

Modeling Particle-Laden Flows: A Research Outlook

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DOI 10.1002/aic.10394

Published online in Wiley InterScience (www.interscience.wiley.com).

Keywords: multiphase, particle, granular flow, fluidization

Introduction

Particle processes pervade the chemical, pharmaceutical, agricultural and mining industries. Many of these processes have significant opportunities for cost savings and productivity enhancements. However, many such advances are currently unrealized due to a lack of understanding of particle flow behavior in industrial scale processes. This lack of understanding results in scale-up failures, decreased reactor conversions, blockages in particle storage devices, and ineffective (from technical and/or economic perspectives) designs of transport systems. Reliable simulation tools can provide valuable insights into particle flow processes and, as a result, accelerate the achievement of substantial process improvements. Recent advancements in computational fluid dynamics (CFD) methods and software can help facilitate these improvements.

The potential for CFD to address interdisciplinary areas (such as those involving particulate flows) was highlighted in the Winter 2002 issue of *The Bridge*, a quarterly journal of the National Academy of Engineering. In an article entitled, "The Role of Computational Fluid Dynamics in the Process Industries" (subtitled: "Computational fluid dynamics has enormous potential for industry in the 21st century"), various applications of CFD were discussed in detail (Davidson, 2002). Adroit use of CFD has already shown much success. For example, a case study on the economic benefits of using CFD in one engineering company concluded that, over a six-year period, the benefits achieved generated approximately a six-fold return on the total investment (including salaries) required in CFD (Davidson, 2001). In another industrial example, an international oil company successfully implemented CFD to model particle-laden flow in a fluid catalytic cracking unit. The result was higher conversion by improving solids distribution in the reactor (Barthod et al., 1999).

As a result of the enormous potential associated with flow simulation technologies, the development of reliable particle flow models within the context of CFD is a subject of very active research. This Perspective is intended to provide an overview of the advances made in the development of these models. Attention is confined to particle flows in which both particle-particle interactions are significant and particle velocity fluctuations are not affected by the presence of the interstitial fluid (i.e., high-particle Stokes number and/or high Bagnold number flows). Solid volume fractions can range from extremely dilute (0.1% solids fraction) to very dense (solids fractions approaching closest packing). Important aspects of these specific types of particle-laden flows are highlighted, and the challenges and opportunities for innovation in model development in these areas are outlined.

Modeling Approaches

Models describing particle-laden flows can be roughly divided into two groups, Lagrangian models and Eulerian models. Lagrangian models, or discrete element models (DEM), calculate the path and motion of each particle. Particle interactions are modeled through specified collision rules. The Eulerian models, or two-fluid models, treat the particle phase as a continuum and the coexisting phases as interacting continua. The most sophisticated Eulerian models describe the particle-phase stress associated with particle interactions using kinetic theory concepts. Using these concepts, a separate energy balance associated with the particle velocity fluctuations that result from particle interactions (the so-called "granular energy balance") is solved in conjunction with particle continuity and momentum balances. An overview of these two approaches can be found in Van Wachem and Almstedt (2003). Figure 1 illustrates these two approaches by comparing results from both a Lagrangian simulation involving 4,100 particles (1b) and an Eulerian simulation (1c) to an experiment (1a) in a bubbling-fluidized bed.

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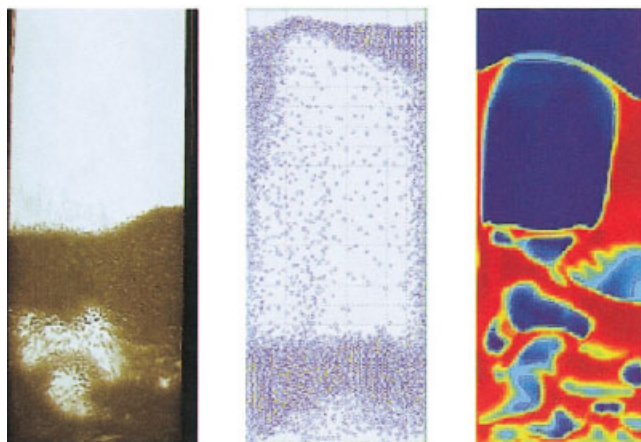


Figure 1. Comparison of modeling approaches.

(a) experiment and (b) Lagrangian simulation (4,100 particles) of a 9cm wide fluidized bed operated at three times the minimum fluidization velocity containing particles of density 1150 kg/m^3 and 1.55 mm dia. (c) Eulerian simulation of a 50cm wide fluidized bed operated at three times the minimum fluidization velocity containing particles of density 2640 kg/m^3 and $480 \text{ }\mu\text{m}$ dia.

An advantage of using the Lagrangian approach is the ability to easily vary the physical properties associated with individual particles (e.g., size or density). Moreover, local physical phenomena related to the particle flow behavior can be easily probed. Hence, these models can be used for validation, testing, and development of continuum models. The primary drawback is the computational effort required to track large numbers of particles. Therefore, the Eulerian approach is the more practical approach for simulating large-scale particle flow processes. However, this approach requires sophisticated modeling in order to describe the key effects and phenomena found in industrial processes. Some of these more critical effects are described more fully in the rest of this article.

Turbulent Gas-Particle Interactions

Interactions between particles and a turbulent gas lead to the changes in the level of the gas-phase turbulent intensity. In dilute-phase particle-laden flow, these changes in the level of the gas-turbulent intensity can produce significant changes in the pressure drop required to convey the material. For example, in some cases involving the transport of finer particles ($20 \text{ }\mu\text{m}$ – $75 \text{ }\mu\text{m}$) at mass loadings (the ratio of solids mass-flow rate to gas mass-flow rate) less than 4, the pressure drop actually decreases with increasing solids concentration. This result is due to a reduction in the gas-phase stress with the addition of particles (Marcus et al., 1990).

