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Reflections on Mathematical Models and Simulation of Gas-Particle Flows

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ABSTRACT

Examples of complex flow characteristics observed in circulating fluidized beds and turbulent fluidized beds are presented. Different gas-particle modeling and simulation approaches that are being pursued to probe these flow characteristics are summarized. Major advances that are likely to emerge within the next decade are discussed.

1. INTRODUCTION

Circulating fluidized beds (CFBs) and turbulent fluidized beds (TFBs) are applied widely in chemical process and energy conversion industries (1). They have been in use in fluid catalytic cracking of gas oil for nearly seven decades, and for lesser duration in many other processes; new processes, such as synthesis of olefins from methanol (2), coal and biomass gasification (3), and CO_2 capture by solid sorbents (4, 5), are under development at the present time. Although the long history of use has led to a wealth of design and operational experience with these systems, confidence to design and build commercial plants without significant levels of pilot scale testing at various intermediate scales is still lacking. This is due to an incomplete understanding of the origin and nature of the inherently complex flow structures observed in these devices, and uncertainties as to how they would change upon scale-up. Advanced experimental characterization and rigorous modeling studies are being pursued to unravel the complexities of these flows in both pilot and commercial scale systems. This article presents briefly the author's perspective on the current status of modeling these flows and the advances that can be expected to emerge in the near future.

Section 2 outlines a few illustrative examples of intriguing behavior of CFBs and TFBs, and what one would like to model and understand. This is followed by a brief discussion of why modeling them is difficult. Section 3 attempts to explain why effective fluid-particle drag force model is a critical element in accurate and yet affordable simulations. Section 4 is devoted to advances being made in different modeling approaches. Section 5 touches very briefly on role of gas turbulence. Section 6 outlines some additional data that can benefit modeling efforts. Section 7 provides an outlook of what advances in modeling and simulations can be expected in the next 5-10 years.

2. SOME FLOW CHARACTERISTICS TO UNDERSTAND AND MODEL

In its simplest form, a CFB consists of a riser tube where particles are transported up by co-flowing gas, a device to separate the gas and particles at the top, a standpipe to return the particles to the bottom of the riser and a suitable valve to control the delivery of the particles to the bottom of the riser. The volume fraction of particles in the riser is generally small enough that the particles interact with each other primarily through collisions, while in standpipes it is usually high enough that stress transmission can occur through collisions as well as sustained frictional contact between the particles and between the particles and the wall. More elaborate CFBs would include additional devices such as fluidized beds (e.g., FCC regenerator), leading to more complex flow loops for the particles. Let us briefly review a few flow characteristics that one would like to be able to understand and model.

a) In tall CFBs, operating at near atmospheric pressures, the gas pressure can increase appreciably from the top of the standpipe to the bottom resulting in loss of gas volume through compression; to compensate for the adverse effect of this compression, aeration gas is added at a number of elevations along the standpipe. At low aeration levels, stick-slip flow is often observed in the standpipe. Increasing the aeration level enables smoother flow and improved solids circulation rate. However, beyond some threshold aeration level, the flow becomes unstable and the circulation rate becomes very erratic, which is unacceptable (6). How does the onset of this instability depend on the manner in which aeration is administered and the scale of the CFB?
b) The flow characteristics in the riser are complex even under stable operating conditions. Risers typically operate in the so-called fast-fluidization regime where there is a denser bottom region, transitioning to a more dilute flow at the top. Furthermore, the time-averaged particle volume fraction and gas and particle mass fluxes manifest significant lateral variations; particle volume fractions generally tend to be high near the riser walls where the mass flux of particles is frequently negative (i.e. downflow) even though the cross-sectionally averaged mass flux of particles is positive (7). The particles tend to drag the gas downward in the wall region, and so there can be significant internal recirculation of both particles and gas in the riser. At very high gas velocities, the downflow disappears and one can even get a higher mass flux of particles at the wall region than the core (8). How well can we capture these trends in models and how confident are we in predicting the flow pattern changes that will come about upon scale-up, flow rates or modifications to the flow device?
c) Since risers are often used to carry out (catalytic or non-catalytic) chemical reactions involving the gas and particles, one can anticipate that these persistent macro-scale non-uniformities would affect the effective contact between particles and the gas, and hence the conversion and selectivities. How well can we model these effects and propose design choices to maximize conversion and/or selectivity?
d) Gas by-passing is a common concern in the operation of turbulent fluidized beds and the beds are extensively baffled to mitigate this problem. Deep beds operating at low (say, near-atmospheric) pressures are particularly

susceptible to local defluidization and gulf-streaming (9). Can we capture such flows in models and simulations, and predict how they will change upon scale-up and process modifications (such as the introduction of baffles)? When such inhomogeneous flows arise in chemical reactors, they can affect conversions and selectivities; they can also lead to reactant breakthrough to the top of the bed and cause unwanted freeboard reactions. For example, in FCC regenerators, oxygen breakthrough causes CO combustion in the freeboard leading to high temperatures that favor NO_x formation (10). Can such problems be detected in simulations in a reliable manner?

