile. Different flow regimes have recently been simulated and analysed in relation to drum rotation speed and material properties (Yang et al., 2008c; McElroy et al., 2008) Also, extensive comparison has been made between simulated and measured results and shown a good agreement in terms of flow or mixing pattern (Yamane et al., 1998; Yamane, 2001), angle of repose (Yamane et al., 1998; Yamane, 2001; Yang et al., 2003b), and velocity field (Yamane, 2001; Yang et al., 2003b), as, for example, shown in Fig. 27. These studies confirm the applicability of DEM to the study of particle flow in drums.

The flow patterns in a rotating drum is heavily dependent on particle shape. For example, the inclination with non-circular particles are observed to be approximately twice of that with circular ones (Buchholtz et al., 1995; Poschel and Buchholtz, 1995). Simulations with non-spherical particles can reproduce the stick-slip mode which is unable to be achieved for spherical particles (Poschel and Buchholtz, 1995). It is believed that mircostructures of spherical particles have very weak resistance to shear and the particle assembly flows partly by avalanching and partly by slumping. This slumping reduces the frequency of avalanches, the proportion of

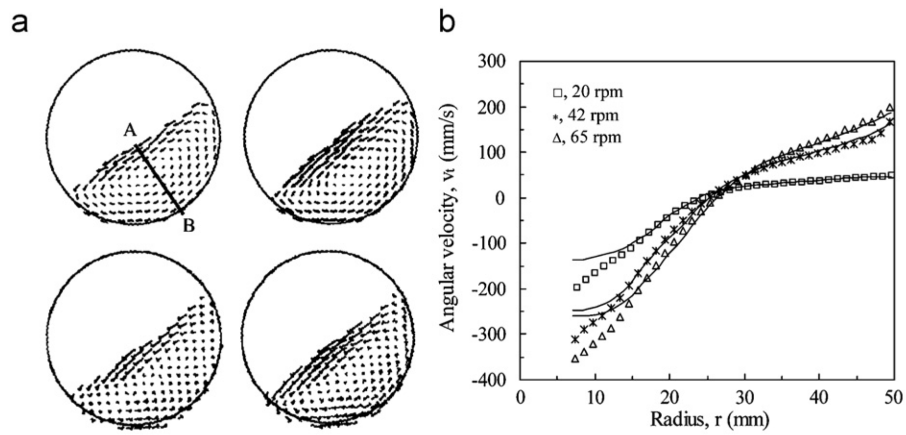

Fig. 27. (a) Velocity fields in a plane section taken from simulation (top) and PEPT experiment (bottom) at rotation speeds of 20 rpm (left) and 42 rpm (right); (b) angular velocity along the radius perpendicular to the flowing surface (line AB in the left figure) at different rotation speeds. Points are the simulation results, and solid lines are the PEPT measurements (Yang et al., 2003b).

avalanches with both materials present, and the energy available in each avalanche (Cleary, 2000).

Mixing is one of the significant phenomena in particle flow in rotating drum, which has been extensively studied (Ristow, 1996; Wightman et al., 1998; Cleary, 2000; Schutyser et al., 2001; Finnie et al., 2005; Kwapinska et al., 2006; Taberlet and Richard, 2006; Van Puyvelde, 2006). In horizontal rotating drums, there are generally two types of mixing: longitudinal and transverse. Finnie et al. (2005) suggested that mixing in the longitudinal direction could be described by the diffusion equation. The diffusion coefficient is shown to increase linearly with rotational speed, while the influence of the filling degree is relatively small. On the other hand, mixing in the transverse plane is much faster and can be characterized by an "entropy"-like mixing index. Their simulation results also show that this mixing index varies exponentially with the number of revolutions of the rotating drum. This transverse mixing speed decreases with increasing rotational speed and filling degree.

Particles may segregate if they are different (Cleary, 1998; Shoichi, 1998; Yamane, 2001, 2004; Rapaport, 2002, 2007; Taberlet et al., 2004). Similar to mixing, there are two types of segregation in rotating drums: radial and axial segregation. Radial segregation can be caused by difference in particle size or density (Ristow, 1994; Yamane, 2001; Dury and Ristow, 1999a,b). Ristow (1994) considered the effect of density and found that the heavier ones of equal-size particles were located near the mass centre of the particles in a drum. Dury and Ristow (1999a) studied the dynamics of size segregation of binary particle mixtures, and showed that particles had maximum segregation for a more than half-filled drum due to the non-zero width of the fluidized layer, radial segregation occurred for any arbitrary small particle size difference, and the final degree of segregation was linearly dependent on the size ratio of the two particle species. These authors further investigated the combined size and density effect by simulating radial segregation of a binary mixture in a three-dimensional cylinder (Dury and Ristow, 1999b). By fixing the size ratio of a binary particle mixture and varying the density of the smaller particles, they found a surprising segregation dynamics in the case of a counterbalance of size segregation by density segregation. The system was prepared to have a sharp interface of small and large particles initially. If the smaller particles also had the higher density, the radial segregation process was enhanced. On the other hand, if the smaller particles had the lower density, the radial segregation could be counterbalanced leading to a well-mixed final state.

Under suitable conditions, axial segregation can occur, with the particles separating into a series of bands perpendicular to the axis. The formation of axially segregated bands is the most basic of the effects, and the fact that segregation occurs under a variety of conditions is a measure of the success of the model (Rapaport, 2002). Shoichi (1998) demonstrated that particles of different sizes and different surface roughness segregate into bands in axial direction. His results suggested that segregated narrow bands were formed by diffusion process and avalanches, and that the cohesive forces operating at the boundaries stabilize them. The significant role of both avalanches and diffusion has also been observed by Rapaport (2002). Taberlet et al. (2004) showed that axial segregation may occur in a mixture of two species of particles differing by size only (i.e., equal densities, frictional properties, Young's modulus, etc.). They introduced a segregation function to measure the degree of axial segregation in the medium, which allows for precise measurement of the period of band oscillations and showed that the coarsening process can stop or slow dramatically when the radial core breaks. Fig. 28a is a space–time diagram and the pixel is black if the concentration in small beads is higher than its average value showing the evolution of this system. The plot shows bands appearing shortly after the rotation starts, with bands disappearing and merging with one another. Fig. 28b shows the snapshots of the drum at different times during the coarsening, clearly indicating the birth and merging of bands. Furthermore, Taberlet and Richard (2006) showed that the diffusion coefficient is independent of particle size.

The microdynamic structure of particles in drum was analysed by Yang et al. (2003b). Based on the DEM data, both spatial and statistical distributions of microdynamic variables related to flow structure such as porosity and CN, and force structure such as particle interaction forces, relative collision velocity and collision frequency have been established. Fig. 29 gives an illustrative example. The dependence of flow behaviour on rotation speed was also analysed. These authors demonstrated that the resulting microdynamic information is useful in understanding the observed effect of rotation speed on agglomeration.

Mills, extended from rotating drums, are the primary grinding equipments in industries. They consume a large amount of energy, and consequently, the power cost can be as high as half the total processing cost (Prasher, 1987). Mill operators often have to assess the power consumption of mills for an entirely different set of operating conditions or for a reconfigured circuit. Therefore, understanding the dynamics of particle flow in mills is critical to mill design and optimization. Much of the previous research on DEM simulation is aimed at the flow pattern, power draw, intensity of collisions and wear rate of liners. Mishra (2003a,b) has given a detailed review in this aspect. Here, we only briefly highlight several key issues.

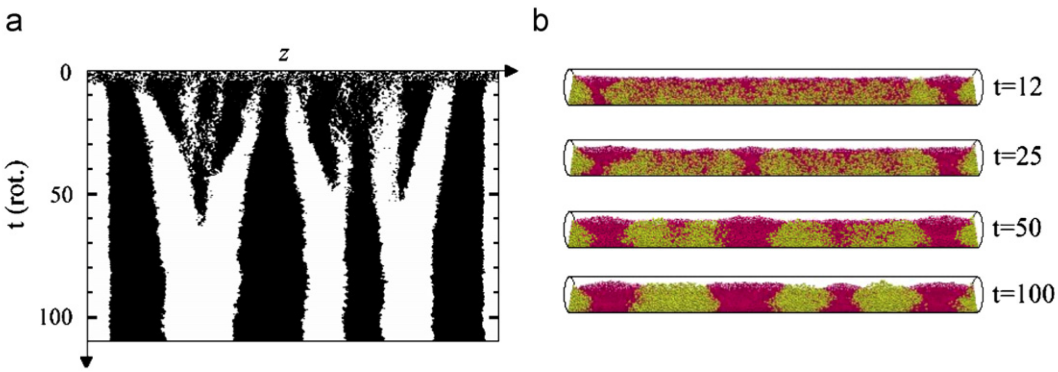

Fig. 28. (a) Space–time plot showing regions of high small-bead concentration and (b) snapshots of the drum during the coarsening (Taberlet et al., 2004).

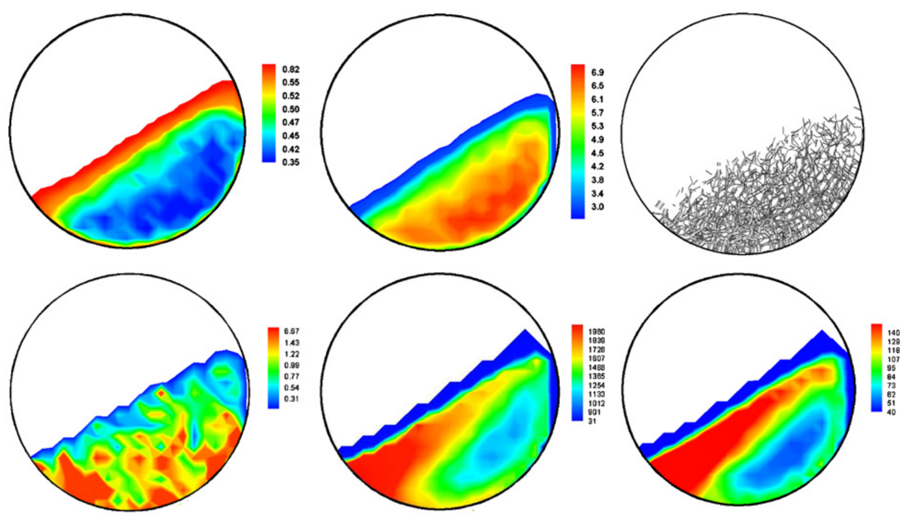

Fig. 29. Time-averaged spatial distribution of (from left to right and from top to bottom): porosity, coordination number, (snapshot) force network, total force (mg), collision velocity (m/s), and collision frequency (1/s) in a cylindrical rotating drum for granulation when rotation speed is 20 rpm (Yang et al., 2003b).

Flow pattern: Mishra and Rajamani (1994) performed two-dimensional simulation of the ball charge motion in a ball mill, compared the observed toe and shoulder positions of the charge with experiments and found a good agreement between the numerical and experimental results. They also pointed out that, to produce mostly cascading motion and very little tararatting of balls, the mill should be operated at an intermediate speed. Cleary (1998) showed that there were two basic mechanisms producing size segregation in mills: at low speeds the segregation is produced by percolation of fines through the surface avalanching layers. This causes large particles to migrate to the outside of the charge. Within a deforming or flowing granular medium, the second mechanism (Brazil nut effect) causes large particles to move against the acceleration field and smaller particles to move in its direction. Jayasundra et al. (2006) considered a stirred mill, i.e., the so-called Isamill, where particles are driven by rotating discs with holes, and showed that the particles in the mill are drawn into disc holes at the lower radius side, and then ejected back into the bulk of particles from the upper radius of the disc, causing circulating flow.