Particle size, particle density, and solids mass loading are all known to influence the gas-phase turbulence modulation in the presence of particles. These effects have been studied extensively, typically using laser Doppler velocimetry. In general, enhancement of gas-phase turbulence is observed in the presence of large particles, with attenuation of turbulence observed in the presence of smaller particles. Increases in the solids loadings for smaller particles tend to further decrease the gas turbulent intensity, and increases in the solids loadings for larger particles tend to further increase the gas turbulent inten-

sity. Recently, the effect of Reynolds number has been also shown to be a significant factor in gas turbulence modulation (Hadinoto et al., 2004b). For a given particulate material and solids loading, gas velocity fluctuations increase with increasing Reynolds number. Hence, the same particulate material can cause both a reduction in gas turbulence at a lower Reynolds number and an enhancement in gas turbulence at a higher Reynolds number.

In dense-phase particle-laden flows, an inspection of the magnitude of forces influencing the motion of the gas phase shows the gas-phase stress to be two orders of magnitude smaller than the drag force (Hrenya and Sinclair, 1997). Hence, the development of a model for predicting the behavior of such flows does not require a description for the turbulent gas-particle interactions. However, in dilute-phase flow, the gas-phase stress and the drag force are comparable in magnitude. Thus, an accurate description for the gas-phase stress is critical in order to accurately predict the flow behavior of the suspension.

In order to predict dilute-phase flows in industrial operations, two-phase flow models are based on Reynolds-averaged conservation equations (RANS) in connection with appropriate turbulence models (e.g., k - ϵ model, Reynolds stress model, etc.). Such a RANS model formulation was first developed in the work of Elghobashi and Abou-Arab (1983). This time-averaging procedure generates a number of terms, describing fluid-particle interactions, which require closure. Various proposals for these resulting turbulent correlations have been put forth in the literature. However, none of them to date encompass the full range—either in magnitude or type (damping or enhancement)—of gas turbulence modulation observed in practice (Crowe, 2000). RANS models either treat the particle phase as a continuum (e.g., Louge et al., 1991; Balzer et al., 1996) or in a Lagrangian fashion (e.g., Lain et al., 2002; Lain and Sommerfeld, 2003). In Lagrangian RANS models, trajectories of computational particles, or “parcels”, are followed in order to describe flows of engineering relevance (typically those with higher solids concentration). These “parcel” trajectories are proposed to represent a number of real particles with the same size and velocity.

Lagrangian models have also been used to simulate interactions between particles and an instantaneous gas velocity field obtained by either direct numerical simulation or large eddy simulation (Boivin et al., 1998). However, to date, only simple turbulent flows and extremely dilute concentrations have been considered. In addition, the particles are treated as point particles in terms their effect on the gas turbulence. The flow around individual particles is not resolved. Consideration of the influence of finite particle size and the influence of particle-particle collisions is a more recent research advance in this approach. These methods hold much promise for developing model closures, describing turbulent gas-particle interactions, that can be applied in continuum-based frameworks.

Particle Clustering

One of the most interesting and significant features of particle-laden flow is the phenomenon of particles temporarily coming together and forming larger structures. These clusters (also known as streamers) of particles continuously break up and recombine in a seemingly random pattern during particu-

late mixture flow. Particle clustering can be readily observed visually in gas-particle flows present in risers and downcomers, most typically when the solids volume fraction exceeds 1%. However, the exact solids fraction at which these clusters appear is uncertain, and the solids fraction at which the clusters can be observed visually varies with particle properties, among other variables. Since the behavior of these clusters significantly influences fluid-solids contacting, solid segregation patterns, and particle mixing, it is critically important to understand the mechanisms causing particle cluster formation in order to model the particle flow patterns accurately. For example, if particle clustering is not accounted for in models simulating vertical pneumatic conveying of solids, an incorrect solids segregation pattern is predicted. These incomplete models show particles segregating preferentially toward the core of the pipe—a segregation pattern opposite to what is observed in practice (particles segregating toward the pipe wall).

Particle clusters arise as a result of local instabilities. For smaller particles, clustering is caused by inertial instabilities associated with both gas-particle slip and inelastic particle collisions. Clusters, or meso-scale structures, have been obtained in highly resolved two-phase shear flow simulations involving the kinetic theory model (Sundaresan, 2000; Andrews et al., 2004). However, it is not yet understood how these simulated structures scale with domain size. Such an understanding is necessary for the development of sub-grid drag and stress models before these models can be reliably employed in continuum-based model simulations. In addition, it is unclear how to incorporate the effects of variations in particle size and density that occur within a particle mixture into these highly resolved, two-phase simulations. Future work in this area will improve the ability to develop sub-grid models that better account for the presence of clusters.

In the case of the flow of larger particles in a gas, instabilities in the particle phase alone, due to inelastic particle collisions, lead to the formation of particle clusters. Under these particle flow conditions, the discrete element method (DEM) is an excellent tool for probing particle clustering phenomenon at the level of individual particles. Using this method, the effects of varying properties of the particle mixture can be easily incorporated. The results of DEM simulations can then be used to devise appropriate closure relations for continuum-based models.