e) Cyclones play vital functions in CFBs in capturing and returning the particles and minimizing particle emissions. The mass loading of particles in the stream entering the cyclones varies appreciably from stage to stage. The separation efficiency of cyclones is determined by the competition between the swirling flow which aids particle separation and turbulent dispersion which results in re-entrainment of particles into the gas (11, 12). Mass loading of particles affects both the strength of the swirl and turbulent intensity (13-15); how well can we model and simulate these effects?

f) In some processes carried out in CFBs and TFBs, liquid is intentionally injected (16) either as a reactant or for coating purposes. In such systems, one can readily expect that in some regions of the bed (e.g., close to where the liquid is injected), the particles will be coated with a liquid and this can lead to agglomeration of the particles. These agglomerates are likely to induce local defluidization and cause secondary flow structures in the CFBs and TFBs (17). How well do we understand these secondary flow structures and their effects on conversions and selectivities (or coating uniformity)?

The above list, though incomplete, illustrates some characteristics that one would like to understand and model with confidence, so that the models can then be used as tools to test design options for new plants as well modifications to existing units. More specifically, the models should help us understand the macroscale flow behavior and allow us to perform computational experiments exploring means of manipulating the flow to maximize a desired set of objectives, such as conversion, selectivity and operational stability.

What makes modeling difficult? One can readily list a number of reasons, a few of which are described below.

a) Circulating fluidized beds typically consist of a number of devices, as mentioned above, and regions with widely different particle volume fractions are encountered in the flow loop. As a result, the manner in which stress is transmitted through the particles changes significantly from location to location. For example, such stress transmission occurs predominantly by collisions in the riser, while in the standpipe and slide (or “L”) valves stresses transmitted through enduring contact become important. As the overall performance involves a complex interaction of various devices in the circulation loop, a good model should account for the effect of stress transmission through particles via collisions as well as enduring contact.

b) Meso-scale structures form as a result of the instability of two-phase fluidized flow when the particle volume fraction becomes too small to support sustained force chains (18); the point at which this occurs depends on particle roughness, size (which affects the importance of cohesion) and shape. These meso-scale structures take the form of bubble-like voids at high mean particle volume fractions (approximately greater than 0.40) and clusters and streamers at low mean particle volume fractions (approximately less than 0.25) (19). In the intermediate region, a turbulent state exists where the meso-scale structure changes rapidly between bubble-like voids and clusters and streamers. These structures are generally difficult to resolve in computations; yet, they affect the gas-particle interactions (such as the effective fluid-particle drag, the heat and mass transfer rates, and the stress transmission in the particle and fluid phases).

c) The particles invariably have a distribution of sizes that evolve naturally through attrition, or develop because of reactions occurring in the fluidized beds. Accounting for the particle size distribution (PSD) is critical to predict accurately the rate of elutriation from turbulent fluidized beds, cyclone efficiency, etc.

3. THE FLUID-PARTICLE DRAG

It is easy to understand that one must include gravity (which pulls the particles to the bottom of any device), pressure gradient (which establishes motion of the gas relative to the particles) and fluid-particle drag (which is the principal means by which particles can be suspended against gravity) in any model to capture the flow of fluidized suspensions. The accuracy with which the fluid-particle drag can be determined is critically important in modeling of fluidized suspension flows. A number of empirical constitutive models for the fluid-particle drag in homogeneous suspensions of uniformly sized spherical particles are available in the literature (20); a prominent example is the widely used correlation due to Wen & Yu (21). A practical difficulty comes about when we apply such correlations developed for (nearly) homogeneous suspensions to flows of fluidized gas-particle mixtures.

As noted earlier, fluidized suspensions readily form inhomogeneities that span a wide range of length and time scales. As a result of these inhomogeneities, flows in turbulent fluidized beds and risers are invariably multi-dimensional. Furthermore, when the particles and the gas move around from one location to another in a device, inertia should be included in the models. Inertia – especially, the particle phase inertia – is important to capture the formation of flow inhomogeneities such as bubbles, clusters and streamers. As a result of the multi-dimensionality and inclusion of inertia, the models are invariably solved numerically on suitable spatial grids (more on solution methods later). Such computations resolve the flow at scales larger than the grid resolution, but not those occurring at a sub-grid scale. Using extremely fine grid resolution to resolve all the flow structures is often not practical.

