



Appendix 2: Report of study group on disperse flow [☆]

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Abstract

In this report, we have outlined a number of scientific challenges which represent building blocks for the comprehensive understanding of disperse flows encountered in a variety of technologies and in nature. In dilute particle-laden turbulent flows, we see a need for more realistic descriptions of particle–fluid and particle–particle interactions that would ultimately be suitable for incorporation in large eddy simulations. Experiments are needed to clarify the mechanisms by which particles modulate turbulence. Progress in computer simulation methods and kinetic-theory analyses are leading to new opportunities to obtain the equations of motion for more concentrated multiphase flows which are strongly influenced by or dominated by the disperse phase. However, instabilities inherent to the multiphase nature of these flows lead to the very complex behavior of industrial scale multiphase flows. We require a better understanding of these instabilities as well as coarse-grained models for the average multiphase flows at larger scales. A major issue in dense granular flows is to elucidate the manner in which particle–particle frictional interactions can lead either to mixing or segregation of different particle species.

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1. Introduction

This article outlines some outstanding problems in the area of disperse flows where the loading of the disperse phase ranges from dilute to dense. The systems considered include

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fluid–particle mixtures (where we consider the entire range of particle volume fractions from dilute to random close packing condition), dilute droplet laden gas flows (where the liquid droplets can essentially be treated as particles) and bubbly suspensions. Important challenges ahead of us in the area of disperse flow include:

- (a) Understanding and quantitative modeling of gas–particle interactions when the particle size is larger than the Kolmogorov scale,
- (b) development of averaged equations of motion and associated closure for situations where the continuous phase inertia associated with the relative motion between the continuous and dispersed phases is important,
- (c) understanding the statistical characteristics of fluctuations resulting from instabilities associated with the inertia of relative motion between the phases and development of coarsened equations of motion,
- (d) development of quantitative models for contact stresses in dense granular assemblies resulting from frictional and cohesive interactions between the particles, and
- (e) a thorough understanding of the competition between mixing and segregation in granular systems, including techniques to control these through manipulation of interparticle cohesive interactions.

These are discussed in a greater detail below. This report groups the systems in terms of disperse phase loading levels as follows:

- (a) Dilute particle-laden flows, where the influence of particles on fluid turbulence and the effect of fluid turbulence on particle motion are principal issues,
- (b) suspensions at modest to high particle loading levels, where the issues range from formulation of averaged (two-fluid) equations of motion and associated constitutive relations to instabilities and their consequences to suspension flow,
- (c) mixing, segregation and flow of dense particulate systems with enduring contact between particles and between particles and bounding surfaces, where the particle interactions, cohesion and size/shape/density distribution influence the way particles pack and respond to imposed stresses, and segregate/mix.

2. Dilute particle laden flows

Here we focus exclusively on dilute particle or droplet-laden gas flows, where the volume fraction of particles is very small, but the mass loading ratio may be as large as unity or even greater. Strong two-way coupling, where the motion of the fluid has a significant effect on the particle motion and vice versa, is present. Interparticle collisions may also be significant.

Such dilute particle-laden gas flows are found in nature and technology, e.g. sand and rain storms, coal combustors, paint sprayers, cyclone separators, and liquid-fuel combustors. The regime may extend to fast-fluidized beds, grain conveying systems, and snow avalanches. Most or all of these flows are turbulent. While, geometric parameters and the overall Rey-

nolds number usually are sufficient to describe the baseline single phase flow, the addition of the particle phase adds several more parameters including the mass loading ratio, the Stokes number (particle time constant/fluid time scale), the particle Reynolds number based on particle diameter and mean relative velocity of particles and fluid, and the particle diameter normalized by an appropriate length scale (commonly, the Kolmogorov length scale).

2.1. Large-eddy simulations

A large fraction of recent CFD development work for particle-laden flow is centered on extending existing single-phase large-eddy simulation or direct numerical simulation codes by the addition of particle tracking and back momentum coupling (through point-force approximation). These codes can track several million individual particles simultaneously and have recently been applied to the computation of complex geometry systems (e.g., stirred reactors) (Wu et al., 2001) and also in simple geometries to explore basic phenomena such as fuel droplet clustering in spray combustors (Oefelein, 1998).