Initial DEM simulations, such as the work of Walton and Braun (1986), employed up to a few hundred particles. No particle clustering was observed in these simulations involving such a low number of particles. Since the particles in these simulations did not exhibit clustering, the predicted particle-phase stress resulting from these simulations showed good agreement with the stress for slightly inelastic particles that was predicted by the kinetic theory model of Lun et al. (1984). However, in the two-dimensional (2-D) shear flow simulation of Hopkins and Louge (1991) (which involved 2,600 particles), clustering was observed—with the clusters oriented at 45° with respect to the stream-wise direction. These simulations were carried out for highly inelastic particles with a coefficient of restitution e equal to 0.2 and a solids volume fraction ϕ of 0.3. When the coefficient of restitution of the particles was increased, simulations involving a larger number of particles were required in order to reproduce the clustering phenomena observed in practice. For example, 200,000 particles were

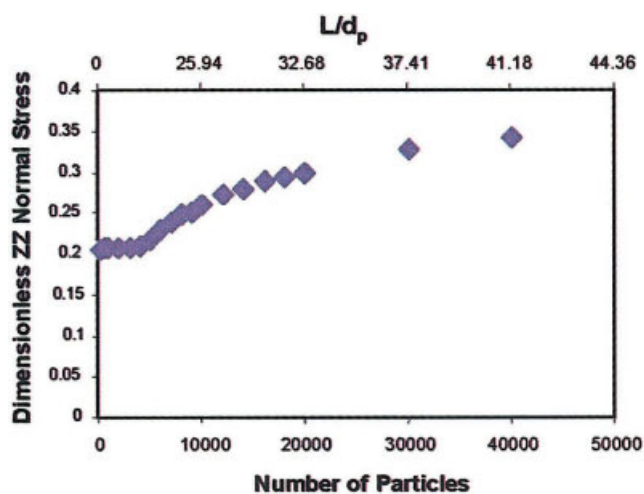


Figure 2. Dimensionless normal stress as a function of number of simulated particles ($e = 0.6$, $\phi = 0.3$).

necessary in the 2-D shear flow simulations of Tan and Goldhirsch (1997) in order to observe clustering when the particle coefficient of restitution was 0.6 and the solids fraction was 0.05.

In 3-D shear flow simulations, the same trend has been demonstrated—particle clustering is observed, provided the DEM simulations involve a sufficiently large number of particles. This point is illustrated in Figure 2, which shows a plot of the dimensionless normal stress (stress component perpendicular to the shearing plane) as a function of both the number of simulated particles and the relative system size, L/d_p , with L the characteristic length of the system and d_p the particle diameter (Lasinski et al., 2004). Increases in the particle-phase stress are evident, provided a sufficiently large number of particles are simulated. Figures 3a–3c show the segregation patterns of the particles at various system sizes. It is clear from these figures that particle clustering is responsible for the significant variation in the particle-phase stress. Regions of high-particle density and low-particle density appear in bands along the stream-wise axis of the system, provided a sufficiently large number of particles are simulated. In simulations, such as that shown in Figure 3a involving a small number of particles, the clustering behavior is not captured and particles are uniformly distributed. Particle clustering is also present in nearly elastic systems; the system size needed to manifest clustering in the simulations merely increases as the coefficient of restitution increases.

In systems with a binary distribution of particle sizes (50/50 mix by volume), particle clustering is also present. This clustering is illustrated by the figures on the cover of this issue. For these figures, the restitution coefficient is 0.6. The simulations on the top row are for particle-size ratio equal to 2 and mean solids fraction equal to 0.1. The simulations on the bottom row are for a particle size ratio equal to 3 and a mean solids fraction equal to 0.3. While the smaller-sized particles exhibit the same clustering pattern as the larger particles, they are less segregated than the larger particles. In addition, the overall stress in the clustered particle mix is reduced with increasing size ratio. Simulations also show that the particle-phase stress increases

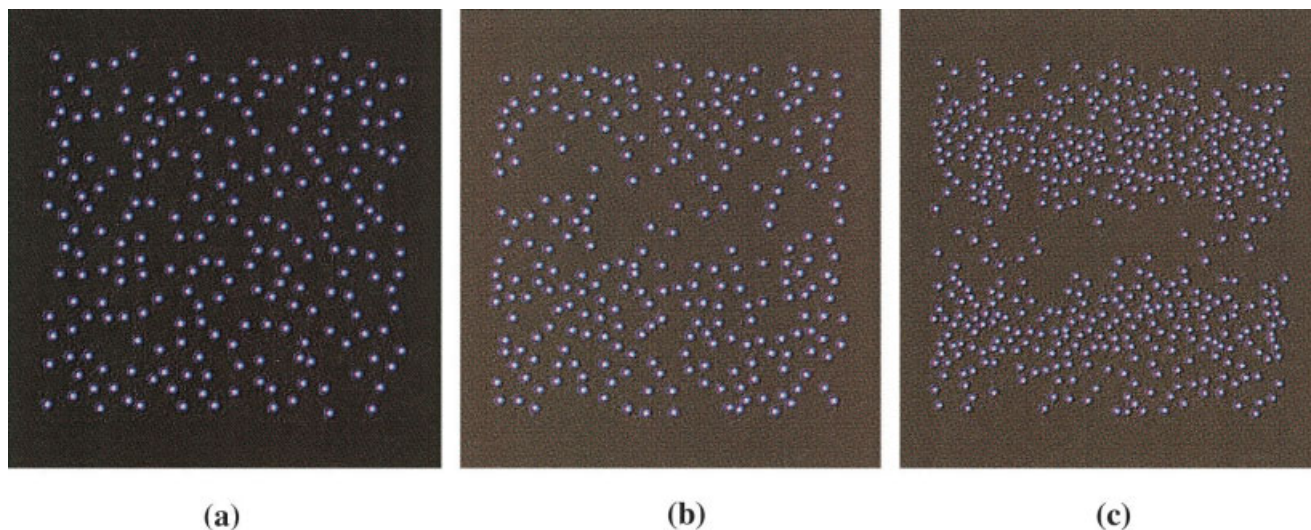


Figure 3. Particle segregation patterns at the center of the simulation domain ($e = 0.6$, $\phi = 0.3$) (a) 4,000 particles, (b) 6,000 particles, (c) 20,000 particles.

less rapidly with system size as the particle-size ratio is increased.