The challenge in accounting for the effective drag force accurately can be illustrated as follows. Consider a zero-dimensional (0D) model for a turbulent fluidized bed, i.e. the entire bed is simulated using a single numerical grid cell. Such a 0D model ignores all the flow structures present in the bed and reduces to a force balance over a uniformly fluidized bed. If drag force correlations intended for homogeneous suspensions are employed, one readily concludes that the superficial gas velocity must remain well below the terminal settling velocity (v_t) of the particles in the bed; however, this is almost never the case and most turbulent fluidized beds operate at velocities in excess of v_t. This difference is primarily due to the fact that the inhomogeneities, which were not resolved in this 0D analysis, result in a decrease in the fluid-particle drag and it has not been properly accounted for in the analysis. To capture the particle volume fraction in the bed correctly using such a 0D model, one must modify the drag force correlation to reflect the effects of unresolved flow inhomogeneities. If one analyzes the same system as an unsteady flow problem using several numerical grid cells, then some of the flow inhomogeneities will be resolved, and so the modification to the drag force correlation will now be different; as the number of grids increases, the required modification to the drag force correlation decreases. Knowing what inhomogeneous flow structures have not been resolved and how one should account for their effects on the effective fluid-particle interaction (drag) force is a challenge. This issue has been addressed in the literature. O'Brien & Syamlal (22) and Heynderickx *et al.* (23) corrected the drag coefficient at very low particle volume fractions to account for the consequence of clustering. McKeen & Pugsley (24) used an apparent cluster size in an effective drag coefficient closure. Li and coworkers (25) deduced corrections to the drag coefficient using an Energy Minimization Multi-Scale approach. Filtered models, where the effects of sub-filter scale inhomogeneities on the drag force are modeled by introducing a filter size dependent drag law, are being developed (26, 27); Parmentier *et al.* (27) have presented an additional advance where the filter size dependent drag force is dynamically corrected in simulation of filtered model simulations. The development of these filtered models is still in the early stage, and many more validation studies are needed to test and refine these models.

All the modifications to the drag law that have been described in the literature, which are intended to correct for unresolved structures, are for uniformly sized particles. Drag laws for homogeneous suspensions of particles having a distribution of sizes are described in the literature (28); however, little has been published in the literature on modifying these drag force correlations to correct for unresolved structures.

4. FORM OF THE MODEL FOR GAS-PARTICLE FLOWS

The above discussion touched upon numerical computations without making specific reference to the form of the models for gas-particle flows. All the models for gas-particle flows solve the Eulerian form of the continuity and momentum balance equations for the gas phase on a fixed spatial grid, and so the unresolved structures discussed above are obviously relevant. When solving for the particle phase, there are multiple options.

4.1. Eulerian treatment of the particle phase(s)

In two-fluid models, Eulerian continuity and momentum balance equations are formulated for the particle phase as well, and are solved using the same grids (as for the gas phase). This approach (also referred to as the Eulerian-Eulerian model) has a long history of development and analysis. When multiple types of particles are present, they can be generalized as multi-fluid models, where each particle type is treated as a separate phase, interacting with all the other phases.

Two-fluid models have served well in our quest to understand the underlying mechanisms leading to inhomogeneous structures. For example, one can readily find the solution of two-fluid model equations corresponding to the state of uniform fluidization analytically, and examine its linear stability to pinpoint the origin of instability leading to bubble-like voids in dense suspensions, as well as clusters and streamers in dilute suspensions (19, 29, 30), and the characteristic length and time scales associated with the dominant instability mode. It has also helped advance simple qualitative arguments explaining why particles segregate towards the walls in riser flows (31).

The two-fluid model equation for the particle phase allows for stress transmission through the particle phase. Over the past three decades, researchers have adapted the kinetic theory of dense gases and developed constitutive models for the rheology of assemblies of monodisperse, spherical and inelastic particles interacting through binary collisions (32, 33). Such models, generally referred to as kinetic theory of granular materials, require solution of an additional scalar equation for the kinetic energy per unit mass associated with the fluctuating motion of the particles relative to the local average velocity of the particle phase (a.k.a. granular temperature); the particle phase stress is then expressed in terms of local particle volume fraction, granular temperature and local rate of deformation of the particle phase.

The kinetic theory models have also been generalized for mixtures of different types of particles (32-37). These multi-fluid models can take one of two forms:

(a) Separate continuity, momentum and granular energy balance equations are formulated for each particle phase, and solved. In this approach, if there are N different particle phases, one has to solve (N+1) continuity equations, d(N+1) momentum balances (where d denotes the number of spatial dimensions involved in the problem) and N granular energy balance equations (34, 35).
(b) Continuity equations are formulated for the N different particle species, along with a single momentum balance equation and a single granular energy balance equation for the particle mixture; these are supplemented by algebraic models for the granular temperatures of the different particle species and the “diffusive” flux of each particle species relative to the mixture flow. In this approach, one has to solve (N+1) continuity equations 2d momentum balances, one granular energy balance equation, along with a set of algebraic equations to determine the diffusive fluxes (36, 37).

A recent study comparing these two approaches found that both approaches yield similar predictions for binary particle mixtures, with the latter approach requiring less computational time (38); the advantage is likely to be more significant when the number of particle species increases.