These codes assume that the particle Reynolds numbers are small and that the particles are much smaller than the Kolmogorov scale. However, in many applications, particle Reynolds numbers are in the range of 0.1–100 and the particle diameter is comparable to or even greater than the Kolmogorov length scale. An important challenge is to understand the fluid/particle interactions in such a parameter range and develop validated models (for use in the CFD codes). Specific examples of the shortcomings of the current CFD codes are illustrated below.

- Particle tracking in these codes is done using highly simplified equations of motion; generally, the resolved fluid velocity field is interpolated to the position of the particle and an analytical or empirical drag law is applied assuming that the particle is moving in a locally uniform velocity field. This neglects the fact that the flow is turbulent and may have motions with the same scale as the particle. Published large eddy simulations, rarely, if ever, include any effect of the sub-grid scale turbulence on either the overall drag or on motions transverse to the inferred relative velocity.
- The drag laws used in most simulations accounting for two-way coupling are based on the undisturbed relative velocity. However, when two-way coupling is implemented in the code, the undisturbed velocity is not available. Simple calculations suggest that the standard technique can cause very large particle tracking errors (Burton and Eaton, 2001). New analytical research is needed to develop an appropriate way to use the self-disturbed velocity field to calculate the particle drag.
- The existing codes ignore the effect of particles on small-scale turbulence that is modeled in large-eddy simulations. However, it is difficult to argue that this effect is insignificant in flows where the turbulence is modified strongly by the particles.
- Large-eddy simulations require very fine grids near solid boundaries, and in many cases, the grid spacing is smaller than the particle diameter. Implementation of standard particle-tracking and back-coupling algorithms is clearly not appropriate.

2.2. Fluid–particle interactions

The issue of accurate particle drag laws which are applicable even in flows where the particle diameter is of the same order as the Kolmogorov length scale is of fundamental interest and goes beyond use in CFD codes. There is little information in the analytical, computational, or experimental literature to guide us in formulation of these drag laws. One can imagine that turbulent eddies on the same scale as the particle would have a significant effect on the drag applied on the particle and on motions transverse to the average relative velocity. The drag on a particle with Reynolds number of order 10 is likely to be sensitive to the details of the particle wake. Those details could be modified significantly by small-scale turbulence. Highly resolved computations and experiments are required to assess the importance of this issue and to guide the development of models.

2.3. Particle–particle interactions

Collisions between particles may be significant in this flow regime. Several workers have used detailed simulations to study the statistics of particle collisions in simple turbulent flows (e.g., see Sundaram and Collins, 1997; Reade and Collins, 2000), where the particles are small compared to the Kolmogorov scale. Collisional and hydrodynamic interactions between particles, when the particle size is not small compared to the Kolmogorov scale, represent fertile areas of research.

Due to the potential importance of collisions and the growing importance of codes tracking millions of particles, research into efficient models to represent the effects of collisions is imperative. Detailed experiments should be proposed to examine collision statistics in a dilute turbulent gas flow. Three-dimensional particle-tracking velocimetry seems to offer an appropriate vehicle to study this.

2.4. Turbulence modification by particles

One of the most important problems in dilute particle-laden flows is turbulence modification. In some simple turbulent flows, reductions of the turbulent kinetic energy by greater than 80% have been observed at mass loading ratios below 0.5 (Kulick et al., 1994), see Figs. 1 and 2. Such dramatic changes in the turbulent kinetic energy (shown in Fig. 1) may be expected to have pronounced impact on heat and mass transfer characteristics. Simultaneous measurements of turbulence and heat transfer characteristics of particle-laden flows (e.g., see Yarin and Hetsroni, 1994a,b,c) should be made to explore and understand this coupling.

Other quite similar flows reveal almost no turbulence modification up to fairly high mass loading ratios (Fessler and Eaton, 1999). Some other flows containing large particles exhibit substantial enhancement of turbulence (Gore and Crowe, 1989; Parthasarathy and Faeth, 1990). Turbulence attenuation can have enormous effects on device performance, yet there is no theory or model that allows consistently accurate predictions of turbulence modification. The physical mechanisms are so poorly understood that experts in the field cannot predict if turbulence attenuation will occur in a given flow.