Lasinski et al. (2004) have conducted DEM simulations involving up to 300,000 particles. Both the nature of clustering and the particle-phase stress continue to change with system size. The challenge ahead is to formulate scaling rules, based on these simulations, so that appropriate closure relations for the particle-phase stress can be developed. Otherwise, simulations of extremely large systems of particles will be necessary in order to accurately describe the clustering behavior.

Frictional Effects

Frictional stresses are particulate-phase stresses that are associated with the local deformation and long-term interaction of particles. These stresses are important in very dense particle flows (e.g., flows in which the solids volume fraction typically exceeds 30%), such as those found in hoppers, chutes, and fluidized beds. The particle stresses associated with these long-term interactions are not described at all by kinetic theory. In fact, the particle stresses associated with particle velocity fluctuations and collisions alone are often negligible compared to the actual stresses present in highly dense-phase systems. Hence, when frictional effects are not included in the modeling of such flows, the particle-phase stresses are underpredicted. Figure 4 illustrates this point by showing predicted solids volume fractions in hopper flow—both without (Figure 4a) and with (Figure 4b) frictional stress included in the model formulation. The predicted particle flow patterns from the simulation without frictional stress exhibit too much of a “water-like” behavior, with particle velocities higher than observed in practice.

In continuum-based treatments for particle flow, the models currently employed to describe the higher stresses encountered in frictional flows originate from the geo-mechanical research community and follow a rigid-plastic rheology assumption (e.g., models proposed by Schaeffer (1987), Tardos (1997), and Jackson (1982)). The particle stresses have a order-zero dependency on the rate of strain, which is typical for quasi-static

flows. These models employ the so-called “critical state” theory, which assumes that the principal stress and deformation direction must coincide. In continuum-based treatments, the frictional stresses represented by these models are simply added to the kinetic and collisional stresses as described by kinetic theory. Although there is no physical basis for this assumption of additivity, dense-phase flow behavior over a range of solids volume fractions seems to be accurately captured by employing this assumption of additivity (Van Wachem et al. 2001a).

In many industrial particle flows, static (not flowing) regions exist, such as those found at the shoulders of a funnel flow hopper exhibiting “ratholing”. These stagnant particle regions produce a singularity in the critical state theory, resulting in models predicting infinitely high stresses. Srivastava (2001) has applied a frictional-collisional model, based on the work of Savage (1998), which does not exhibit such a singularity. Unfortunately, this model still incorrectly predicts the behavior of stagnant regions and over-predicts hopper discharge rate.

An alternate approach to describing long-term particle interactions is to analyze these interactions in detail at the level of individual particles. In the seminal work of Mindlin and Deresiewicz (1953), the time-dependent interaction of elastic spheres is considered. The local deformation during interaction is described by the contact theory of Hertz, in which the forces resulting from the deformation are described by Poisson’s ratio and Young’s modulus for the specific particulate material. Cundall and Strack (1979) simplified the Mindlin and Deresiewicz theory by describing the forces associated with particle interactions via three mechanical elements—a spring, dashpot, and slider—which are integrated in time for each particle. This method of describing the particle interactions is often referred to as the “soft-sphere” model and is the most common DEM approach for simulating dense-phase particle flow. Tsuji (1994) has shown, through simulations of hopper flow, that ‘soft-sphere’ models describe the particle interactions on the level of individual particles in very dense-phase flows more accurately than either the kinetic theory of granular

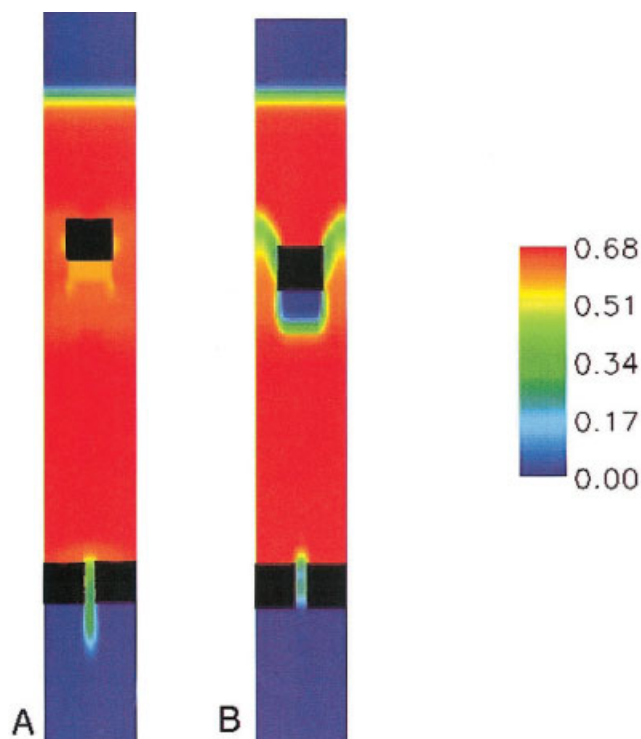


Figure 4. Simulation of a 2-D (20cm x 160cm) hopper flow of 480 μm glass beads (a) without and (b) with frictional stress after 0.15 s of real-time.