Power draw: Power draw is an important parameter to test the validity of DEM models and to characterize the mill performance. Using a particular friction model with the friction coefficient increasing linearly with rotation speed, Mishra and Rajamani (1992) predicted the power draw of production mills with reasonable accuracy over a wide range of speeds. Cleary (1998) observed that the power draw increases linearly with speed until the peak is attained for 80–100% of the critical speed of mill and then decreases (Fig. 30). It is also observed that changing material properties, such as coefficients of restitution and sliding friction, has little effect on the power draw. Jayasundra et al. (2006) compared the power draw of a stirred mill at different speeds and solid loadings. Their work showed that the overall results from simulations and experiments are quite comparable, all indicating that the power draw increases with rotation speed and solid loading. The small discrepancy at high rotation speeds was attributed to the mechanical and other energy losses (e.g., sound and heat) in the experiments, which are not considered in the simulation.

Interparticle collision: Collision frequency and collision energy are two critical parameters to determine milling performance, but are difficult to obtain from experiments. With DEM simulation, this type of information can be readily obtained (Mishra and Rajamani, 1994; Inoue and Okaya, 1996; Cleary, 1998; Inoue et al., 1999; Hoyer, 1999; Yang et al., 2006a; Jayasundara et al., 2006). Inoue and Okaya (1996) and Inoue et al. (1999) studied the energy distribution in a centrifugal mill and found that the energy dissipation was maximal at filling level of 0.6–0.8, depending on the mill parameter and also other parameters. Hoyer (1999) showed that the collision energy distribution can be fitted by a Gaussian distribution and varied with ball size and density, mill speed and mill diameter. Jayasundara et al. (2006) suggested that the collision energy is related to the collisional force, which can be used as indicators of breakage and attrition (Fig. 31).

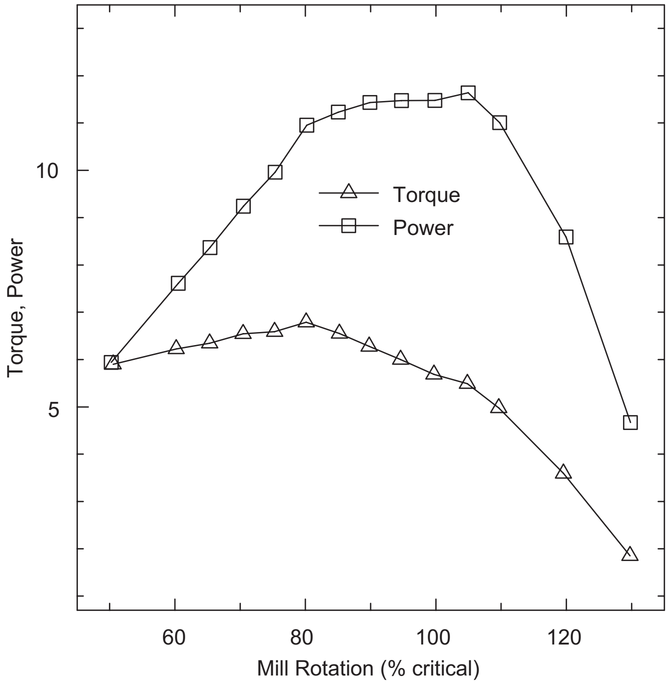

Fig. 30. Average torque and power as a function of rotation speed of a ball mill (Cleary, 1998).

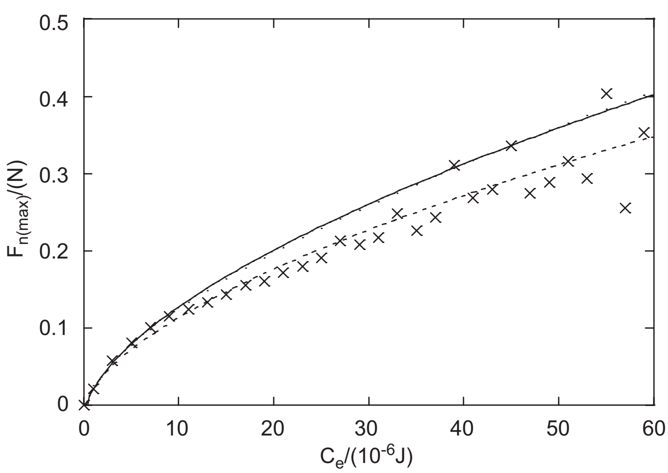

Fig. 31. Relationship between the collision energy and the maximum force. The cross symbols and the dotted line represent the numerical results, and the solid line represents the theoretical results (Jayasundara et al., 2006).

They also observed that the impact energy intensity (i.e., the total collision energy per unit time per particle), which was demonstrated to have a linear correlation with grinding rate (Kano and Saito, 1998), is a useful parameter to characterize the grinding process.

Liner wear: The wear of liners affects the load behaviour and the performance of mills. The accurate prediction of the evolving mill liner profile due to wear is therefore important. For example, it can be used to determine the optimal initial lifter design for a particular operation. Cleary (1998) modelled the evolution of the liner profile to predict the lifter life cycle and its effect on the mill operation. Djordjevic et al. (2004) found that the distribution of the impact energy is affected by the number of lifters, lifter height, mill speed and mill filling. Furthermore, Kalala and Moys (2004) and Kalala et al. (2005b) proposed a mathematical model based on DEM results, taking into account adhesion, abrasion and impact wear to predict the loss of material on liners.

3.3. Summary and discussion

The intrinsic macroscopic characteristics of materials, as the main aspect of the earlier experimental and analytical approaches, have been extensively studied by DEM for various simplified particle systems. These studies mainly focus on the evolution of volumetric strain and stress during deformation, dependence of stress on strain and its gradients, the relationship of axial strain with volumetric strain and void ratio, and other intrinsic characteristics of particle flow. Such a study takes into account the discrete nature of granular materials without requiring any global assumption needed in the previous macroscopic approaches and thus allows a better understanding of the fundamental mechanisms of particle flow. Moreover, DEM results have also been increasingly used to test the conventional theoretical approaches on macroscopic description of particle system based on some assumptions. Some theories have been shown to agree with DEM results under some conditions, while the shortcomings of these theories have also been shown in this comparison exercise.

Nonetheless, particle flows related to various industrial problems have been studied by DEM to elucidate the mechanisms governing the dynamics of granular materials. Compared with the traditional studies, the advantage of DEM simulation study is obvious, as the flow pattern, velocity field, solid fraction, granular temperature and force structure can be readily obtained. Various comparisons of DEM results with experimental data have been conducted. It has been reported that the flow patterns and velocity distributions from DEM simulations are in good agreement with the experimental results in various cases, which validate the applicability of DEM to these systems. The microscopic analysis is mainly focused on two aspects of these properties: spatial and statistical distributions, which has been demonstrated to be very important to understanding the physics of particle flow. New insights about the microscopic origins of the macroscopic properties of particle flows have been obtained from the analysis of the microstructures such as displacement fields and force transmission.

The behaviour of particle flows is affected by many variables related to system geometry, operational condition and material properties. Some variables are difficult to investigate experimentally. But this difficulty can be overcome readily in numerical experiments. The influence of some properties on the dynamic behaviour of particle flows under different conditions has been quantified by means of DEM simulations. It is expected that DEM will play a more and more significant role in the research of this type.

Clearly, DEM is a very useful technique to study the physics of particle flow. However, there are still limitations in the previous work. For example, the number of particles that can be dealt with at the moment is limited, and most studies are focused on spherical particles. So, future effort will be made to develop more robust models and efficient computer codes so that the particle scale simulation can be extended to process simulation to meet real engineering needs. In the mean time, as an effective technique, DEM will continue to play an important role in the study of the physics and long-standing fundamental problems of particle flow.

One of the main challenging tasks is to develop a proper constitutive relationship for the macroscopic description of particle flow. In the past, various models have been proposed to derive the constitutive equations for the rate-independent deformation and rapid flow of granular materials. However, to date, there is no accepted continuum theory applicable to the transitional regime that heavily involves both collisional and frictional mechanisms. Such work is highly demanded, because the majority of particle flows in practice are in this regime. The new theory should remove the restrictions of the traditional analysis and theory, reflect the influence of physical properties of particles and their interactions, and be suitable for general application. DEM offers a very promising opportunity to generate a solution to this important problem.

4. Particle-fluid flow

Particle flow is often coupled with fluid (gas and/or liquid) flow. In fact, coupled particle–fluid flow can be observed 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 formulation of strategies for process development and control. This necessitates a multiscale approach to understand the phenomena at different length and time scales (see, for example, Villermaux, 1996; Xu and Yu, 1997; Li, 2000; Yu and Xu, 2003; Li et al., 2004a; Tsuji, 2007). In the past, many studies have been done at either atomic/molecular scales related to the thermodynamics and kinetics or large scales related to the macroscopic performance of an operational unit or plant. However, what is missing is the quantitative understanding of microscale phenomena related to the behaviour of particles, droplets and bubbles. Without this information, it is difficult to establish a general method for reliable scale-up, design and control of particulate processes of different types. Therefore, particle scale modelling of particle–fluid flow has been a research focus in the past decade. DEM plays an important role in this development (Yu and Xu, 2003; Yu, 2004). When applied to particle–fluid flow, the fluid phase can be modelled at different time and length scales from discrete (e.g. molecular dynamics simulation (MDS), lattice-Boltzman (LB), pseudo-particle method (PPM)) to continuum (direct numerical simulation (DNS), large eddy simulation (LES), and other conventional CFD techniques including two fluid model (TFM) description). The advantages/disadvantages of different model combinations have been discussed (Zhu et al., 2007). As pointed out by Yu and Xu (2003), at this stage of development, the difficulty in particle–fluid flow modelling is mainly related to solid phase rather than fluid phase. Therefore, the CFD-DEM approach 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. In the approach, the motion of individual particles is obtained by solving Newton's equations of motion while the flow of continuum gas is determined by the CFD on a computational cell scale (Tsuji et al., 1993; Hoomans et al., 1996; Xu and Yu, 1997, 1998).

The theoretical treatments of CFD-DEM have been extensively reviewed in our previous work (Zhu et al., 2007). Therefore, the present review is mainly focused on the application of the CFD-DEM approach to the study of particle–fluid flows. It is an extension of the previous reviews (Yu and Xu 2003; Deen et al., 2007). For convenience, the previous studies are divided into three categories: fluidization, pneumatic conveying/pipeline flows, and process studies.