Turbulence modification is apparently a strong function of the particle Stokes number. A few experiments (Eaton, 1994) suggest that attenuation is largest for Stokes numbers based on the

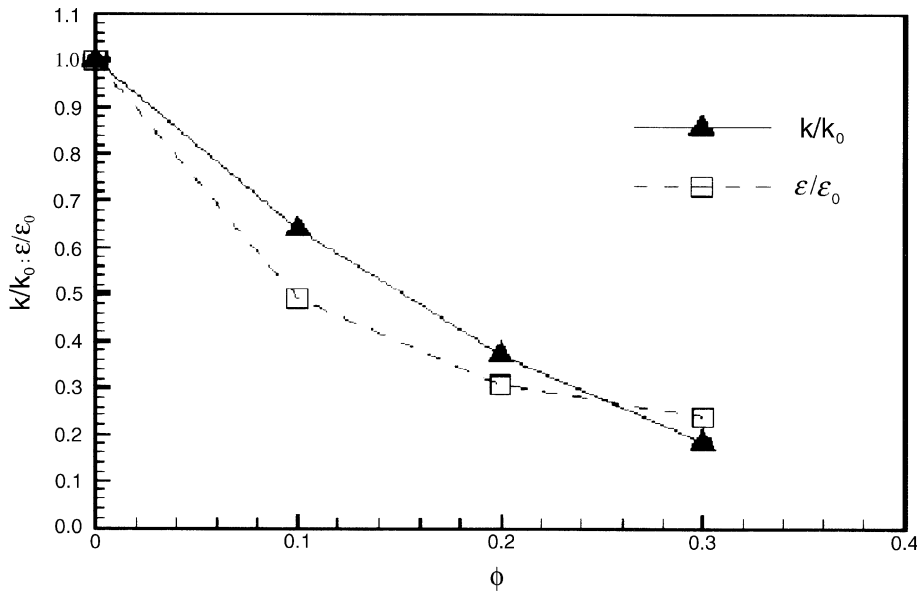


Fig. 1. Turbulent kinetic energy and rate of viscous dissipation as functions of mass loading ratio. These quantities are scaled with respect to corresponding quantities of zero mass loading. Data were obtained in the center plane of a fully developed channel flow of air with uniform loading of $150\ \mu\text{m}$ glass spheres, with resolution down to the Kolmogorov scale (but not to the particle scale). The channel flow Reynolds number based on the half width and the mean velocity was 13,800. Constant mass flow of gas was maintained. Stokes number based on the Kolmogorov time scale is 50. Particle diameter/Kolmogorov length scale = 0.88 (source: Paris et al., 2001).

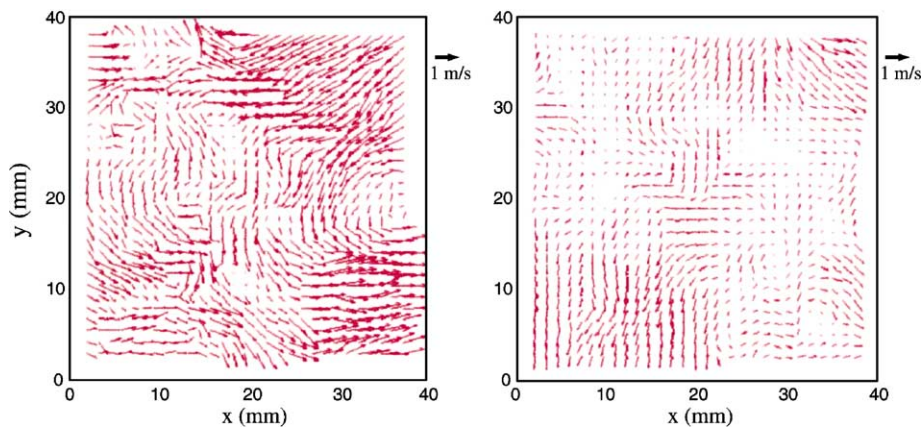


Fig. 2. Instantaneous snapshots of gas velocity fields. (a) Unladen flow with a Taylor microscale Reynolds number is 470, (b) with $150\ \mu\text{m}$ glass spheres at a mass loading of 0.3. Data obtained in a forced homogeneous/isotropic turbulence chamber operated under micro-gravity conditions. The scales in both figures are the same, and the strong attenuation due to the particles is evident. Particle phase velocities are not shown. Stokes number based on the Kolmogorov time scale is 79. Particle diameter/Kolmogorov length scale = 1.1 (source: unpublished work of Hwang, W. and Eaton, J.K., 2002).