The legend indicates the solids volume fraction.

flow or the hard-sphere Lagrangian models. However, the results from “soft-sphere” models are sensitive to the selection of collision parameters, such as the spring stiffness. In addition, the selection of these collision parameters appears rather arbitrary in much of the DEM research published to date. Hence, recent work is aimed at developing guidelines for assigning these parameters (Ketterhagen et al., 2004).

On the basis of numerous other investigations, it is clear the “soft-sphere” models of both Mindlin and Deresiewicz (1953) and Cundall and Strack (1979) incorporate the correct physics for individual particle interactions in the frictional flow regime. Unfortunately, it is difficult to statistically “coarse-grain” the soft-sphere approach due to the strong time dependency of individual particle collisions. This is a challenge that lies ahead - to capture the behavior of individual particles undergoing long-term interactions into a model which can be applied on a higher, continuum scale.

Particle Shape

Particle-laden flow processes involving nonspherical particles can behave very differently than systems involving particles that are generally spherical in shape. In conveying systems, for example, the higher drag forces associated with nonspherical particles cause higher pressure drops compared to systems conveying spheres having the same equivalent volume. For highly nonspherical particles, such as flakes and fibers, this increase in pressure drop can be particularly significant. For example, Henthorn et al. (2005) measured a pressure drop 50% higher for lean-phase, vertical pneumatic conveying

of flake-like particles (sphericity of 0.39) than for spherical particles with the same equivalent volume diameter and density.

Although, very few engineering processes involve perfect spheres, the bulk of modeling efforts to date has been directed at spherical particles. However, when nonspherical particles are studied in continuum-based models, particle shape is typically accounted for in the model formulation through use of a nonspherical drag coefficient. There are many such drag coefficient correlations for nonspherical particles available in the literature; an excellent review of these correlations is given by Chhabra et al. (1999). Most of these correlations are based on measurements of particle terminal velocity in settling experiments for a wide range of particle shapes and orientations.

Typically, drag coefficient correlations relate drag to particle sphericity and particle Reynolds number based on the equivalent volume sphere diameter. In general, the lower the particle sphericity, the poorer is the correlation to the particle settling velocity data. Henthorn et al. (2005) recently tested the predictive ability of one of these commonly-used correlations by comparing measurements of pressure drop for flake-like particles and spheres to predictions from a two-fluid, kinetic theory model (Hadinoto and Curtis, 2004a). While the model predictions showed excellent agreement with the pressure drop measurements for spherical particles, the model did not capture the significantly higher pressure drops observed for flake-like particles.

The failure to predict the observed pressure drops for nonspherical particles may also be due to the fact that particle shape is not accounted for when describing particle-phase stress. Several research efforts have been aimed at understanding the influence of particle shape on particle-particle interactions. Walton and Braun (1993) simulated various particle shapes using different arrangements of rigid clusters of spheres. They showed an increase in the angle of repose for nonspherical particles in rotating cylinders. Park (2003) used the same approach as Walton and Braun, but allowed the clusters to deform as they interacted. Cleary and Sawley (2002) simulated 2-D hopper flow with particles modeled as superquadrics with various aspect ratios and angularities. They showed an increase in stress in the nonspherical particle mixture, and a decrease in hopper discharge rate compared to the discharge rate for perfect spheres. Based on the results of these investigations, it is likely that an increase in particle stress arising from interactions between nonspherical particles is also contributing to the significantly larger pressure drops observed. However, stress closure models for nonspherical particles remain to be developed.

Particle-Size Distribution Effects

Particle-size distribution (PSD) plays an important role in the behavior of particle-laden flows. In fluidized beds, for example, Morse and Ballou (1951) found that the uniformity of fluidization improves as the PSD is widened, leading to improved reactor performance. In addition, the minimum fluidization velocity decreases and the bed expansion increases as the PSD widens (De Groot, 1967; Grace and Sun, 1991). In circulating fluidized beds, the solids circulation rate increases when the PSD is widened (Horio et al., 1986), gas-solid contacting is improved, and, relative to the smaller particles, a

higher concentration of the larger particles is measured near riser walls (Mathiesen et al., 2000a).