4.1. Fluidization

Gas fluidization is observed when gas continuously flows upward through a bed of particles at an appropriate flow rate. It exhibits complex and intriguing flow patterns. The mutual interaction between the discrete particles and continuum gas provides an ideal environment for rapid heat and mass transfer, good mixing of solids and fast chemical reaction inside a fluidized bed. These features are very desirable for many industrial applications. There have been extensive research activities in the area of gas fluidization over the past few decades (see, for example, Davidson et al., 1985; Grace, 1986; Bi and Grace, 1995). As noted by Xu and Yu (1997), although a large amount of data have been accumulated from both laboratory experiment and plant practice, a comprehensive interpretation of these data is difficult, if not impossible, as the information obtained from an experiment is usually incomplete due to the limitation of measurement technique. To date, information on the transient forces acting on individual particles during fluidization is still unavailable. These forces are believed to be key factors responsible for the complex flow phenomena in a fluidized bed. Information about the flow mechanisms is expected to obtain with the aid of mathematical modelling. The TFM approach, as summarized by Gidaspow (1994), can provide useful information about the gas–solid flow and has actually dominated the modelling of fluidization processes for years. However, in addition to the difficulty of providing constitutive correlations for the inter-phase transfer of mass, momentum and energy within its continuum framework, this approach is unable to model the discrete flow characteristics of particles of different properties. But these problems can be readily overcome by the coupled approach of CFD-DEM (Zhu et al., 2007). Therefore, CFD-DEM has been widely used to investigate the gas fluidization under various conditions, which mainly includes:

- *Cohesionless particles* including monosized particle systems (Tsuji et al., 1993, 1998, 1999, 2008; Tanaka et al., 1993; Hoomans et al., 1996, 1998, 2000, 2001; Xu and Yu, 1997, 1998; Gera et al., 1998; Ouyang and Li, 1999; Jie and Li, 1999; Xu et al., 2000, 2001a; Kawaguchi et al., 1998, 2000a; Lu et al., 1999; Yuu et al., 2000a; Rong et al., 1999; Rong and Horio, 2001; Goldschmidt et al., 2002, 2004; Kafui et al., 2002; Bin et al., 2003; Wang and Rhodes, 2003, 2004, 2005; Zhou et al., 2003a, 2004a–c; Takeuchi et al., 2004, 2005, 2008a; Feng and Yu, 2004a; Swasdisevi et al., 2004, 2005; Lu et al., 2005, 2006; Link et al., 2005; Chiesa et al., 2005; Wen et al., 2005; Zhong et al., 2006; Chaikittisilp et al., 2006; Li and Kuipers, 2007; Weber and Hrenya, 2007; Tian et al., 2007; Sun et al., 2007; Nakamura et al., 2007; Nakamura and Watano, 2007; Di Renzo and Di Maio, 2007; Deen et al., 2007; van der Hoef et al., 2008; Zhao et al., 2008a,b; Müller et al., 2008; Godlieb et al., 2008; Di Renzo et al., 2008;Chu and Yu, 2008) and multi-sized particle systems (Hoomans et al., 2000; Rhodes et al., 2001b; Limtrakul et al., 2003, 2004; Bokkers et al., 2004; Feng et al., 2004b; Feng and Yu, 2004b, 2007; Dahl and Hrenya, 2005; Lu et al., 2007; Beetstra et al., 2007; Link et al., 2008a,b; Christensen et al., 2008; Gui et al., 2008).
- *Cohesive particles* (Umekage et al., 1998; Mikami et al., 1998; Xu et al., 1999, 2001b, 2002a; Rhodes et al., 2001a,c; Kuwagi and Horio, 2002; Xu and Yu, 2002; Yu and Xu, 2003; Ye et al., 2004, 2005a,b; Zhang et al., 2005; Pandit et al., 2005, 2006, 2007; Limtrakul et al., 2007; Moreno-Atanasio et al., 2007).

Recently, CFD-DEM has been further extended to study heat transfer and combustion in different particle–fluid flow systems (Kaneko et al., 1999; Li and Mason, 2000, 2002; Peters, 2002; Li et al., 2003a,b; Zhou et al., 2003a, 2004c, 2006, 2007; Swasdisevi et al., 2005; Malone and Xu, 2008; Feng et al., 2008).

4.1.1. Fluidization of cohesionless particles

The applicability of the CFD-DEM modelling in gas fluidization has been verified by extensive comparison with experimental results either qualitatively or quantitatively. There are many case studies showing that CFD-DEM can reproduce the flow patterns observed under different experimental conditions (Tsuji et al., 1993, 1999; Tanaka et al., 1993; Hoomans et al., 1996; Xu and Yu, 1997, 2002; Kawaguchi et al., 1998; Lu et al., 1999, 2005; Yuu et al., 2000a; Xu et al., 2001a; Limtrakul et al., 2003; Feng et al., 2004b). As an example, Fig. 32 shows the comparison between physical and numerical experiments for size segregation in gas fluidization of binary mixtures of particles (Feng et al., 2004b), while Fig. 33 shows the calculated and measured flow patterns of the gas–solid flow under

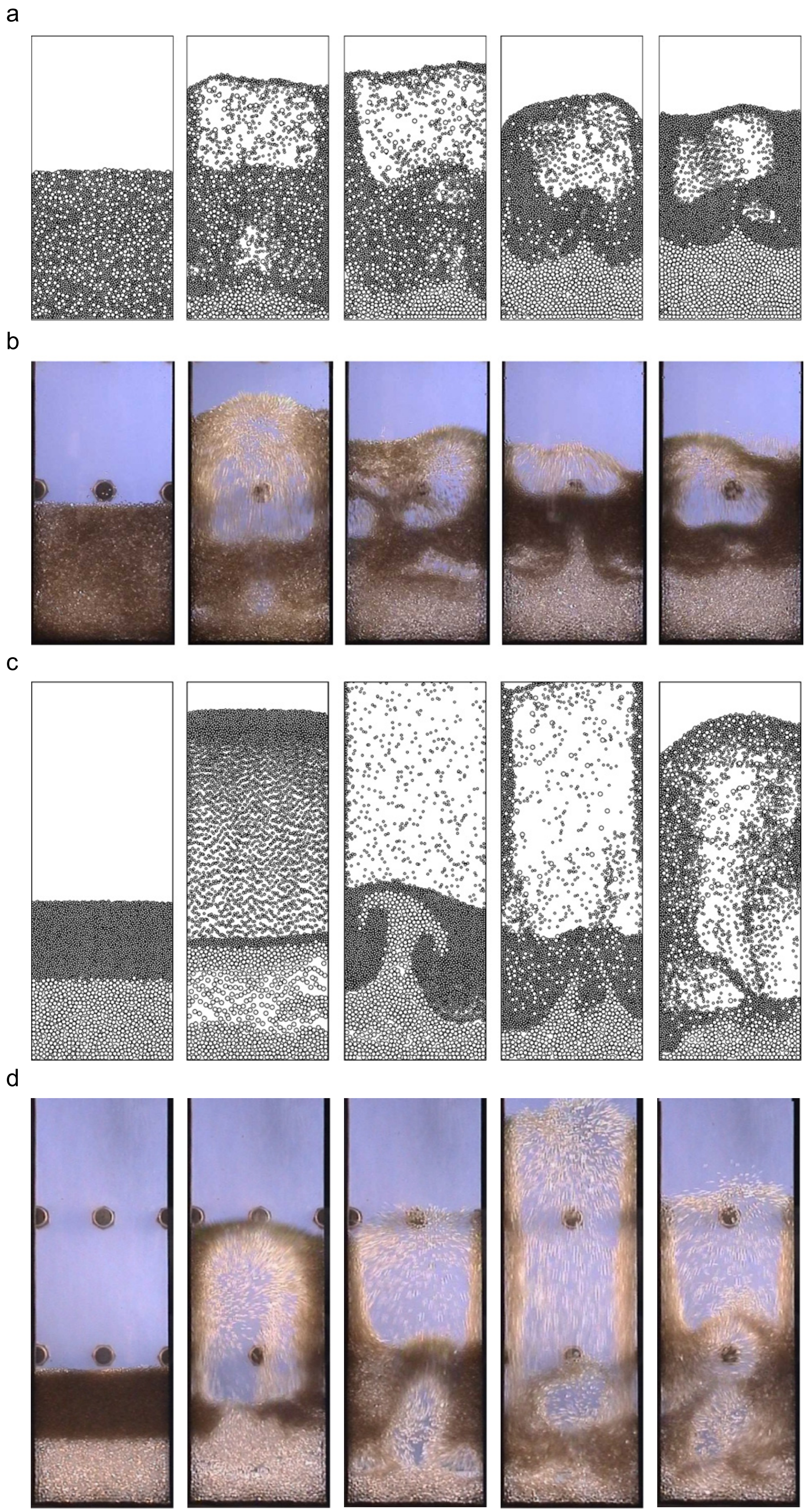

Fig. 32. Snapshots for size segregation in gas fluidization of binary mixtures of particles: (a) the simulated, and (b) the experimental snapshots when gas superficial velocity is 1.3 m/s, and initial state is well mixed; (c) the simulated and (d) the experimental snapshots when gas superficial velocity is 1.8 m/s, and initial state is fully segregated (Feng et al., 2004b).

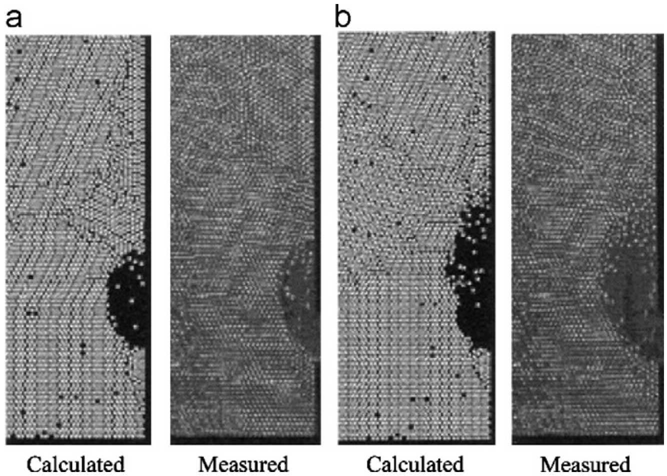

Fig. 33. Comparison between the simulated and measured internal circulating flow of particles when the gas velocity is laterally blasted into a packed bed at different velocity: (a) 25 m/s and (b) 26 m/s. The measured results are obtained by means of a high speed digital video camera (Xu et al., 2001a).

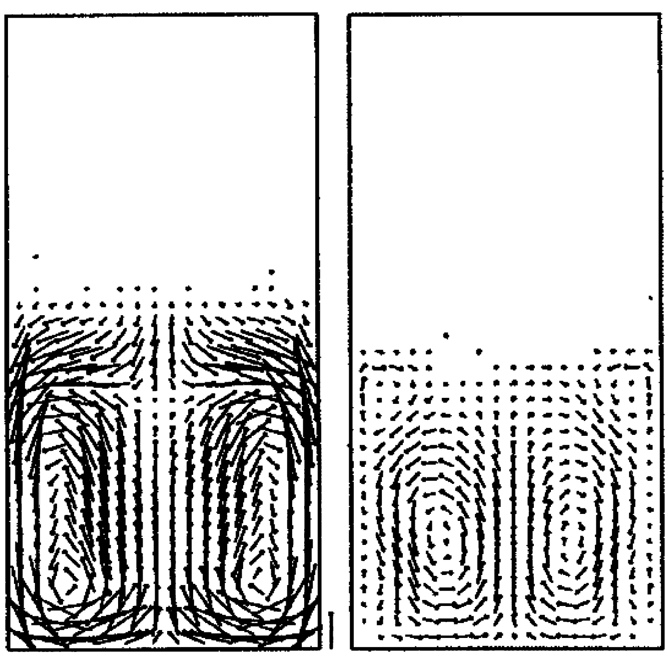

Fig. 34. Velocity map obtained from the PEPT data (left) compared with the velocity map of the simulation assuming fully elastic, perfectly smooth collisions (right) (Hoomans et al., 2001).

raceway conditions (Xu et al., 2001a). Quantitatively, good agreement between the simulated and measured velocity fields has also been observed. For example, Hoomans et al. (2001) showed that the velocity map obtained from the PEPT is similar to that simulated (Fig. 34). In addition, the trajectory of selected individual particles has also been compared. For example, Xu and Yu (1997) showed that the trajectory of a particle initially located in the jet region of a fluidized bed wandered everywhere in the bed. Although dominated by the up-and-down movement, the particle can shift from left to right or vice versa. These observations are qualitatively consistent with the PEPT findings obtained by Seville et al. (1995).

It is generally believed that continuum-based models, e.g., TFM, are limited by the shortage of reliable constitutive correlations in modelling particle–fluid flow. The discrete approach such as CFD-DEM can generate rich information about the hydrodynamics of particle–fluid flow, which can be used for the establishment of improved constitutive correlations for continuum models (Zhu et al., 2007). The generated results by two approaches have been compared (Tsuji et al., 1998; Chiesa et al., 2005; Goldschmidt et al., 2002, 2004). For example, as revealed by Goldschmidt et al. (2004), continuum models can predict the right fluidization regime and trends in bubble sizes and bed expansion, but the predicted bed expansion dynamics differ significantly from the experimental results. However, CFD-DEM can produce superior resemblance with the experimental results.