Kolmogorov time scale of the order of 10 and particle diameters of the same order as the Kolmogorov length scale. Fundamental studies of turbulence modification in recent years have centered on the use of direct numerical simulation codes with the addition of point-force coupled particles or very recently using two-fluid models (Squires and Eaton, 1990; Ahmed and Elghobashi, 2000; Boivin et al., 1998). Both make major assumptions in their formulations that are not valid in the parameter regime noted above. Specifically, for the point-force coupling to apply, the particles must be much smaller than the grid scale. This cannot be achieved if the particle diameter is approximately the same as the Kolmogorov scale. In the Reynolds averaged modeling arena, most effort has been directed at correctly computing the so-called extra-dissipation due to particles in the kinetic energy transport equation. However, this term has been measured experimentally, and it does not correlate well with observations of turbulence attenuation (Paris and Eaton, 2001; Longmire and Khalitov, 2002).

New experiments and or analyses are needed to cast light on the important phenomena that cause turbulence attenuation. In the experimental arena, measurements are needed that allow us to understand the scaling of turbulence attenuation with the various dimensionless parameters discussed above. Experiments should be conducted in simple turbulent flows such as grid turbulence, fully developed pipe or channel flow, or simple axisymmetric jets. Regardless of geometry, experiments must include a wide range of particle parameters in a single fixed facility. Ideally, the particle size would range from particles so small that they act as flow tracers and do not cause attenuation up to particles that are so large that they cause turbulence augmentation. (The experiments should also explore the effect of particle size distribution.) Flow parameters, especially the Reynolds number should be varied to assess the importance of the range of turbulent length scales in setting turbulence attenuation. Measurements should include at a minimum the mean and second order turbulent statistics for both phases, as well as particle/fluid velocity correlations.

More detailed experiments may be possible that cast light directly on mechanisms of turbulence modification. These would involve observations of the distortion of turbulent eddies in the neighborhood of particles. One of the biggest questions is how sub-Kolmogorov scale particles can affect energy containing eddies. Early thinking was that they only affected those eddies by collective action, similar to changes caused by an increase in viscosity. However, some recent results suggest that individual particles may substantially distort energy containing eddies (Eaton et al., 1999; Hishida and Sato, 2001). This may be the key to understanding turbulence attenuation. Detailed simulations that resolve the flow around each particle may also contribute to our understanding of turbulence attenuation.

2.5. Transition to turbulence

The addition of particles and bubbles will modify instabilities such as the transition to turbulence that occur in a single-phase flow. Particles enhance the effective viscosity of a suspension and this may be expected to delay the transition to turbulence. On the other hand, particles create a disturbance in the fluid. Since the instability of single-phase pressure-driven channel flow is subcritical and laminar planar Couette flow and pressure driven pipe flow are stable to infinitesimal disturbances for all Reynolds numbers, the finite amplitude disturbances produced by particles may play an important role in triggering a transition to turbulence (Matas et al., 2003). Particles

may also modify the mean velocity profile and thereby influence flow transitions. An important challenge in performing experiments to test the effects of particles on the transition to turbulence is to identify diagnostics that can indicate the transition even in the presence of particles that cause fluid velocity fluctuations in a laminar flow.

3. Concentrated “fluid-like” suspensions

3.1. Derivation of equations of motion and constitutive equations

Although general conservation laws for the mass and momentum of each phase (or of the dispersed phase and the mixture) can be derived readily, these two-fluid model equations are not closed. A simple starting place for considering the constitutive equations is to study the interaction of a single particle, drop, or bubble with the continuous phase. Much progress has been made at this level, whose validity is necessarily limited to very dilute systems. Even here, issues related to carrier phase turbulence (discussed above) remain unsolved.

A greater challenge concerns more concentrated suspensions where particle–particle interactions (both hydrodynamic interactions mediated by the continuous-phase fluid motion and direct collisions) play an important role. The understanding of the rheology of low Reynolds number suspensions has benefited greatly from consideration of simple model suspensions and simple flows for which analytical theories can be developed, tested, and then generalized to more complex systems. These studies often include direct comparison between theory, many-particle simulations, and ideal experiments specifically designed to test the theories. The time is ripe for applying a similar approach to multiphase flows where inertial effects are important on the particle length scale.