There are two modeling approaches used in the Eulerian framework for simulating large-scale particle-laden flow processes involving a distribution of particle sizes (or densities). The first approach is characterized by a separate momentum equation for each particle species. In order to describe the particle-phase stress associated with each species, a granular energy balance for each species is also required. The drawback of this approach is that each species requires closure for both the fluctuating particle velocities and the interactions between these fluctuating particle velocities. These closures are based on the kinetic theory approach, which allows for the granular energy of the various particles to be different (i.e., the theory does not assume equipartition of granular energy). However, all kinetic theories published to date that allow for a difference in granular energy between unlike particles assume a Maxwellian particle velocity distribution. This assumption, as demonstrated by Willits and Arnarson (1999) via their DEM simulations of shear flow, is highly inaccurate, and results in an under-prediction of the particle-phase stress in a binary mixture. Hence, the incorporation of a non-Maxwellian velocity distribution appears to be necessary for reliable stress predictions. In the second approach, averaged mixture properties from the individual particles are defined, and a mixture momentum and granular energy balance are employed. These average mixture properties are locally updated by determining their local diffusion velocities as described by the kinetic theory for multiple components. Particle-phase stress closure models associated with this approach rely on the assumption of an equipartition of granular energy, but do allow for a non-Maxwellian particle velocity distribution. While experimental measurements clearly indicate a difference in granular temperature between particle species (Huilin et al., 2001), the impact of this difference on the accuracy of stress predictions in nonsegregating particulate systems is not significant. Clelland and Hrenya (2002) showed via DEM simulations that the energy equipartition kinetic theory model of Willits and Arnarson (1999) generates good predictions for the particle-phase stress of a binary mixture over the range of parameters investigated (particle size ratios up to 5 and restitution coefficients greater than 0.8). However, the validity of the equipartition assumption rapidly deteriorates as the coefficient of restitution is decreased, and this effect is magnified as the particle size ratio increases. Furthermore, the impact of the granular temperature difference between particle species on the particle-phase stress in segregating systems is not yet known.

Each of these modeling approaches has recently been applied separately to simulate particle flow patterns within fluidized beds and risers containing particles possessing a size distribution. The first approach, based on the assumption of a Maxwellian velocity distribution, has been employed by Mathiesen et al. (2000b) to model flow in a circulating fluidized bed with three different solid phases. This approach was also applied by Huilin et al. (2003) to model the flow of a binary mixture of solids in a fluidized bed. Both investigations report good agreement between model predictions and a limited set of experimental measurements. Van Wachem et al. (2001b) have employed the second approach, the one involving a mixture momentum balance, to predict the flow of a binary particle mixture in a fluidized bed. Although no comparisons of

model predictions to experimental measurements were made in this particular work, the key qualitative flow features associated with a widening of the PSD were predicted. For example, widening the PSD resulted in model predictions of decreased required minimum fluidization velocity, as well as increased bed expansion (up to 40% higher than predictions generated by a monodispersed particle model). In addition, the well-known phenomenon of “bed inversion” in binary mixtures of small/heavy particles and large/light particles was also reproduced. At low fluidization velocities, small/heavy particles preferentially segregate toward the bottom of the bed, with large/light particles toward the top. At higher fluidization velocities, however, the opposite segregation pattern occurred.

Given the limited number of simulations involving PSDs that have been performed in research conducted to date, it is not clear how accurate either of these approaches is at predicting the flow behavior of a particle mixture over a broad range of particle properties and operating conditions. Ideally, a more complete theory for stress in a particle mixture would account for both a non-Maxwellian particle-velocity distribution and a nonequipartition of granular energy between the particle species. However, derivation of such a complete theory is very complex. To date, such a theory has been developed only for very dilute phase flows (Garzo and Dufty, 2002). The future may hold promise for extending this theory to more dense-phase flows. In parallel, the individual approaches already mentioned previously will need to be more fully explored in order to test their predictive ability over a wider range of experimental conditions.

Evolving Particle-Size Distribution

In many industrial applications, such as fluidized-bed reactors or pneumatic conveying, the PSD of moving particles evolves with time due to chemical reaction, agglomeration, or attrition. In order to model such flows, the population balance equation (often called the general dynamic equation) must be solved in conjunction with a hydrodynamic model that accounts for the effect of PSD. The population balance equation has been applied extensively to flows involving a dispersed phase assumed to be inertialess (e.g., as in aerosol dynamics), but only recently have investigators focused on particle motion dictated by a separate balance of momentum.

Brown (1996) solved the population balance equation using the method of moments, in conjunction with a simplified two-fluid model, to describe the deposition of particles in gas turbines (Brown et al., 1994). A log-normal distribution for the particle phase was assumed, in which the number of particles, the mean particle size, and the standard deviation of the distribution all varied with time (i.e., three moments). Thus, the application of this model formulation to other processes is limited to those processes which retain the same form for the PSD over time (so-called “self-similar” processes). It cannot be applied, for example, to processes involving particle attrition, in which the PSD often converts from log-normal to bimodal. In general, moment methods suffer from closure problems unless a distribution is assumed.

A very promising method for circumventing this closure problem is the quadrature method of moments, which is based on an approximation of the unclosed terms by using an ad hoc quadrature formula. Fox and coworkers (Fan et al., 2004) have

developed an extension of the quadrature method of moments, known as the direct quadrature method of moments (DQMOM). In DQMOM, the particle distribution function is represented by a summation of Dirac delta functions. This approach is computationally efficient and effective in modeling the evolving particle-size distribution associated with a polymerization reaction occurring in a fluidized bed. The only minor drawback associated with this approach is the limited amount of information that is known about the true particle-size distribution, which is represented by several delta functions. Theoretically, an infinite number of moments is required to completely determine a distribution (Hamilton *et al.*, 2003). A calculation involving such a large number of moments is not practical given current computational capabilities. Nevertheless, the development and application of the DQMOM approach represents a significant advancement in the range of particle-laden flow processes which can now be modeled.

Implications

For industrial operations involving particle-particle interactions, particle flow models are generally reliable provided that the particles are rounded in shape and do not possess a wide or evolving particle-size distribution. Such models have been incorporated into commercial CFD codes, such as Fluent and CFX. The more complex aspects of particle-laden flows that have been discussed in this article require additional investigation. Ongoing research into Lagrangian/DEM approaches is important at the microscale level, while advancements in continuum models are critical for improving large-scale processes. The areas covered by this article offer opportunities for academic and industrial researchers to gain fundamental insights into key aspects of particle-laden flows, especially how microscale phenomena are linked to the types of macroscale challenges faced by industry.