The particle–fluid flow behaviour in a fluidized bed can be very complex as, for example, demonstrated by the varying anisotropic particle velocity distributions (Lu et al., 2005; Goldschmidt et al., 2002, 2004; Li and Kuipers, 2003, 2005). Clusters and bubbles are the two most common features observed in gas fluidization, which have significant influence on the performance of a fluidized bed (Yuu et al., 2001b). Traditionally, the formation of bubbles has been studied using continuum approaches by, for example, Ding and Gidaspow (1990), Kuipers et al. (1992), Pain et al. (2001), and Guenther and Syamlal (2001). But the mechanisms of the bubble dynamics have not been identified in these studies due to the limitation of the adopted approaches. The CFD-DEM simulations have shown that it is achievable to examine the mechanisms of the various bubble dynamics, for example, bubble formation, coalescence and disruption in a bubbling fluidized bed (Yuu et al., 2001a,b, 2005a; Ouyang and Li, 2001; Annaland et al., 2006). In particular, it has been suggested that the very high air fluctuating kinetic energy in the fluidized bed is mainly yielded by the pressure gradient velocity correlations and dissipated by the air particle interactions (Yuu et al., 2001a, 2005a). This indicates that the suitable expression of the pressure term in a continuum model is very important for the correct description of particle phase in a fluidized bed.

The flow behaviour in fluidization is affected by operational conditions, particle characteristics and bed geometry. CFD-DEM can be used to examine the effects of variables of interest under well-controlled conditions. For example, Li and Kuipers (2002) observed that an elevated pressure reduces the incipient fluidization velocity, widens the uniform fluidization regime, shortens the bubbling regime and leads to a quick transition to the turbulent regime. Liu et al. (2002) revealed that the minimum fluidization velocity decreases with increasing ambient air temperature for Geldart B particles, while it increases for Geldart D particles. Wang and Rhodes (2004) presented an investigation of the effect of increased "gravity" on the characteristics of gas fluidization, indicating that the effect resembles that caused by increasing particle density, and it is closely associated with the need for increase in superficial gas velocity. Recently, Kleijn van Willigen et al. (2008) studied an electric-field enhanced fluidized bed, and revealed a significant reduction of bubble size, both for horizontal and vertical electric fields. When the field strength is strongly increased, particles form strings in the direction of the field. Kawaguchi et al. (2000a) and Takeuchi et al. (2004, 2005, 2008a) studied spouted beds with different geometry. The spouted beds are conical or conical–cylindrical vessels having a small opening for gas injection at the centre of its bottom. It has been shown that the typical flow pattern of a spouted bed can be reproduced, including stable spout, fountain and annulus with a taper bottom (Kawaguchi et al., 2000a) or flat bottom (Takeuchi et al., 2004, 2005). The installation of a draft reduces the minimum spouting velocity and pressure drop, and increases the maximum spoutable bed height (Swasdisevi et al., 2004; Zhao et al., 2008b). The more detailed gas–particle behaviours in spouted beds, including velocity, collision and forces, have been investigated by Zhong et al. (2006).

Microscopically, the flow behaviour of gas and particle in fluidization is controlled by the interactions between particles, between

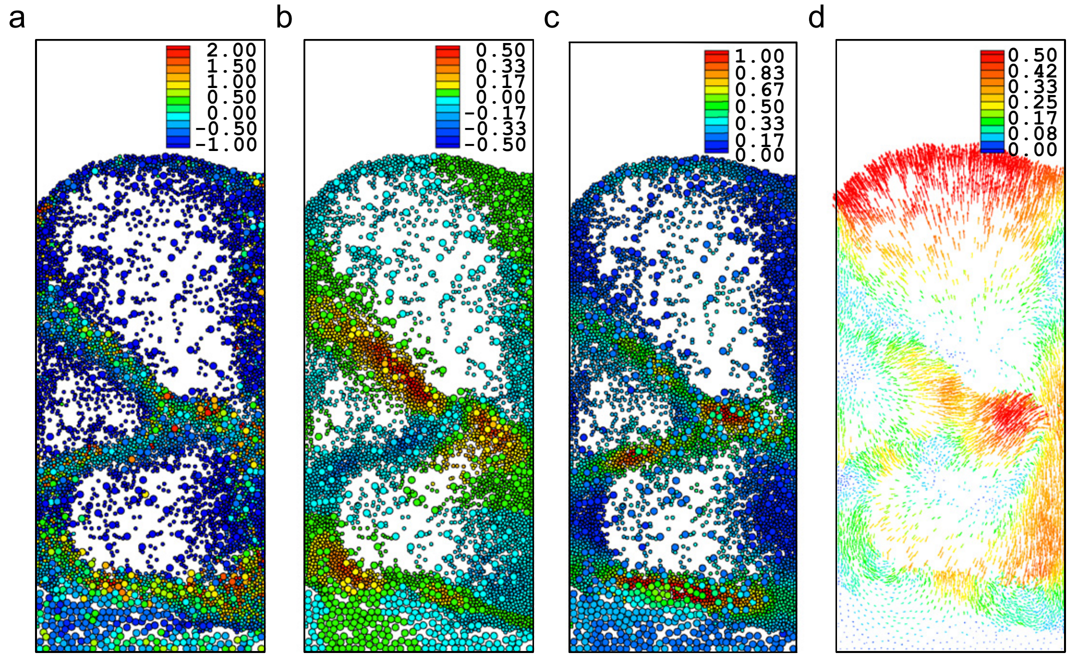

Fig. 35. Snapshots showing the spatial distribution of forces and velocities when $t = 3.5$ s, $v = 1.4$ m/s, initial state is well mixed: (a) particle–particle contact force in logarithmic scale; (b) fluid drag force in horizontal direction; (c) fluid drag force in vertical direction; and (d) particle velocity (*note*: the forces are non-dimensionized by their respective gravity force) (Feng et al., 2004b).

particles and fluid, and between particles and wall, in addition to the gravitational force. The analysis of these interaction forces is therefore key to developing a better understanding of the underlying mechanisms. CFD-DEM simulations have shown to have advantages for such research. For example, Fig. 35 shows the spatial distributions of velocity and force fields of particles in a fluidized bed (Feng et al., 2004b). The results highlight that rich dynamic information can be generated from a CFD-DEM simulation. According to Fig. 35(a), large contact forces are found mainly in the area where particles are crowded, and the magnitude of such a force on a particle can be hundreds of times of its weight due to the high relative velocity between particles. On the other hand, Figs. 35(b) and (c) suggest that the drag force in a dense area is larger than that in a loose area, both horizontally and vertically, due to the difference in porosity and permeability. As a consequence of force differences, vigorous particle motion is observed, producing good mixing, as shown in Fig. 35(d).

For a multi-sized particle system, mixing and segregation often occur, and can be either detrimental or beneficial, depending on specific applications. The knowledge of the fundamentals governing segregation or mixing is important for better use of these phenomena to enhance the performance of operations. Because of the complexity of such a problem, in practice the previous models are not reliable for general application (for example, Beeckmans, 1984; Hoffmann et al., 1993). Particle scale modelling and analysis is helpful to the elucidation of the mechanisms governing mixing/segregation. In recent years, CFD-DEM has been more and more widely used in this area (Hoomans et al., 2000; Rhodes et al., 2001b; Limtrakul et al., 2003; Feng et al., 2004b; Bokkers et al., 2004; Chaikittisilp et al., 2006; Beetstra et al., 2007; Lu et al., 2007; Tian et al., 2007; Feng and Yu, 2007; Di Renzo et al., 2008). In general, the degree of mixing/segregation can be quantified by the so-called Lacey mixing index or its variants (Lacey, 1954; Poux et al., 1991). CFD-DEM simulations show that the mixing is affected by initial packing structure, gas velocity and particle properties. The final equilibrium state is not significantly affected by the initial packing of particles (Rhodes et al., 2001b; Feng et al., 2004b; Bokkers et al., 2004). The rate and the degree of mixing increase with gas velocity for fluidized beds, but decrease with the increase of particle diameter. Dahl and Hrenya (2005) further examined the effect of size distribution on segregation, and showed that the degree of segregation increases with an increase in the width of particle size distribution, and segregation is attenuated as bubbling becomes more vigorous. Moreover, the shape of the local size distribution (i.e., Gaussian or lognormal) is found to mimic that of the overall size distribution in most regions of the fluidized bed, a finding which needs further verification under different conditions.

The mechanisms of mixing/segregation have also been analysed from the information about the interaction forces between particles and between particles and fluid (Feng et al., 2004b; Feng and Yu, 2007). As an example, Figs. 36 and 37 show the information of interaction forces between particle–fluid, particle–particle and particle–wall. The difference in the upward drag force on flotsam and jetsam particles produces separation in the loose regions (Fig. 36). Fig. 37 further shows that, at the start of gas injection, the upward fluid drag force is greater than the gravity force for flotsam and less than the gravity force for jetsam. This will provide a driving force for segregation, with flotsam rising to the top and the jetsam sinking to the bottom of the bed. Two stages can be identified: transient stage and stable stage. At the transient stage, the drag force decreases for flotsam and increases for jetsam. This should correspond to the rearrangement and segregation process of particles in the bed. Consequently, the interaction force between flotsam and jetsam decreases. After about 20s, the forces simply fluctuate around their mean values, and a macroscopically stable stage is reached.

4.1.2. Fluidization of cohesive particles

Cohesion between particles will affect gas–solid flow in gas fluidization. The cohesive forces involved in fluidization typically include liquid bridge force for wet particles and van der Waals force for fine particles. The continuum approach in modelling cohesive particles has to adopt extra constitutive equations related to cohesive forces, which is far difficult to deal with. But for discrete approach, it is rational and straightforward to take those forces into account,

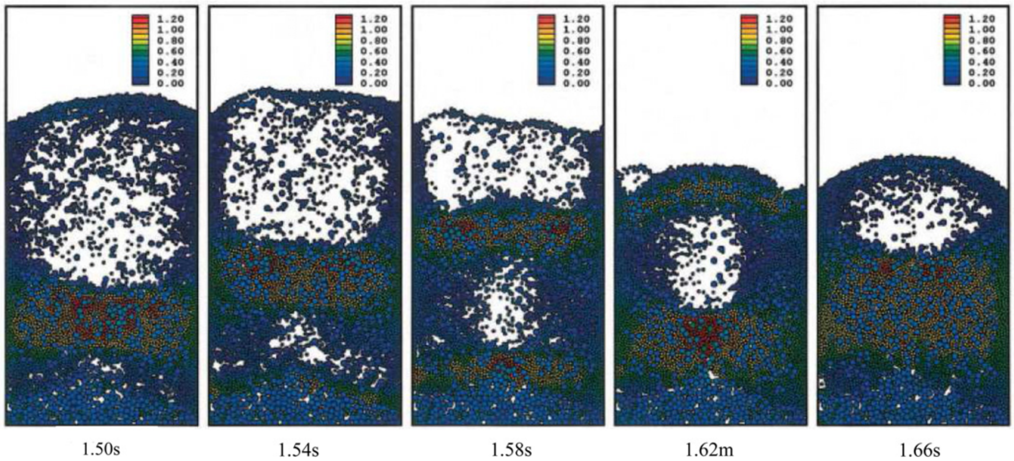

Fig. 36. Transition of the spatial distribution of vertical drag force when $v = 1.0\,m/s$ and the initial state is well mixed (*note*: the forces are non-dimensionized by their respective gravity force) (Feng et al., 2004b).