Theories have been developed for three special cases of inertial multiphase flow: rapid granular flows, gas–solid suspensions, and suspensions of high Reynolds number, nearly spherical bubbles (Lun et al., 1984; Sangani et al., 1996; Spelt and Sangani, 1998; Koch and Sangani, 1999). The latter theory allows for relative motion of the continuous and disperse phases as well as shearing of the suspension. These theories are based on analogies with the kinetic theory of dense gases but allow for the dissipative effects of fluid viscosity and inelastic particle collisions. The theory of rapid granular flow assumes that particles undergo only instantaneous collisions (and not enduring solid-body contacts) and neglects all effects of the continuous phase. Theories of gas–solid suspensions have added the effect of a low Reynolds number gas, while assuming the particle Stokes number is large—a situation made possible by the large ratio of densities of the two phases (Sangani et al., 1996). Theories for bubble suspensions are limited to potential flow interactions among essentially spherical bubbles (Spelt and Sangani, 1998). Although the simplest formulations of the theories consider nearly Maxwellian particle (or bubble) velocity distributions and Newtonian constitutive equations, more complex rheology including normal stress differences and viscoelastic responses can be captured by solving dynamic equations for all the components of the second moment tensor for the particle velocity distribution.

These theories have been validated extensively by comparison with many-particle numerical simulations based on the same physical assumptions as the theories (e.g., see Sangani et al., 1996), but the comparison with experiment is quite limited. There is a need for careful experiments involving homogeneous flow to test the theories described above.

To develop a more general theory for disperse multiphase flows, a three-pronged strategy would be useful.

- (a) We should extend the theories for weakly dissipative multiphase flows to include stronger dissipative effects. For example, one can allow for finite Reynolds number effects in the theory for a gas–solid suspension by allowing for the enhanced viscous dissipation of particle kinetic energy at finite Reynolds number, including the Reynolds stresses of the gas, and considering the viscous force dipoles acting on the particles.
- (b) Theories for Stokes flow suspensions provide an opposite limiting case where viscous dissipation dominates over particle inertia. We should consider the first effects of fluid inertia on the rheology of a suspension at small, but non-zero Reynolds number, and establish a second beachhead in our attempt to understand moderately dissipative systems (Lin et al., 1970).
- (c) It is now possible to simulate the dynamics of particle or bubble suspensions (Bunner and Tryggvason, 1999). Much of the earlier work has been aimed at developing the numerical methods and verifying the accuracy of their predictions for a given initial particle configuration. We should perform more extensive simulations with adequate time and/or ensemble averaging and a closer connection between simulation and averaged-equation modeling to reap the full benefit of these numerical simulation methods. The results of these simulations can be used to test approximate theories that are developed as extensions of the exact asymptotic results that can be obtained in the weak and strong dissipation limits.

It is vital to test theory and simulation against physical experiments. Such comparisons are beginning to appear (Bizon et al., 1998; Bougie et al., 2002) for the case of rapid granular flows (see Figs. 3 and 4), but remain to be performed in multiphase flows. As discussed below, instabilities may occur in these suspensions on a length scale of the order of 10–50 particle diameters, so a narrow-gap channel or Couette, in which the gap thickness is only 5–10 particle diameters, may be necessary to achieve a stable flow. A good understanding of the boundary conditions on the averaged equations of motion is essential to achieve a quantitative comparison of theory and experiment. Boundary conditions for granular flows have received much attention (Hui et al., 1984; Jenkins, 1992; Louge, 1994), but the current understanding of boundary conditions in two-phase flows is more limited.

The shear flow of neutrally buoyant solid particles over a wide range of particle Reynolds numbers warrants careful study. A recent investigation by Hunt et al. (2002) shows that the classic experiment of Bagnold (1954) on high Reynolds number neutrally buoyant particle shear flow did not truly probe the effects of the particle phase on the suspension rheology.

Present theories of multiphase flow typically do not incorporate effects of bubble or drop deformation. It is now possible to simulate interacting deformable bubbles (Esmaceli and Tryggvason, 1999), but we require a theoretical framework that accounts for bubble deformation. There is a mean bubble shape that is induced by the mean relative motion of the phases and the shear flow and this has a large effect on the drag, added mass and lift forces acting on the bubbles (Magnaudet and Eames, 2000; Sankaranarayanan et al., 2002; Sankaranarayanan and Sundaresan, 2002). However, there may also be important effects of bubble shape oscillations induced by the hydrodynamic disturbances caused by the bubbles and by bubble–bubble collisions.