Literature Cited

- Andrews, A., P. Loezos, and S. Sundaresan, "Coarse-Grid Simulation of Gas-Particle Flow in Vertical Risers," *I&EC Research*, submitted (2004).
- Balzer, G., O. Simonin, A. Boelle, and J. Lavieville, "A Unifying Modelling Approach for the Numerical Prediction of Dilute and Dense Gas-Solid Two Phase Flow," *Proc. of the 5th Int. Conf. on Circulating Fluidized Beds*, Beijing, China (1996).
- Barthod, D., M. Pozo, and C. Mirgrain, "CFD Aided Design Improves FCC Performance," *Oil & Gas J.*, **5**, 66 (1999).
- Boivin, M., O. Simonin, and K. Squires, "Direct Numerical Simulation of Turbulence Modulation by Particles in Isotropic Turbulence," *J. Fluid Mech.*, **375**, 235 (1998).
- Brown, D. P., "Development of a Three-Dimension Coupled Flow, Species and Aerosol Model: Applications to Particle Deposition in Gas Turbines and Aerosol Formation and Growth in Jet Engine Exhausts," PhD Thesis, University of Cincinnati, Cincinnati, OH (1996).
- Brown, D. P., P. Biswas, and S. G. Rubin, "Transport and Deposition of Particles in Gas Turbines: Effects of Convection, Diffusion, Thermophoresis, Inertial Impaction and Coagulation," FACT-Vol.18, Combustion Modeling, Scaling and Air Toxins, ASME (1994).
- Chhabra, R., L. Agarwal, and N. Sinha, "Drag on Non-Spherical Particles: An Evaluation of Available Methods," *Powder Tech.*, **101**, 288 (1999).
- Cleary, P., and M. Sawley, "DEM Modeling of Industrial Granular Flows: 3D Case Studies and the Effect of Particle Shape on Hopper Discharge," *Applied Math. Modelling*, **26**, 89 (2002).
- Clelland, R. and C. Hrenya, "Simulations of a Binary-Sized Mixture of Inelastic Grains in Rapid Shear Flow," *Phys. Rev. E.*, **65**, 031301 (2002).
- Crowe, C., "On Models for Turbulence Modulation in Fluid-Particle Flows," *Int. J. Multiphase Flow*, **26**, 719 (2000).
- Cundall, P. A., and O. D. Strack, "A Discrete Numerical Model for Granular Assemblies," *Geotechnique*, **29**, 47 (1979).
- Davidson, D. L., "The Enterprise-Wide Application of Computational Fluid Dynamics in the Chemicals Industry," *Proc. of the 6th World Congress of Chem. Eng.*, Melbourne, Australia (2001).
- Davidson, D. L., "The Role of Computational Fluid Dynamics in Process Industries," *The Bridge*, **32**, 4 (2002).
- De Groot, J., "Scaling-up of Gas-Fluidized Bed Reactors," *Proc. of the Int. Symp. on Fluidization*, Amsterdam, A. A. H. Drinkenberg, ed., Netherlands University Press, Amsterdam, 348 (1967).
- Elghobashi, S. E., and T. W. Abou-Arab, "A Two-Equation Turbulence Model for Two-Phase Flows," *Phys. Fluids*, **26**, 931 (1983).
- Fan, R., D. Marchisio, and R. Fox, "Application of the Direct Quadrature Method of Moments to Polydisperse Gas-Solid Fluidized Beds," *Powder Tech.*, **139**, 7 (2004).
- Garzo, V., and J. Dufty, "Hydrodynamics for a Granular Binary Mixture at Low Density," *Phys. Fluids*, **14**, 1476 (2002).
- Grace, J., and G. Sun, "Influence of Particle Size Distribution on the Performance of Fluidized Bed Reactors," *Can. J. Chem. Eng.*, **69**, 1126 (1991).
- Hadinoto, K., and J. Curtis, "Effect of Interstitial Fluid on Particle-Particle Interactions in Kinetic Theory," *I & EC Research*, **43**, 3604 (2004a).
- Hadinoto, K., E. Jones, C. Yurteri, and J. Curtis, "Reynolds Number Dependence of Gas-Phase Turbulence in Gas-Particle Flows," *Int. J. Multiphase Flow*, submitted (2004b).
- Hamilton, R., D. Ramkrishna, and J. Curtis, "Beyond Log-Normal Distributions: A Hermite Spectral Method for Solving Population Balance Equations," *AIChE J.*, **49**, 2327 (2003).
- Henthorn, K., K. Park, and J. Curtis, "Measurement and Prediction of Pressure Drop in Pneumatic Conveying: Effect of Particle Characteristics, Mass Loading, and Reynolds Number," *I & EC Research*, in press (2005).
- Hopkins, M., and M. Louge, "Inelastic Microstructure in Rapid Granular Flows of Smooth Disks," *Phys. Fluids A*, **3**, 47 (1991).
- Horio, M., K. Morishita, and O. Tachibana, "Dynamics of Particles in Circulating Fluidized Beds," *World Congress III of Chem. Eng.*, Tokyo, 536 (1986).
- Hrenya, C. M., and J. L. Sinclair, "On the Effects of Particle Turbulence in Dense Gas-Solids Flow," *AIChE J.*, **43**, 853 (1997).
- Huilin, L., D. Gidaspow, and E. Manger, "Kinetic Theory of