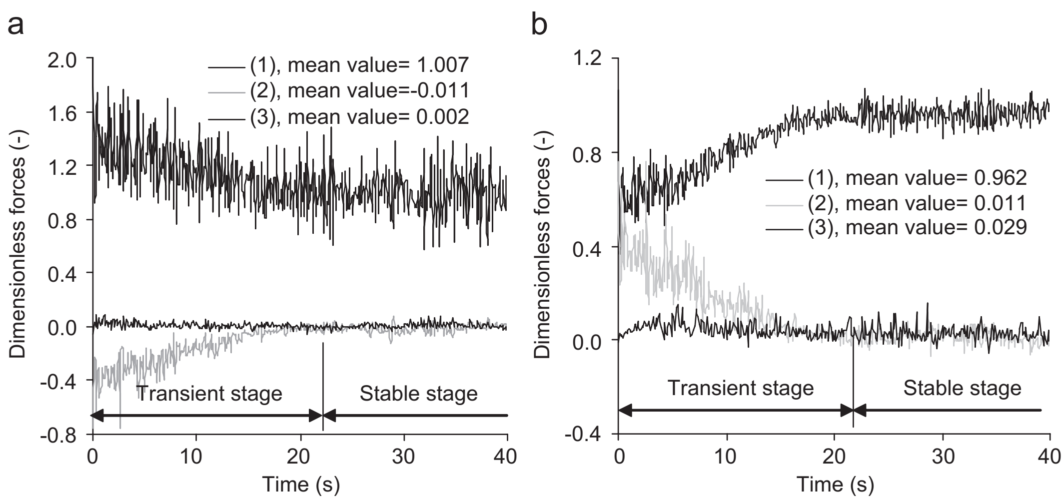

Fig. 37. Variation of mean interaction forces with time at vertical direction when gas velocity is 1.0 m/s and the initial state is well mixed: (a) flotsam; (b) jetsam (*note*: line 1, particle–fluid interaction force; line 2, particle–particle interaction force; line 3, particle–wall interaction force; and the forces are non-dimensionized by their respective gravity force) (Feng et al., 2004b).

as discussed elsewhere (Zhu et al., 2007). To date, the main findings from CFD-DEM simulations include the following aspects.

With the presence of liquid bridge force, the bed behaviour can significantly change, depending on the amount of liquid and other parameters such as particle properties (Xu et al., 1999; Pandit et al., 2006, 2007; Limtrakul et al., 2007; Moreno-Atanasio et al., 2007). In particular, the minimum fluidizing velocity for wet particles is higher than that for dry particles (Mikami et al., 1998; Xu et al., 1999). The formation of agglomerates in wet particle fluidization and its mechanisms have been examined (Kuwagi and Horio, 2002; Goldschmidt et al., 2003). The effect of other forces such as metallic bridging (Kuwagi et al., 2000) or lubrication force (Zhang et al., 2005) has also been investigated.

The effect of van der Waals force on fluidization behaviour is obvious. It has been shown that Geldart B particles will bubble immediately when the superficial gas velocity exceeds the minimum fluidization velocity, whereas Geldart A particles display an interval of non-bubbling expansion (homogeneous fluidization), which is affected by gas and particle properties (Ye et al., 2005b). Typical characteristics of cohesive behaviour have been observed, including throwing of particles high into the freeboard, lumping of particles, channelling of the bed, and formation of a fixed structure (Rhodes et al., 2001a,b; Xu et al., 2001b, 2002a; Yu and Xu, 2003; Ye et al., 2004; Pandit et al., 2005). As an example, Fig. 38 shows the effect of the van der Waals force on flow patterns. Three regimes of fluidization can be identified: good fluidization, quasi-fluidization and defluidization, depending on the ratio of van der Waals force to particle gravity. In particular, when the ratio is beyond 300, the fluidization is impossible by normal means.

A new stability criterion has been established to quantify the transition between fixed, expanded and fluidized bed based on the fact that the existence of an expanded bed must be associated with the balance between the van der Waals force and contact force (Xu and Yu, 2002; Yu and Xu, 2003). Such a view has been further confirmed by Ye et al. (2004) and Pandit et al. (2005). Fig. 39 shows the variation of the time- and ensemble-averaged van der Waals force, contact force and fluid drag force with superficial gas velocity. The plot clearly indicates that the fixed bed ends at the minimum fluidization velocity at which the effective contact force decreases to zero, and the fluidized bed starts at the minimum bubbling velocity when the effective contact force starts to increase from zero. Between the two velocities, there exist expanded beds where the effective

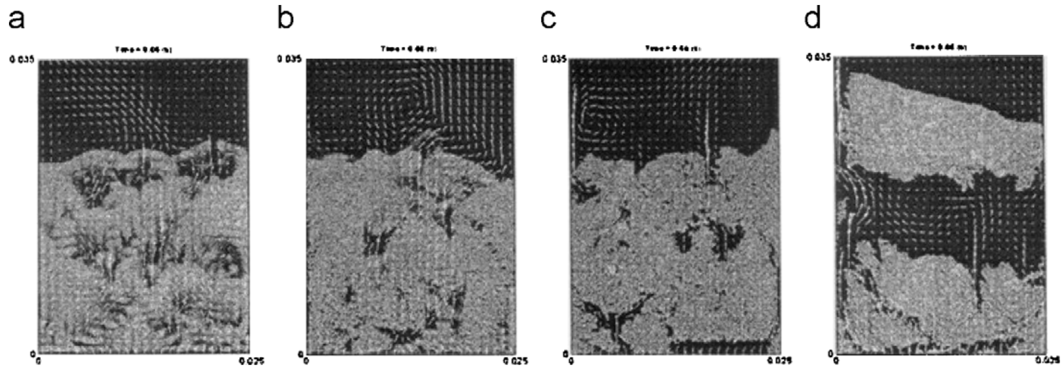

Fig. 38. Effect of the interparticle forces on powder fluidization behaviour when the superficial gas velocity is 0.048 m/s at different ratio of the van der Waals forces to particle gravity: (a) 12; (b) 42; (c) 113; and (d) 400 (Yu and Xu, 2003).

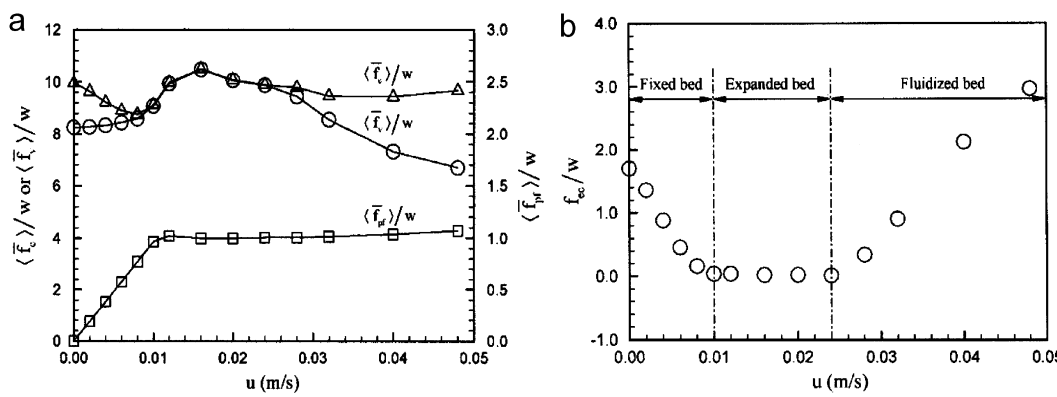

Fig. 39. (a) The dimensionless time- and ensemble-averaged contact force, van der Waals force and fluid drag force as a function of superficial gas velocity and (b) transition between fixed, expanded and fluidized beds identified in the relationship between the effective contact force and superficial gas velocity (Yu and Xu, 2003).

contact force is zero as the van der Waals force balances the contact force to counteract the disturbance induced by gas flow. Therefore, to form an expanded bed, not only the van der Waals force but also the frictional force must be present among particles and between a particle and a wall. If the van der Waals force or frictional force is absent, fluidization starts as soon as the superficial gas velocity exceeds the minimum fluidization velocity.

4.1.3. Other applications in fluidization

Attempts have also been made to apply the CFD-DEM approach to study liquid fluidization. Bubble wake is the dominating factor responsible for inherent transport properties in such a flow system. Therefore, it is important to understand the fundamentals involved in the bubble wake. Several CFD models (Gidaspow et al., 1994; Grevskott et al., 1996; Mitra-Majumdar et al., 1997) have been proposed for this purpose, in which both the gas and solid phases are treated as pseudo-continuous phases. However, such treatment usually experiences the difficulty to enclose the governing equations. DEM has been illustrated to be a good alternative to investigate the bubble wake structure and the bed stabilities (Li et al., 1999,2001) Zhang et al., 2000; Wen et al., 2005; Annaland et al., 2005; Di Renzo and Di Maio, 2007; Lim et al., 2007; Mukhejee and Mishra, 2007; Malone and Xu, 2008; Takeuchi et al., 2008b). In addition, Ushijima and Nezu (2002) examined the mixing and segregation of granular mixture included in gas and liquid flows. The nearly uniform mixing and particle segregation in oscillating liquid flows observed in physical experiments were successfully reproduced. Potic et al. (2005) investigated the fluidization behaviour with hot compressed water in micro-reactors. The calculated minimum fluidization and bubbling velocities were shown to be in good agreement with the measured ones.

Heat transfer in a gas fluidization is also an important phenomenon. Macroscopic studies, as reviewed by Botterill (1975), Wakao and Kaguei (1982), Kunii and Levenspiel (1991), mainly focused on the overall heat transfer behaviour in terms of correlations which often have limited applicability. To overcome this limitation, well-controlled experiments have been carried out focusing on the behaviour of selected particles (Prins et al., 1986; Baskakov et al., 1987; Agarwal, 1991; Parmar and Hayhurst, 2002; Collier et al., 2004; Scott et al., 2004), but information related to the underlying mechanisms is still difficult to determine. CFD-DEM, coupled with the proper heat transfer models, can overcome such a difficulty readily. Different heat transfer conduction mechanisms, such as conduction through the gas lens (Delvosalle and Vanderschuren, 1985; Rong and Horio, 1999), and direct conduction due to elastic deformation during impact (Sun and Chen, 1988; Li and Mason, 2000; Lathouwers and Bellan, 2001; Zhou et al., 2003a, 2004c) have been examined. Recently, a more comprehensive model in dealing heat transfer is proposed (Zhou et al., 2006, 2007), and more detailed analysis of heat transfer mechanisms in packed or fluidized beds has been performed on this basis. It is revealed that conductive heat transfer by either conduction through the gas lens, or direct conduction due to elastic deformation during impact is relatively weak compared with particle–fluid convection heat transfer in fluidized beds. But in a packed bed, conduction contribution to overall heat transfer could be significant, mainly depending on the particle and fluid properties, e.g., thermal conductivities (Cheng et al., 1999; Zhou et al., 2006, 2007).

4.2. Pneumatic conveying and pipeline flow

Pneumatic transport of granular material is a common operation frequently employed to transport solid particles from one location to another in chemical, process and agricultural industries. It is environment friendly, flexible and can be fully automated. But it may involve various problems such as high power consumption, wear, blockage and particle degradation. Depending on the system geometry, gas velocities, and material properties of the solid particles to be transported, such transportation processes can take place in different modes, usually referred to as dense or dilute phase conveying. The former is usually the preferred method for handling solids that are sensitive to abrasion as shear and collisional forces are generally lower. The latter mode, where particles are dispersed as a suspension in gas, is known to be a more stable mode, with lower fluctuations and excursions in gas pressures (Lim et al., 2006a). An understanding of the differences between the various flow regimes found in pneumatic conveying of granular material is therefore important to industrial applications with regards to the optimality of operation, ease of control, and extent of damage inflicted on the solid particles as well as the conveying lines. The CFD-DEM approach can generate rich microscopic information, and has hence been extensively used to study the flows in pneumatic pipelines. The resulting findings are briefly discussed in the following.