While the kinetic theory has given us a good handle on particle phase stress resulting from particle streaming and collisions, models for stress in the dense, quasi-static flow regime where the particles make enduring contacts with multiple neighbors and stress is transmitted largely through force chains are by and large phenomenological (39-41).

Distribution of particle sizes is handled in the Eulerian modeling approach in several different ways. In one approach, the particles are divided into a number of cuts, each representing a size range and each cut is treated as a separate particle phase. Multi-fluid models are solved to determine the flow behavior. In the other approach – discrete quadrature method-of moment – the actual PSD is replaced by a sum of delta functions placed at judiciously selected particle sizes (quadrature nodes); these quadrature nodes are allowed to change temporally and spatially to capture agglomeration and break-up, change in size by chemical reactions, etc. (42). The number of different particle phases that are needed to capture the effect of PSD will clearly depend on the nature of the PSD; studies addressing how the predictions change as more and more particle phases are used to approximate a given PSD are beginning to appear in the literature (43).

The development of software platforms for solving multi-fluid models has progressed appreciably over the past two decades. The open-domain code MFIX developed at NETL (22) and commercial software (e.g., ANSYS Fluent®) are widely used by many research groups around the world to study reacting multiphase flows. Many research groups also employ in-house codes to solve such models (e.g., Neptune in the research group of Olivier Simonin).

Application of multi-fluid models to simulate gas-particle flows does raise questions and also poses a number of challenges. Let us consider the two-fluid model where the all the particles are treated as a single particle phase and examine the issues:

a) A basic question that one can raise concerns the validity of treatment of the particle phase via a continuum model. In writing such a model, it is presumed that the particles interact with each other rapidly, thus endowing the particle phase with a pressure and a viscosity. In normal fluids, we are able to do this for low Mach number flows as there is a clear separation of scales between the random motion of the molecules that gives rise to pressure and viscosity, and the mean velocity of the fluid phase. It is not at all obvious that such a separation of scales exists for the particle phase in most gas-particle flows where the particles interact via binary collisions. In such situations, the low order moments of the particle velocity distribution function - namely, mass, momentum and fluctuation energy - which are evolved through the particle phase continuity, momentum and granular energy balance equations - may not adequately define the full flow problem.
b) High resolution simulations of gas-particle flows via two-fluid models yield fine structures at length scales as small as 10 particle diameters, and it is argued by some that these fine structures are not real features of gas-particle flows and that it is manifestation of the inadequacy of the continuum treatment of particle phase in the two-fluid model.
c) The existence of such fine structure raises the issue on the required grid resolution. Resolving all the fine structures contained in the two-fluid model equations requires numerical computations using extremely fine grids. These are simply unaffordable. This necessitates development of filtered two-fluid models where the fine structures are smoothed out and their effects on the resolved flow are modeled. While some progress has been made on the hydrodynamic aspect of filtered two-fluid models, corresponding thermal energy and species balance equations have not yet been developed and validated.
d) Handling PSD using multi-fluid models, especially when the PSD is changing due to reactions, break-up, etc., remains a challenge.
e) Three-dimensional simulations using two-fluid models of large process units remain expensive (unless one uses filtered models that permit coarse grids); multi-fluid models increase the computational cost significantly.

f) Boundary conditions for multi-fluid models at solid surfaces are still primitive.
g) The continuum hydrodynamic model for the particle phase is obtained by taking the low-order moments of the Boltzmann equation for the particle distribution functions; such an approach usually emphasizes dominant aspects of flow. In some engineering applications, one would like to understand relatively rare events (such as formation of hard particle agglomerates in fluid cokers); two-fluid models are not useful for such inquiries.

4.2. Lagrangian treatment of the particle phase(s)

Here one formulates and solves Newton's equations for the motion of particles. Also, the particles are not restricted to be on an Eulerian mesh (e.g., the one used to solve for the gas phase variables). The fluid velocity and pressure gradient at the particle locations, required to solve the particle momentum balance, are readily obtained from the Eulerian (fluid phase) mesh via interpolation. Similarly, the force on the fluid due to the particles can readily be mapped to the Eulerian mesh from the particle locations. Such Lagrangian treatment offers several advantages, while also placing some limitations, as discussed below.

At very low volume fractions where inter-particle collisions are rare and unimportant, one can formally ignore collisions and employ a point-particle approximation. Such an approach is used extensively in the literature in studies on particle-turbulence interactions. In the context of CFBs, it is employed in (secondary and tertiary) cyclones. Typically 1-50 million point particles can be tracked in practical simulations and so it is possible to follow all the particles in modestly sized devices only at extremely low particle volume fractions.