- Fluidized Binary Granular Mixtures," *Phys. Rev. E.*, **64**, 061301 (2001).
- Huilin, L., H. Yurong, D. Gidaspow, Y. Lidan, and Q. Yukun, "Size Segregation of Binary Mixture of Solids in Bubbling Fluidized Beds," *Powder Tech.*, **134**, 86 (2003).
- Jackson, R., "Some Mathematical and Physical Aspects of Continuum Models for the Motion of Granular Materials," *Theory of Dispersed Multiphase Flows*, R. Meyer, ed., Academic Press, New York, 291 (1982).
- Ketterhagen, W., J. Curtis, and C. Wassgren, "Stress Results from 2-D Granular Shear Flow Simulations Using Various Collision Models," *Phys. Rev. E.*, submitted (2004).
- Lain, S., M. Sommerfeld, and J. Kussin, "Experimental Studies and Modelling of Four-Way Coupling in Particle-Laden Horizontal Channel Flow," *Int. J. Heat Fluid Flow*, **23**, 647 (2002).
- Lain, S., and M. Sommerfeld, "Turbulence Modulation in Dispersed Two-Phase Flow Laden with Solids from a Lagrangian Perspective," *Int. J. Heat Fluid Flow*, **24**, 616 (2003).
- Lasinski, M., J. Curtis, and J. Pekny, "Effect of System Size on Particle-Phase Stress and Microstructure Formation," *Phys. Fluids*, **16**, 265 (2004).
- Louge, M.Y., E. Mastorakos, and J. T. Jenkins, "The Role of Particle Collisions in Pneumatic Transport," *J. Fluid Mech.*, **231**, 345 (1991).
- Lun, C., S. Savage, D. Jeffrey, and N. Chepurniy, "Kinetic Theories for Granular Flow - Inelastic Particles in Couette Flow and Slightly Inelastic Particles in a General Flow Field," *J. Fluid Mech.*, **140**, 223 (1984).
- Marcus, R., L. Leung, G. Klinzing, and F. Rizk, *Pneumatic Conveying of Solids*, Chapman and Hall, London (1990).
- Mathiesen, V., T. Solberg, and B. Hjertager, "An Experimental and Computational Study of Multiphase Flow Behavior in a Circulating Fluidized Bed," *Int. J. Multiphase Flow*, **26**, 387 (2000a).
- Mathiesen, V., T. Solberg, and B. Hjertager, "Predictions of Gas/Particle Flow with an Eulerian Model Including a Realistic Particle Size Distribution," *Powder Tech.*, **112**, 34 (2000b).
- Mindlin, R. D., and H. Deresiewicz, "Elastic Spheres in Contact under Varying Oblique Forces," *J. Appl. Mech.*, **20**, 327 (1953).
- Morse, R., and C. Ballou, "The Uniformity of Fluidization - Its Measurement and Use", *Chem. Eng. Prog.*, **47**, 199 (1951).
- Park, J., "Modeling the Dynamics of Fabric in a Rotating Horizontal Drum," PhD Thesis, School of Mechanical Engineering, Purdue University, West Lafayette, IN (2003).
- Savage, S. B., "Analyses of Slow, High-Concentration Flows of Granular Materials," *J. Fluid Mech.*, **377**, 1 (1998).
- Schaeffer, D. G., "Instability in the Evolution of Equations Describing Incompressible Granular Flow," *J. Differential Equations*, **66**, 19 (1987).
- Srivastava, A., "Dense-Phase Gas-Solid Flows in Circulating Fluidized Beds," PhD Thesis, Dept. of Chemical Engineering, Princeton University (2001).
- Sundaresan, S., "Modeling the Hydrodynamics of Multiphase Flow Reactors: Current Status and Challenges," *AIChE J.*, **46**, 1102 (2000).
- Tardos, G. I., "A Fluid Mechanistic Approach to Slow, Frictional Flow of Powders," *Powder Tech.*, **92**, 61 (1997).
- Tan, M., and I. Goldhirsch, "Intercluster Interactions in Rapid Granular Shear Flows," *Phys. Fluids*, **9**, 856 (1997).
- Tsuji, Y., "Discrete Particle Simulation of Gas-Solid Flows," *KONA Powder and Particle*, **11**, 57 (1994).
- Van Wachem, B. G. M., J. C. Schouten, R. Krishna, C. M. van den Bleek, and J. L. Sinclair, "Comparative Analysis of CFD Models for Dense Gas-Solid Systems," *AIChE J.*, **47**, 1035, (2001a).
- Van Wachem, B., J. Schouten, C. van den Bleek, R. Krishna, and J. Sinclair, "CFD Modeling of Fluidized Beds with a Bimodal Particle Mixture," *AIChE J.*, **47**, 1291 (2001b).
- Van Wachem, B. G. M., and A. E. Almstedt, "Methods for Multiphase Computational Fluid Dynamics," *Chem. Eng. J.*, **96**, 81 (2003).
- Walton, O., and R. Braun, "Viscosity, Granular Temperature, and Stress Calculations for Shearing Assemblies of Inelastic, Frictional Disks," *J. Rheol.*, **30**, 949 (1986).
- Walton, O., and R. Braun, "Simulations of Rotary-Drum and Repose Tests for Frictional Spheres and Rigid Sphere Clusters," *Joint DOE/NSF Workshop on Flow of Particulates and Fluids*, Ithaca, NY (1993).
- Willits, J., and B. Arnarson, "Kinetic Theory of a Binary Mixture of Nearly Elastic Disks," *Phys. Fluids*, **11**, 3116 (1999).