4.2.1. Horizontal conveying

Wave-like motion is a typical flow pattern of plug flow in a horizontal pipe. A plug sweeps up the stationary particles in front and leaves behind a stationary layer. The particle velocity in the plug is almost uniform, while particles near the bottom wall have some slip velocity. Such features have been reproduced in the discrete modelling (Tsuji et al., 1992; Xiang and McGlinchey, 2004; Li et al., 2005b; Li and Mason, 2000; Lim et al., 2006a,b; Fraige and Langston, 2006; Zhang et al., 2007; Kuang et al., 2008; Chu and Yu, 2008). The effect of stationary layer at the bottom of a pipe on the transition and flow of slugs along the pipeline has also been examined, and the flow mechanisms have been revealed (Li et al., 2005b). As an example, Fig. 40 shows the formation, collapse, and motion of one plug, and the formed stationary layer. It is shown that there is an intensive exchange of particles between the slug body and the stationary layer as slugs move along the pipeline, and a large variation of solid concentration and pressure and velocity distributions across the slug. A slug wave actually compresses the particle layer just ahead of it, pushing some of the particles up from the layer into the wave. On the other hand, particles at the tail of the slug fall into the bottom part of the pipeline and form a stationary particle layer behind the slug. These phenomena have been confirmed by analysing the recorded video footages. Further study on the horizontal pipe flow is done recently by Fraige and Langston (2006). These investigations give an overview of the effects of material properties on flow behaviour, and possible problems encountered in the CFD-DEM simulation.

Recently, the microscopic and macroscopic structures of slug flow have been analysed by Kuang et al. (2008), as shown in Figs. 41 and 42. The results show that slug velocity linearly increases with gas flow rate but is not sensitive to solid flow rate and slug length increases with both gas and solid flow rates. An empirical correlation is also proposed to approximate the relationship between the number of particles or solid concentration and solid flow rate for different gas flow rates, which is useful to relate CFD-DEM simulations of slug flow to engineering application. Force analysis reveals that the axial particle–fluid force in slug flow is much bigger than the radial one. The movement of a slug is macroscopically controlled by the axial particle–fluid and particle–wall interactions, whereas the particle–particle interaction microscopically causes a slug to sweep up particles in a settled layer. The magnitudes of these interaction forces increase with gas and solid flow rates.

4.2.2. Vertical conveying

CFD-DEM simulations have shown that in a vertical pneumatic conveying, particles tend to be dispersed throughout the pipe for high gas velocities and low solid concentrations, and tend to cluster together and move in the form of a dense plug for low gas velocities and high solid concentrations (Kawaguchi et al., 2000b; Ouyang and Yu, 2005; Lim et al., 2006a; Xu et al., 2007b; Zhang et al., 2008; Chu and Yu, 2008). These flow patterns have been referred to as the dispersed, transition, and plug flow regimes, respectively, as shown in Fig. 43, which agrees well with the experimental observations of Zhu et al. (2003). It has also been suggested that particle breakage and attrition are inevitable phenomena affecting both the conveying characteristics and the quality of particulate materials (Han et al., 2003), and the charged powders due to collisions between powder and equipment wall (Watano, 2006).

The different flow regimes in vertical or horizontal pneumatic conveying arising from the use of different operating conditions can be represented in the form of phase diagrams, which can be established by CFD-DEM simulation, as shown in Fig. 44. Dashed lines in the figures separate approximately the regions representing different flow regimes, while dashed circles enclose regions where transition between two adjacent flow regimes may take place. In vertical pneumatic conveying, the dispersed flow regime is dominant at high gas velocities and low solid concentrations, while the plug flow regime is dominant otherwise (Fig. 44a). This is also generally true for horizontal pneumatic conveying, except at low gas velocities and solid concentrations where the effects of gravitational settling of particles result in the formation of the moving dunes and stratified flow regimes (Fig. 44b). Intermediate values of gas velocities, where transitions between the moving dunes and homogeneous flow regimes (MD/H) and between the stratified and homogeneous flow regimes (S/H) are similarly approximated, and shown by regions enclosed within the dashed circles in Fig. 44b.

4.3. Process studies

The CFD-DEM approach has also been used to study various industrial processes. Representative examples include ironmaking blast furnace, gas cyclone and film coating process, as briefly discussed below.

Ironmaking blast furnace is a multiphase flow system including gas, solid, liquid and powder four-fluid flow (Yagi, 1993; Dong et al., 2007). Although continuum-based mathematical models have been proposed to study this flow system at a macroscopic level, it is necessary to develop a better understanding of flow mechanisms at a particle level for better process efficiency. The most important and interesting part is the raceway region which, as a cavity, forms in the lower part where gas is laterally blasted into a furnace at a very high speed. Xu et al. (2000) first examined the gas and particle flow behaviour in a raceway by means of CFD-DEM. Such efforts have recently extended to include more complicated phenomena (Feng et al., 2003; Nogami et al., 2004; Umekage et al., 2005; Yuu et al., 2005b; Singh et al., 2007). Particle flow in other regions, such as the shaft (Nouchi et al., 2005; Zhou et al., 2005, 2008b; Mio et al., 2007) and hearth (Nouchi et al., 2003a,b) have also been examined.

Cyclones are widely used in industries to separate solids from fluid. The most important performance variables of a gas cyclone are gas pressure drop and solid separation efficiency (Yuu et al., 1978; Hoffmann et al., 1992; Fassani and Goldstein, 2000). Numerical methods such as Lagrangian particle track (LPT) method and CFD-DEM (Chu et al., 2007) have been used to quantify these properties (Yoshida, 1996a; Pant et al., 2002; Derksen et al., 2006; Wang et al.,

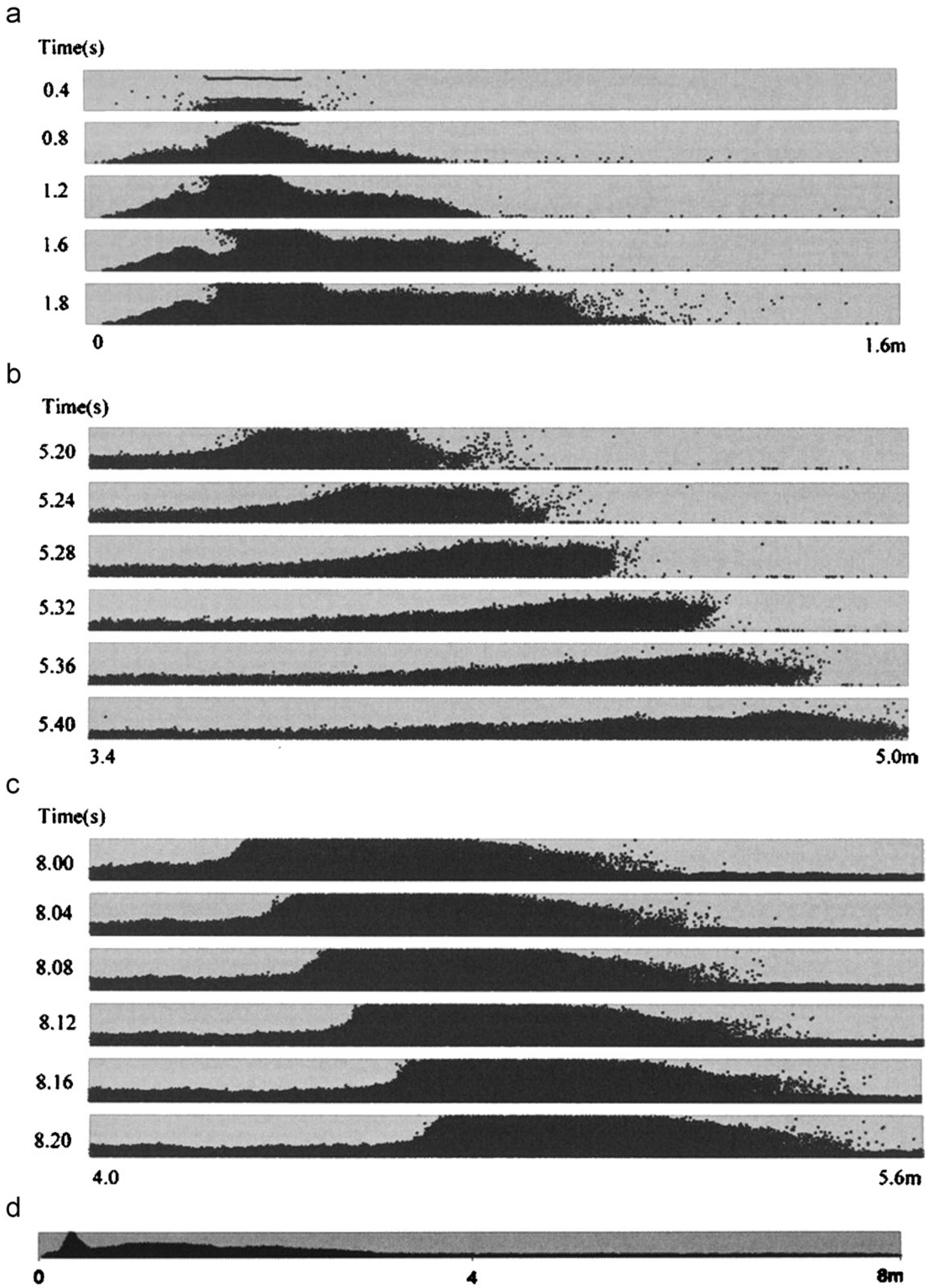

Fig. 40. (a) The formation of plugs; (b) the collapse of one plug; (c) motion of one plug; and (d) the stationary layer after conveying (Xiang and McGlinchey, 2004).

2006). It has been demonstrated that CFD-DEM can capture some key flow features in a cyclone separator, which cannot be satisfactorily obtained by a conventional modelling technique (Chu et al., 2007). The results also suggest that not only the tangential velocity but also the axial and radial velocities change significantly after solids are loaded, which may contribute to the decrease of pressure drop. Recently, the CFD-DEM approach has been extended to study the multiphase flow in dense medium cyclones (Chu et al., 2007; Wang et al., 2007a).