4.2.1. Parcel-based approach

To circumvent this limitation on the number of particles that can be simulated, *parcels* of point particles are simulated. Here each test particle being tracked represents a large number of particles having the same characteristics as the test particle (e.g., see Andrews and O'Rourke (44), or Pantakar and Joseph (45). Such a parcel based approach can appreciably expand the range particle volume fractions that can be handled.

The approach using *parcels* of point particles must be modified when the particle volume fraction becomes sufficiently large that interactions between particles via collisions, sustained force chains, cohesion, etc. become important. In the multi-phase particle-in-cell (MP-PIC) method, the interaction of other particles with a test particle (parcel) is modeled by a force on the test particle that is proportional to the prevailing particle phase volume fraction gradient at the location of the test particle (46-49). Clearly, even though one tracks point particles, it is recognized that each particle has a finite volume; the particle phase volume fraction and its gradient at the location of the test particle affects both the fluid-particle drag and the effective force due to the interaction between particles.

Conceptually, the parcel-based MP-PIC method and the multi-fluid model are equivalent; this has been illustrated recently by direct comparison of the two approaches on a model flow problem (50). Nevertheless, there are clear differences in the advantages offered by the two approaches. As noted earlier, the two-fluid model approach is readily amenable to stability and simple macroscopic analyses, which have been useful to develop better understanding of the competing forces leading to complex flow structures. The MP-PIC approach always requires a numerical solution and is not well-suited for simple mathematical analyses. On the other hand, the parcel-based MP-PIC approach does have major attractions:

a) Particle size distribution is much more easily handled than in multi-fluid models.
b) In dilute flows where the interaction of particles with bounding surfaces occurs mainly by collisions, boundary conditions are easily implemented.
c) Changing particle properties and size are easily handled.
d) As a large number of parcels are tracked, there is a possibility that rare events can be detected and analyzed.

The parcel-based MP-PIC approach [available commercially, CPFD®] has indeed rapidly emerged as very powerful and is being used more and more in industries. Preliminary versions of this approach are available in MFIX as well. It is now being offered as an option in Fluent® as well. In the opinion of this author, parcel-based MP-PIC method will likely emerge over the next decade as a preferred approach for reasons mentioned above. At the same time, it should be noted that this approach has not been tested as extensively as the two-fluid models. There are relatively few interrogations of the properties of solutions obtained by this approach; for example, studies investigating the influence of grid resolution on the solutions for various classes of flow problems – fluidized beds, risers, etc. – are needed. A limited investigation (50) performed recently shows that at fine grid resolution the parcel based approach yields similar microstructure as the two-fluid model, and so it appears that MP-PIC simulation of flows in large devices using coarse grids will need filtered fluid-particle drag force models (and possibly modifications to the effective particle interaction force as well) – as in the case of multi-fluid models. If this is indeed the case, and if so, what filtered fluid-particle drag force model is appropriate for the parcel-based approach, are not clearly understood at the present time.

It would also be useful to perform more simulations of classical problems to gain better understanding of the parcel-based approach itself, as well as the underlying flow physics. One example would be simulations of fluidization in a vertical pipe over a wide range of gas velocities and particle fluxes, thus generating a map of average pressure gradient vs. gas velocity at different particle mass fluxes. The general character of such *phase diagrams* are well known experimentally: choking, multiplicity of states and carrying capacity of the gas have been widely studied experimentally (51, 52). Demonstrating that such complex phase diagrams can be robustly captured would greatly increase the confidence of the method in the minds of the users, than simply testing the method against a few operating conditions.

4.2.2. Discrete Element Method (DEM) for spherical particles

One can, in principle, circumvent the need to postulate a phenomenological model for the force on a test particle due to interactions with other particles (in the parcel approach) by directly simulating all the finitely sized particles in a region and their interaction via collisions and enduring contacts. Though these simulations may allow for arbitrarily shaped particles, let us focus first on spherical particles, which have been studied the most using granular/molecular dynamics. In assemblies at low particle volume fraction, where the particles interact largely through binary collisions, grains are conveniently modeled as hard particles that experience instantaneous collisions, which are detected using an event-based algorithm. At high volume fractions, where particles tend to make enduring contact, DEM is the preferred approach, where the particles are modeled as soft spheres that can overlap slightly and exert both normal and tangential forces on each other (53). DEM simulations, however, are computationally expensive. In the early 1990's, DEM simulations were limited to about 10^3 particles (54, 55); simulations of millions of soft-sphere particles are now feasible using CPUs with higher clock frequency, as well as computer clusters. Also, significant improvements in commercial (e.g. PFC3D (56)), as well as open-source (e.g., LAMMPS (57)) software make DEM simulations more common. Recent applications of DEM-based simulations of particle flows also include a coupling to computational fluid dynamics (CFD) of the fluid phase, e.g., cyclone separators under high mass loads (58), or the DEM-CFD model recently proposed for fluidized bed reactors including heat, and mass transfer, as well as chemical reactions (59). Computations using Graphic Processing Units (GPUs) have become fashionable after software to use these powerful co-processors was published (60). Tailored applications focusing on single-GPU computations have been developed, enabling a roughly 100-fold speed-up compared to conventional single-CPU calculations (61, 62). Thus, the application of DEM-CFD models is poised to grow rapidly in the years ahead.

DEM is also widely used as a tool to study rheological behavior of dense particle assemblies (63-65). However, most of these studies have been only for spherical particles. Also, these simulations tend to use simple interaction models (e.g., the linear spring-dashpot model of Cundall and Strack (66)). A comprehensive overview of more sophisticated contact force models, e.g. accounting for rolling and twisting resistance between particles, is given by Luding (67). Rarely do all details of these sophisticated contact forces and torques significantly impact granular flow behavior in most of industrial applications of interest; instead, the effect of particle shape has a more severe impact on the static and dynamic features of a granular assembly (53).

4.2.3. DEM for non-spherical particles

The effect of particle shape on flow behavior is currently an active area of research – both from an experimental, as well as modeling point of view. Campbell (68) investigated the flow of prolate spheroidal particles and their effect on granular flow transition; he found that force chain formation, and consequently the stresses in a quasi-static flow situation, depend strongly on particle shape. A specialized algorithm for cylindrical objects has recently been published by Kodam *et al.* (69, 70). In this latter work the particles are described as *true* cylinders (as opposed to spherical particles glued together). Also, Kodam *et al.* provided experimental verification of their approach, as well as a comparison of their simulation with a glued-sphere approach. DEM simulation of non-spherical particles requires significantly more computational resources than a similar simulation of spherical particles. Although various strategies to approximate the true shape of particles exist, they currently cannot compete with the accuracy and details of particle interaction force modeling available for spherical particles. This point is even true for specialized algorithms, e.g., the one used by Kodam *et al.* (70), as the latter did not include rolling or twisting resistance. Thus, there will be always a compromise between particle shape, contact force modeling, as well as time and resources available for the simulation.

While the effect of shape on dry granular flow without interaction with the gas phase has been summarized recently (53), there is much less published on fluidized suspensions; more studies would be useful to fully expose the role of particle shape on fluidization. Recently, Liu et al. (71) measured lower fluidization velocities of non-spherical particles compared to sphere packings. Hilton et al. (72) simulated non-spherical Geldart group D particles using a DEM-CFD approach. Rosendahl and Mando (73) recently reviewed the status of models for non-spherical particle motion in gas-solid flows, and highlighted the importance of the alignment of particles with turbulent vortices. The effect of particle shape on fluidization is likely to be a concern in fluidized beds used to gasify biomass, where degassing of the particles may also alter the effective fluid-particle drag considerably.

4.2.4. More on parcel-based methods

Even with advances in computational power, DEM simulations will remain prohibitive for large process devices. Therefore, a parcel-based approach will remain the method of choice for large scale problems. As noted earlier, in the parcel-based MP-PIC method the particle interaction force is modeled through an empirical particle pressure, while in DEM simulations they are resolved. Researchers have examined if the parcel-based method could be configured in a way that the need for empirical pressure model can be eliminated. Sakai *et al.* (74) as well as Mohktar *et al.* (75) assume that the parcel is represented by a sphere with a volume equivalent to the sum of the volumes of the particles making up the parcel. This requires contact detection between parcels, and hence is computationally more expensive than the parcel-based MP-PIC approach discussed earlier. A primitive form of such contact detection has been already used in the work of Patankar and Joseph (45). Bierwisch *et al.* (76) have shown recently that a parcel-approach with contact detection, when using appropriately scaled interaction parameters, yields simulation results independent of the number of particles making up the parcel. In this approach, one would be performing DEM simulations of the pseudo-particles representing the parcels, where the characteristics of these pseudo-particles are chosen (based on dimensional analysis) such that important features of the flow remain equivalent to the flow of the original particles. Specifically, they show that it is possible to obtain stresses in the quasi-static regime and parcel velocities in all regimes of granular flow, that are independent of the scaling of the system. Analogous scaling can be identified for a linear spring-dashpot model as well (77), whereby properly scaling the spring stiffness, the damping coefficient, as well as cohesive forces, a parcel-based approach can be made to yield the same *quasi-static* flow behavior, stresses, and particle velocities as the original particle system; however, the parcel-based approach with contact detection overestimates the stresses in the inertial regime (78) where stresses are primarily transmitted through collisions and so a correction is needed.

In their latest work, O'Rourke and Snider (46) propose a method to relax the parcel velocities to their local mean value which can be adapted to the parcel-based approach with contact detection to obtain the same particle phase pressure as in the original system of particles (Radl *et al.* (77)). Thus, it seems possible to have a discrete particle method based on parcels that can closely approximate the stresses in the original system of particles across different flow regimes. In the opinion of the author, this approach holds promise for simulations of flows in standpipes, hoppers, spouted beds, dense phase pneumatic conveying, etc.