Particle coating process has been widely employed in many industries, such as food, agriculture, cosmetic and pharmaceutical industries, in order to produce functional materials. Fine particles, having size range from several micrometres down to nanometres, have become a source of major interest in many industries recently. In particular, in the pharmaceutical industry, fine particles have been expected for novel drug delivery systems, such as asthma therapy by inhalation or cancer therapy by transcatheter arterial embolization. Nakamura et al. (2006) made an attempt to

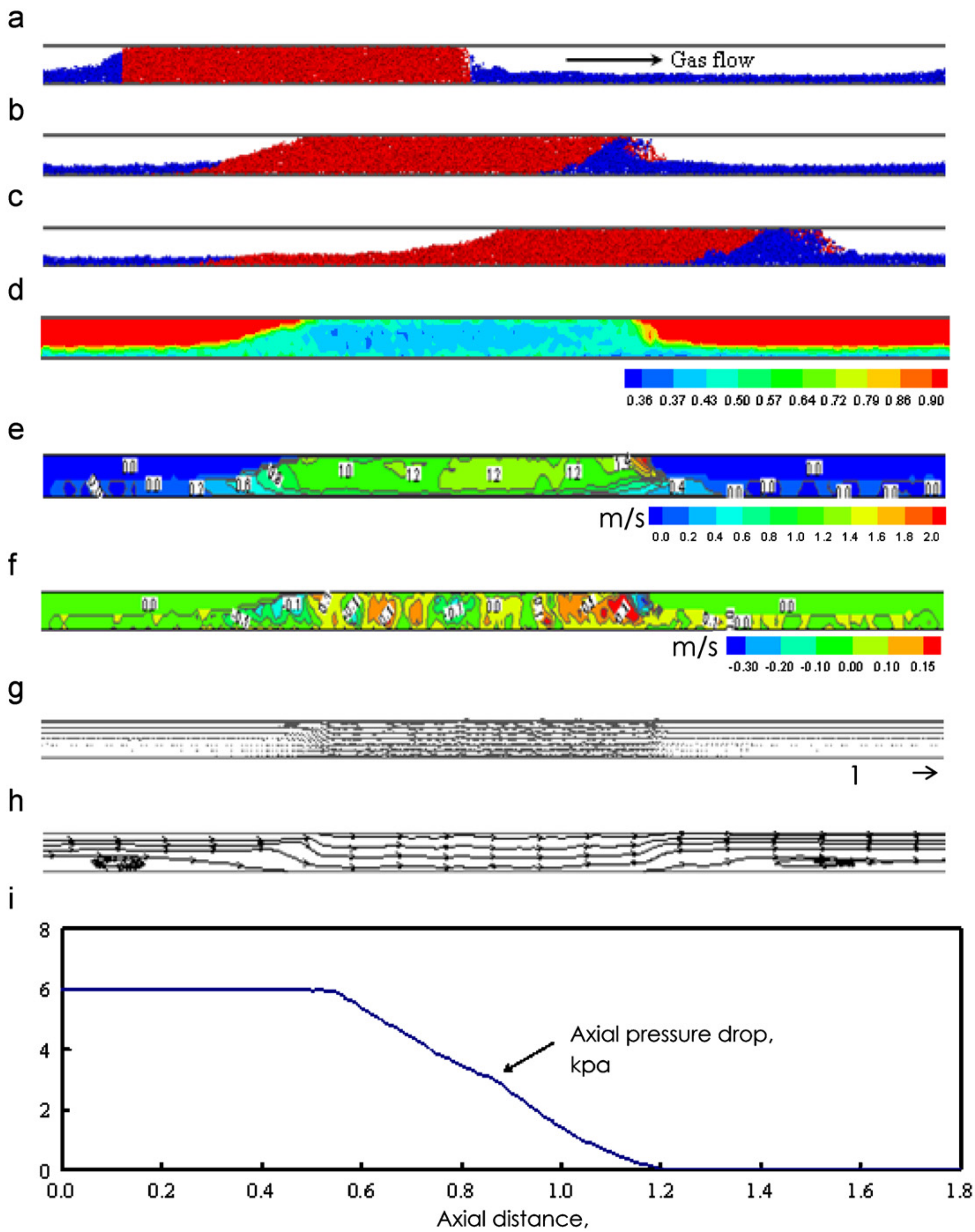

Fig. 41. Snapshots showing the spatial distributions of flow properties when the number of particles is 11,000 and the gas velocity is 2.09 m/s: (a)–(c) particle configurations at 14.236, 14.498, and 14.760 s, respectively; (d) porosity; (e) axial particle velocity; (f) radial particle velocity; (g) gas velocity profile; (h) gas streamlines; and (i) axial pressure drop; (d)–(i) are corresponding to (b) (Kuang et al., 2008).

use CFD-DEM to study film coating process in a rotating fluidized bed (RFB). Visualization of fluidization behaviours and distribution of sprayed material on a single particle was conducted. It has been shown that simulated sprayed material distributions can be expressed by a normal distribution function, which qualitatively agrees with experimental result. The calculated variation coefficient of mass distribution of the sprayed material decreases with an increase in a coating time, gas velocity or centrifugal acceleration.

Other particle–fluid phenomena have also been modelled by CFD-DEM, such as gas-phase olefin polymerization (Kaneko et al., 1999), solid bridging particles (Kuwagi et al., 2000), powder flow (Yuu et al., 2000b; Sugino and Yuu, 2002), cross-flow moving granular filter bed (Chou et al., 2000, 2007), motion of particles during jigging (Mishra and Mehrotra, 2001), drying process (Li and Mason, 2002), particle comminution in jet milling (Han et al., 2002), bed spray granulation (Goldschmidt et al., 2003; Kafui and Thornton, 2008), vapour deposition (Czok et al., 2005), gas–solid injector (Xiong et al., 2005), saturated granular soils (El Shamy and Zeghal, 2005a,b, 2007), granulation in spout-fluid bed (Link et al., 2007), sheet flow of coarse sediments (Calantoni and Puleo, 2006; Calantoni et al., 2006), liquid injection into fluidized beds (Nagaiah et al., 2007), liquefaction of

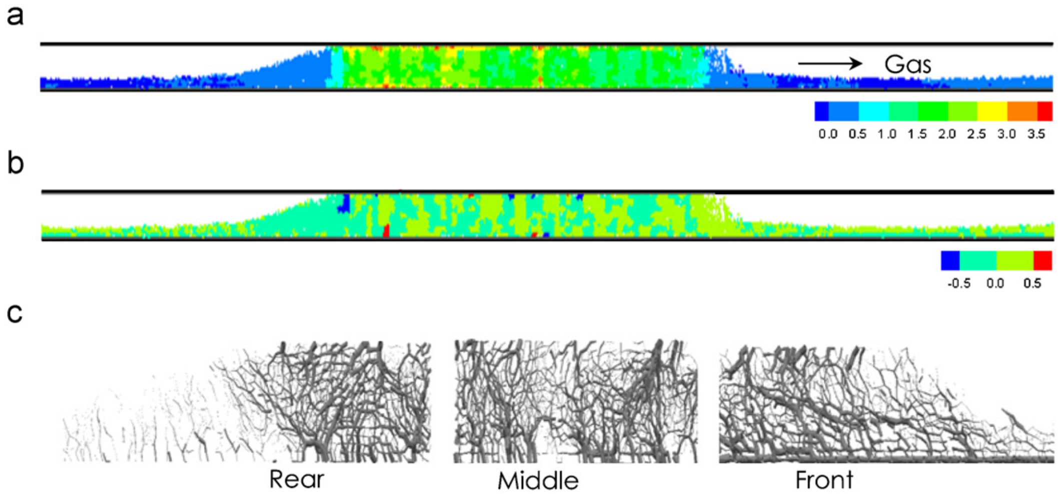

Fig. 42. Snapshots showing spatial distributions of (a) axial particle–fluid force; (b) radial particle–fluid force; and (c) network of normal contact forces, corresponding to Fig. 41(b) (Kuang et al., 2008).

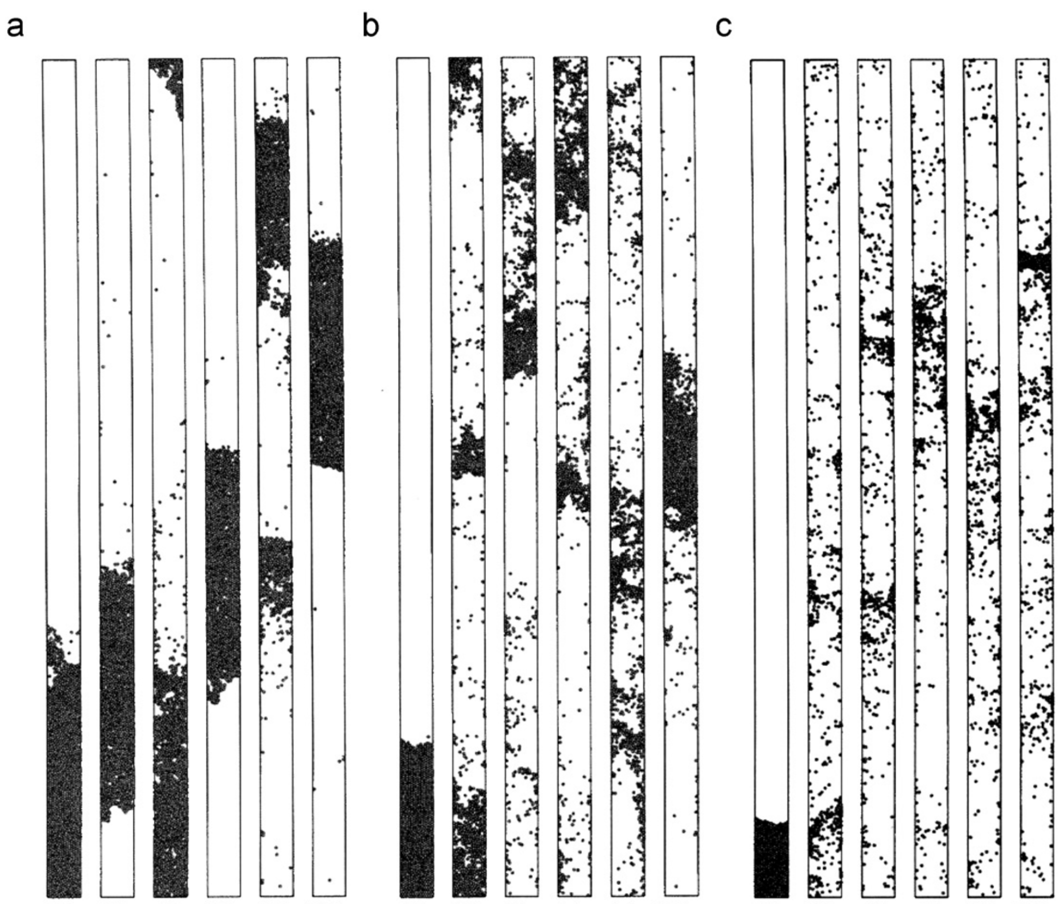

Fig. 43. Vertical pneumatic conveying when gas velocity is 14 m/s: (a) dispersed flow regime with solid concentration 0.08; (b) transition regime between the dispersed and plug flow regimes with solid concentration 0.16; and (c) plug flow regime with solid concentration 0.24 (Lim et al., 2006a).

saturated granular soils (Zeghal and El Shamy, 2008). Attempts have also been made to extend the CFD–DEM approach to study complex processes. As an example, Fig. 45 shows the gas–solid flow in a three-dimensional circulating fluidized bed simulated by Chu and Yu (2008). Under certain conditions, industrial scale simulation is possible. Examples include coal distribution which involves millions of particles and complicated gas–liquid–particle flow (Dong et al., 2008) and dense medium cyclone (Chu et al., 2007). These studies indicate the great potential of the CFD-DEM approach to complex systems.

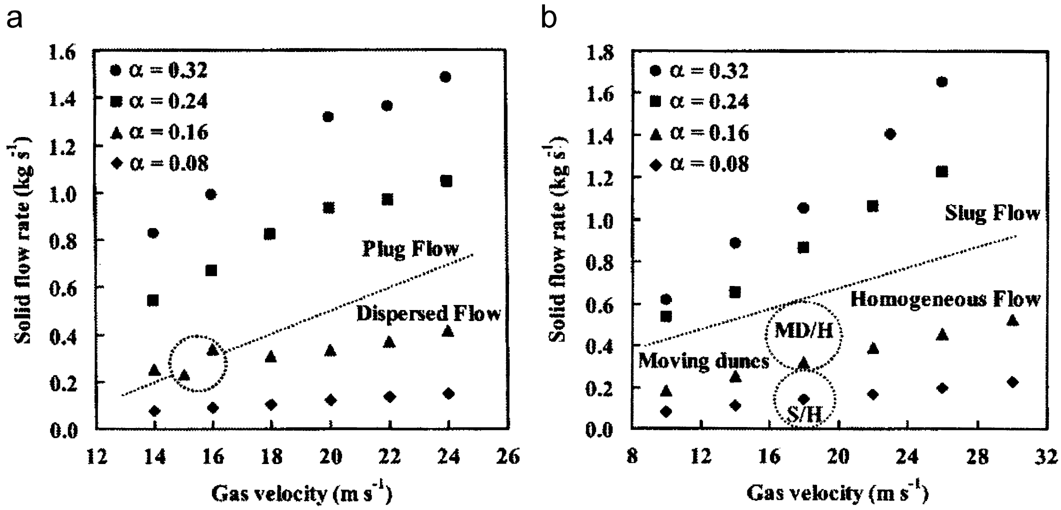

Fig. 44. (a) Phase diagram for vertical pneumatic conveying and (b) phase diagram for horizontal pneumatic conveying (Lim et al., 2006a).