5. ROLE OF GAS TURBULENCES IN CFBs AND TFBs

In turbulent and fast fluidized beds, where the mass loading of particles is often one or more orders of magnitude larger than that of the gas, gas turbulence has only a secondary effect on the flow in most of the regions (in the opinion of this author). Its effect is more likely to be localized in regions where the particle volume fraction is low (for example, in cyclones where turbulent dispersion of particles lead to loss of separation efficiency) and at the interface separating dense and dilute region where it plays an important role in entrainment of particles into the dilute stream (for example, particle pickup by turbulent eddies in pneumatic conveying, and entrainment of particles into jets). Adequate resolution of gas-phase turbulent fluctuations (e.g., via Large Eddy Simulations, or Direct Numerical Simulations) in industrial-scale devices and jets, especially at high particle volume fractions, does not seem feasible for the foreseeable future. We will continue to rely on sub-grid models for the role of gas turbulence in inducing fluctuations in the particle phase. Such models can readily be included in the granular energy equation of the two-fluid model and in parcel-based models (79, 80). This seems adequate for modeling gas-phase stresses in CFB applications, where the mass loading (i.e., the ratio of particle mass flux to gas mass flux) is relatively high.

6. MODEL VERIFICATION AND VALIDATION

It is clear from the discussion above that a variety of different models are being applied to study gas-particle flows, and simulations are based on discretized versions of these models. It is important that the models and the simulators based on these models be subjected to careful verification as well as validation with experimental data. What constitutes verification and what is validation have been discussed in some detail by Grace (81).

Verification is an essential first step and it can take several different forms depending on the model being tested:

a) It is important to demonstrate that simulators based on any model be compared (if possible) with analytically obtainable results for some test problems, even if the problems are highly idealized. For example, in two-fluid models for gas-particle flows, the growth rate of instability modes (starting from a uniformly fluidized state) can be determined readily through linear stability analysis; verifying whether numerical codes can reproduce the analytical results (and if so at what grid resolution and time steps) is a natural test of the fidelity of the code [for example, see ref. (30)].
b) When parcel-based model simulations with collision tracking are formulated, it is important to verify that they yield the expected trends in predictions as one changes parcel size [For example, see ref. (77)].
c) When a filtered two-fluid model is developed by coarse-graining some (say, kinetic theory based) two-fluid model equations, one should verify that simulations of the filtered model yield the same coarse flow structures as the underlying two-fluid model (82).

d) Models invariably involve approximations; frequently different models tend to capture different aspects of physics more accurately. Yet, there must be situations where the different models agree with each other reasonably well; and so, it makes eminent sense to compare predictions of various models. Such predictions fall in the category of verification and not validation. For example, demonstration that two-fluid model and a parcel-based model yield nearly the same results in simulations of a highly idealized flow problem (50) is a useful verification step as it enhances the credibility, establishes equivalence between models and exposes how ideas from one approach can be adapted for the other. Comparison of CFD-DEM and multi-fluid models is also in the same spirit.

e) Comparison of the simulation results obtained at different grid resolutions is also an important verification step. Although this is indeed done in most published articles in an empirical manner (i.e. presenting results obtained at different grid resolutions for one or two test simulations), concrete guidelines on grid resolutions needed to get grid-size independent results are generally not available, with a recent study by Parmentier *et al*. (27) being a welcome exception. As a result even when grid size independence is demonstrated and the simulation is validated against experimental data in a pilot scale unit, practical challenges regarding grid resolution requirements when applying that simulation approach to large scale devices are not fully appreciated. Good verification studies should strive to bring forward simulation issues at different scales.

Even though most of the simulation studies solve the unsteady equations governing the flow, attempts to validate have invariably focused on time-averaged flow characteristics such as axial pressure profile and lateral variation of particle volume fraction and mass flux. Indeed, these quantities arise naturally as the most important ones. Since the flows manifest persistent fluctuations, comparing the power spectra of fluctuations between the models and experiments makes eminent sense (of which differential pressure is the easiest to measure). Since the extent of contact between the gas and the particles is intimately linked to gas dispersion characteristics, they are also important metrics. The challenge problems issued as a part of this CFB-10 conference do indeed focus on validation of models with experimental data on these quantities.

A large number of early studies compared time-averaged results obtained from 2D simulations with experimental data; with increasing computing power, more and more 3D simulations are being done. As one would expect, there are quantitative differences between the results obtained with 2D and 3D simulations, and so true validation does require 3D simulations. However, 3D simulations are very expensive and so demonstrating grid independence of solutions is often prohibitive; in the opinion of this author, it is not at all obvious if some of the published simulation results are truly grid independent. This point is particularly clear from the simulation study of turbulent fluidized beds by Parmentier *et al.* (27) who estimated the grid size needed for nearly grid independent solution of standard two-fluid models used by most researchers; such resolution is often not feasible in commercial scale devices. Based on a recent study (50) comparing the two-fluid model and a parcel based approach, it appears that the grid resolution requirement for the latter approach is also similar. Given this concern (as to whether the computed results are truly grid independent), there is a lingering doubt as to whether favorable comparison of model predictions with experimental data is really indicative of successful validation or a coincidence for the chosen grid resolution. Researchers engaged in simulations certainly understand the need to seek grid independent results, and so the above comment is not intended as a criticism; instead, it is presented as a practical limitation imposed by the size of the problem that one can simulate within the available resources. As clearly demonstrated by Parmentier *et al.* (27), the grid resolution needed to get a grid-independent solution changes appreciably with particle size. Therefore, experimental data on riser flows and turbulent fluidized beds for particles of different sizes would be valuable. The challenge problem (#3) discussed in this conference considers riser flow data for 59 μm (group A) and 802 μm (group B) particles. It would be useful to generate riser flow results for several intermediate sizes as well. The challenge problems include turbulent fluidized bed data for a single particle size (~75-80 μm, with different fines contents); data for somewhat larger particles would be useful as well.

Even if a particular model is validated successfully using pilot scale data (at a certain grid resolution), is there a basis for trusting the simulation results on commercial scale device performance obtained using this model and necessarily coarser grids? This question has been repeatedly posed to the author of this article by researchers in industries (who use the simulation tools to evaluate performance of commercial scale devices). A major concern in scale-up from pilot scale to commercial scale has always been whether the flow characteristics would change qualitatively upon scaleup and lead to serious shortfall in performance. With this in mind, it is suggested that one should compare simulation results obtained at different scales with experimental data. For example, the current challenge problem (#3) considers data obtained in a 30 cm diameter riser; researchers will continue to use these data for many years to further refine their models and simulators. (The data from earlier challenge problems continue to be used for validation studies even today.) It would be useful to collect analogous data on a larger scale unit (say 75 cm diameter riser) for future challenge problems, so that one can evaluate how well the various models and simulation approaches capture both sets of data (30 and 75 cm).

A great deal of current research is aimed at incorporating PSD into models and simulations. To better understand the role of PSD and also validate these models, it would be useful to have data for different PSDs (particularly for group B particles in the size range of commercial interest).

Risers tend to operate in the fast fluidization regime, where (sometimes) there is a dense phase at the bottom transitioning to a dilute phase at higher elevations. Phase diagrams for riser flows suggest that nearly the same combination of riser gas velocity and particle mass flux can yield different pressure drops across the riser depending on the height of the dense region at the bottom. In such situations it is more sensible to specify one of the fluxes and the pressure gradient and calculate the other flux as an output. Most simulators do not perform such computations and part of the reason for poor validation may be due to this. This suggests that it would be useful to have (at least skeletal) performance data at different riser gas velocities (while fixing the solids flux) and generating results akin to the phase diagram mentioned in section 4.2.1). One would then ask how well models and simulations capture a continuous spectrum of operating conditions – this can help assess if the departure between models and experiments is qualitative or quantitative.

In the not too distant future, simulations of the entire CFB loop will become common. It would be of interest to develop good data sets on standpipe operation for models to compare against. The standpipe plays a critical role in stable operation of the CFB loop. Plant operators often seek to increase circulation rate (which is usually tied to productivity of the unit) by improving aeration. Unacceptable failure of the standpipe upon excessive aeration is of practical concern and models and simulations can play a valuable role in understanding this problem and identifying means of improving performance without causing instability. Good data to validate simulations of standpipe flow will help improve confidence in simulations of the full CFB loop.

7. FORWARD LOOK

Within the next 5-10 years, significant advances can be expected in simulation of CFBs and TFBs, because of improved computer resources, as well as better modeling approaches. Three-dimensional simulations of full CFB loops will become more common, and these will pave the way for better understanding of global phenomena such as loop instability. Instead of performing simulations at a small number of operating conditions (in individual units such as risers), researchers will map out model predictions over a range of conditions and examine the robustness of trends and quantify uncertainties in the simulation results.

At a more fundamental level, coarse-grained drag laws for polydisperse systems will emerge along with better understanding of how they should be constructed for the different simulation approaches (multi-fluid models vs. parcel based method). Parcel based methods (with and without collision detection) will likely emerge as the more preferred approach, and it will be studied in greater detail by academic researchers as well, leading to further improvements in the method.

Although not discussed in this article, better understanding of models that one would use for wet systems (such as fluid cokers) where the particles can form agglomerates will also emerge (83). These, in conjunction with flow simulators, will lead to better understanding of secondary flows in such devices. Recent experimental findings, as well as small-scale simulations are a promising starting point to refine our understanding of liquid transport in fluidized beds (84, 85).

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