4.4. Summary and discussion

The CFD-DEM approach has been increasingly used in the study of different particle–fluid systems. The resulting particle scale analysis has shown its value in many aspects, as highlighted as follows.

In fluidization, the complex flow behaviour such as bed dynamics, formation of bubbles and clusters related to different flow conditions has successfully been reproduced in simulation. The behaviour is shown to be controlled by the interactions between particles, between particles and fluid, and between particles and wall. This is clearly demonstrated in the study of mixing and segregation of particle mixtures. It reveals that particle segregation occurs as a result of the strong fluid drag force lifting the flotsam before a dynamical equilibrium state is reached. The particle–particle interaction, like the particle–fluid interaction, plays an important role in achieving uniform fluidization. For Geldart A particles, the bed displays an interval of non-bubbling expansion due to the existence of the van der Waals force. Controlled numerical experiments indicate that an expanded bed forms when the van der Waals force balances the contact force to counteract the disturbance induced by gas flow, so that the transition between fixed, expanded and fluidized beds can be measured by means of a forced-based stability criterion. Better understanding has also been developed about various important aspects, including the bubble wake structure and bed stabilities, formation of agglomerates, heat transfer mechanisms in fluidized beds, and so on.

In pneumatic conveying, some typical flow patterns and regimes observed in horizontal and vertical pipelines have been reproduced and to some degree analysed in relation to the flow structure and force. The study has been extended to more detailed phenomena including the formation and collapse of slugs, formation of stationary layer, and variation of solid concentration, pressure and velocity under different conveying conditions. For example, it is revealed that the movement of a slug is macroscopically controlled by the axial particle–fluid and particle–wall interactions, whereas the particle–particle interaction microscopically causes a slug to sweep up particles in a settled layer. Therefore, new findings from the particle scale analysis are accumulating, which should be useful for generating a more comprehensive understanding of this two-phase flow system.

CFD-DEM has also been successfully used to study particle–fluid flow under different conditions relevant to different engineering applications. Blast furnace, cyclone, film coating, and those mentioned in this review are good examples. Such studies have demonstrated values not only in enhancing fundamental understanding of particle–fluid flow but also in assisting decision-making in the design, control and optimization of a process.

With the rapid development of computer technology, CFD-DEM will become more and more popular in the modelling and simulation of particle–fluid and multiphase flow. To make the full use of this simulation technique, however, a number of obstacles should be overcome. The theoretical developments needed have been discussed in Part I of this review (Zhu et al., 2007). They are certainly very important in order to address problems at different time and length scales in process development and optimization. Furthermore, it is useful to conduct some detailed investigation at a microscopic scale in order to handle particle–fluid flow coupled with heat and mass transfer, and chemical reactions as well. To date, such studies are limited, and there are a lot to do in this direction in the future. For example, a general and convincing correlation to determine the fluid–particle heat transfer coefficient is not available. Most of the correlations proposed in the literature are based on those obtained from macroscopic studies. Some recent attempts have been made to overcome this problem (for example, Zhou et al., 2008a), but there is still lack of accurate theory to calculate the interparticle heat transfer. Also, the validity of various models proposed in the literature needs to be conducted in order to fully verify their applicability in dealing with heat transfer and combustion.

Moreover, in line with the theoretical efforts, development of a robust and general software package for modelling of complex flow systems is also important. In this connection, the recent work of Chu and Yu (2008) to run CFD-DEM simulations on the platform of commercial software package like Fluent may have opened a promising direction for the future developments which, as stressed further in Section 5, should aim to solve particulate and multiphase flow ultimately and generally.

5. Concluding remarks

Understanding and modelling the physics of particulate or granular matter has been a major research focus worldwide, not only in chemical engineering but also in other disciplines (see, e.g. Jaeger and Nagel, 1992; Jaeger et al., 1996). However, progress in this area has been slow in the past. As pointed out by De Gennes (1999) “granular matter is at the level of solid–state physics in 1930”. Particulate and multiphase processing rarely reach more than 60% of the design capacity because of inadequate understanding of the fun-

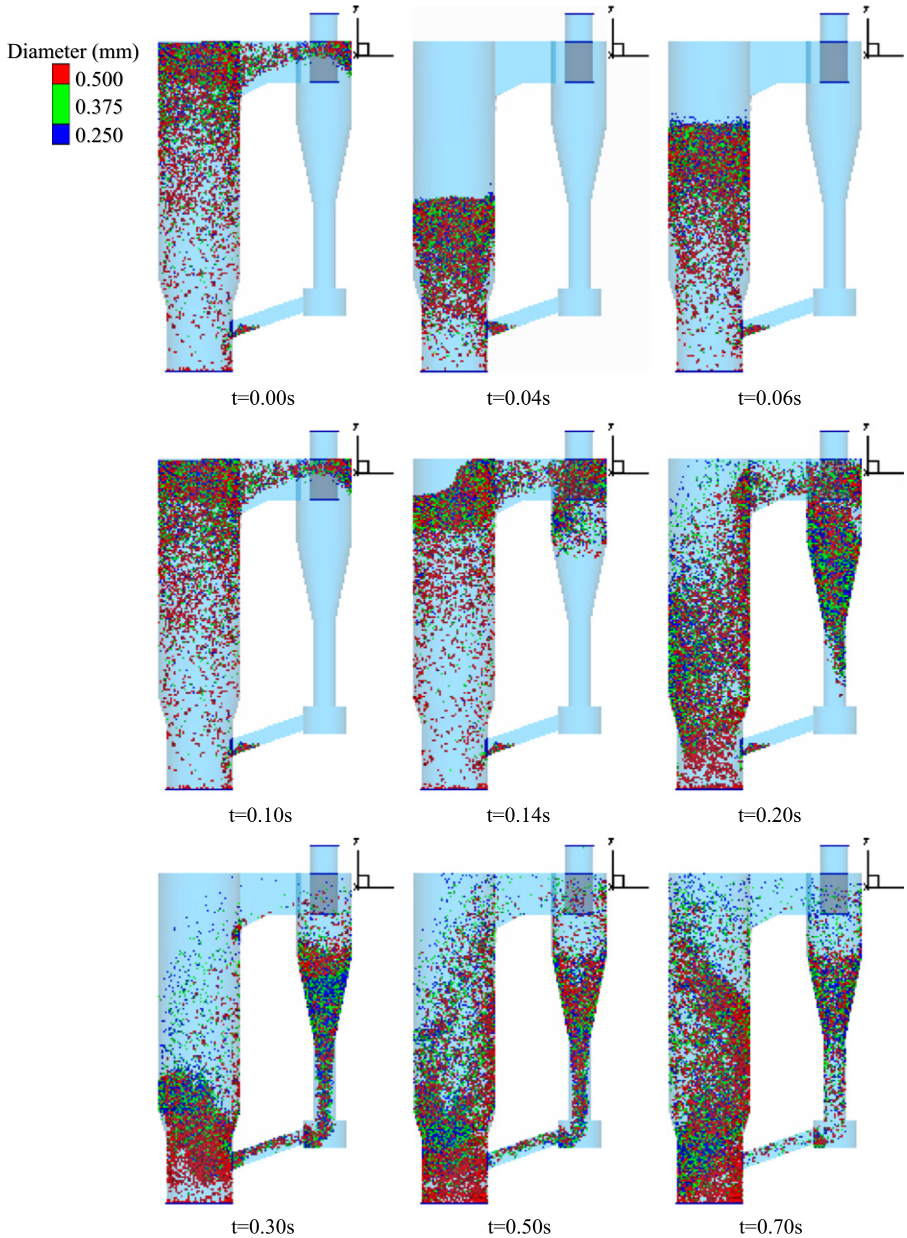

Fig. 45. Snapshots showing the spatial distribution of particles of different sizes in the formation of a simulated CFB (particles are coloured by size) (Chu and Yu, 2008).

damentals (Merrow, 1985; Ennis et al., 1994). Although widely used, many processes are actually operated as "black box" reactors.

A particulate system is always made up of a large number of particles that interact in varying and complex ways. This leads to complex behaviour that is difficult to understand, predict and manage at a macroscopic scale. Chaotic approach may be an approach to describe such a behaviour (see, e.g. Hill et al., 1999). But there is a long way to go before it becomes a general approach. Moreover, conceptually, it is not so advantageous. In fact, the bulk behaviour of granular matter depends on the collected outcomes of the interactions among individual particles, the basic elements in granular matter, indicating that the "chaotic" behaviour can be described as a deterministic process at a microscopic, particle scale. Discrete particle simulation, or granular dynamics simulation to be equivalent to the well-established molecular dynamics simulation for gas, liquid and solid phases, is such an approach to elucidate the underlying fundamentals of granular matter. Therefore, while different studies may have different needs or focuses, it is ultimately because of this function that DEM has been widely adopted and further developed for particulate/granular research, although it was initially proposed for geomechanic research (Cundall and Strack, 1979) or may be extended for research in plant sciences, zoology and social simulation (Richards et al., 2004).

We have indeed seen the rapid development and wide application of discrete particle simulation in the past two decades or so, in parallel to the development of computer technology. This review, together with the first one on theoretical development (Zhu et al., 2007), highlights the major developments and findings. As pointed out by Zhou et al. (2003c), the dynamics of particulate or particle–fluid flow includes at least three aspects: velocity, structure and force. Previous studies have to be limited to velocity 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. DEM or CFD-DEM is an effective technique that can overcome this problem, as demonstrated by many examples summarized in this review. Our discussion of the major findings in the literature is largely along this line.

It should be noted that DEM or CFD-DEM is still a state-of-the-art simulation technique. It needs further developments to meet the research needs corresponding to different time and length scales as discussed elsewhere (Yu, 2004; Zhu et al., 2007). In the mean time, as an effective technique, it has been used and will continue to be used to study the physics of particulate and/or multiphase flow related to various industrial problems. The approach will certainly play a key role in tackling a range of long-standing core problems with particulate/granular matter, including, for example,

- What forces govern particle (including nanoparticle) and particle–fluid flow? And how to describe and implement them in the discrete and continuum simulation of particulate systems?
- What is the role of packing/flow structure in relation to the force structure and the dynamic behaviour of granular materials?
- What are the governing equations and constitutive relations that can be generally used to describe particle packing and flow? Can they be derived generally from discrete particle simulation facilitated by local averaging?
- How to effectively couple the continuum model for multi (continuous) phases with the discrete model for discrete phases for complex flow systems in industry?

In the past, our knowledge of particulate/granular matter has been increased steadily. However, problems encountered may increase at a faster speed because of the rapid development of new products and processes as highlighted by the research and development related to nanoparticles and their applications in, for example, water treatment, pollution control, pharmaceuticals and advanced material manufacturing (Davies, 2001; Roco, 2006). We believe that discrete particle simulation can play an important role in developing a step change to overcome this problem, so that particulate systems can be better designed, controlled and optimized in the future.

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