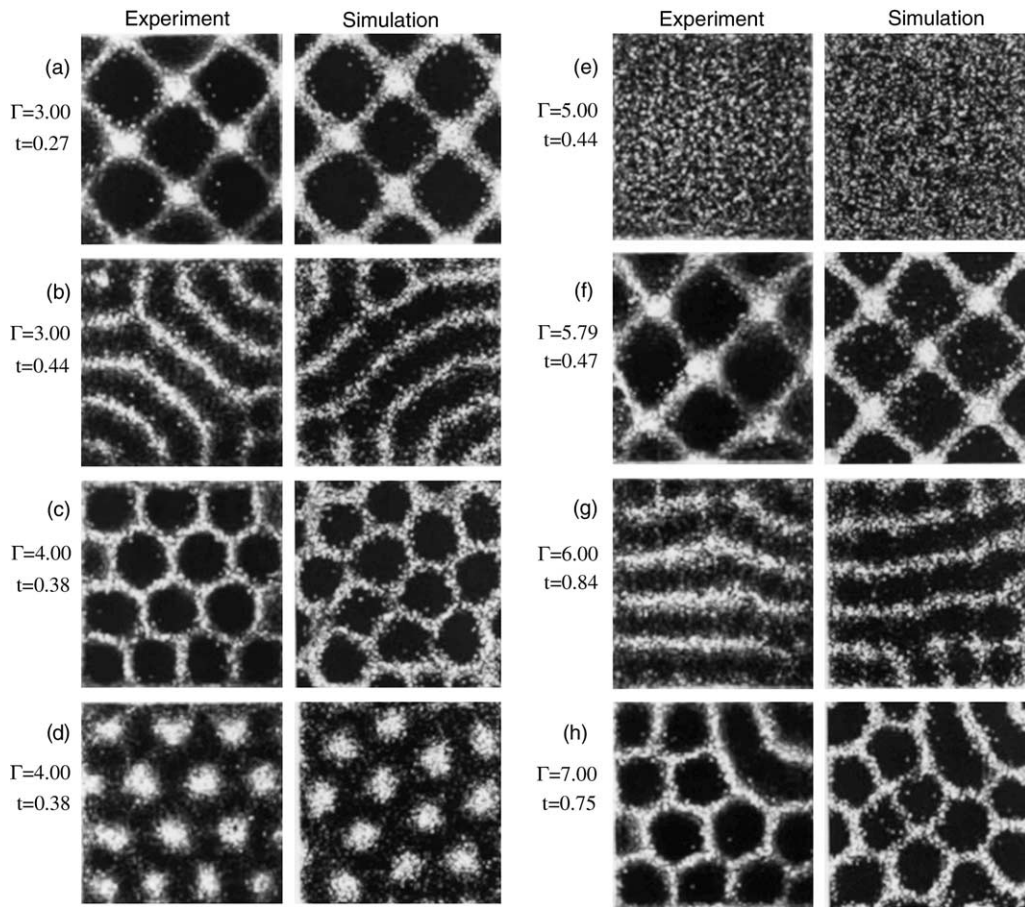


Fig. 3. Patterns obtained in a laboratory experiment and an event-driven particle dynamics simulation of a thin layer of particles in a vertically oscillated container, as a function of the container acceleration amplitude Γ (relative to the gravitational acceleration, g) and the non-dimensional frequency f^* ($= f\sqrt{h/g}$) where f is the frequency and h is the height of the layer. Patterns 9(a)–(e) oscillate at $f/2$, (f)–(h) at $f/4$. The layer was 5.4 particle diameter deep, and the brightness of the photographs indicates height of the layer. The experiment used lead particles (0.5 mm diameter). The same adjustable parameters in the simulation (restitution coefficient = 0.7 and coefficient of friction = 0.5) yield good agreement with experiment over the entire range of conditions shown, suggesting that simulations can capture the experimental results (source: Bizon et al., 1998).

It is well known that the dynamics of fluidized gas–solid suspensions can be altered profoundly by the addition of fines, which alter the particle size distribution. Theories for the effect of particle size distribution on the rheological behavior of the fluid–solid suspension must be developed and validated.

3.2. Instabilities of multiphase flows

It is unusual to achieve a homogeneous, laminar multiphase flow when inertia is important on the particle or bubble length scale. The homogeneous state of a particle suspension translating

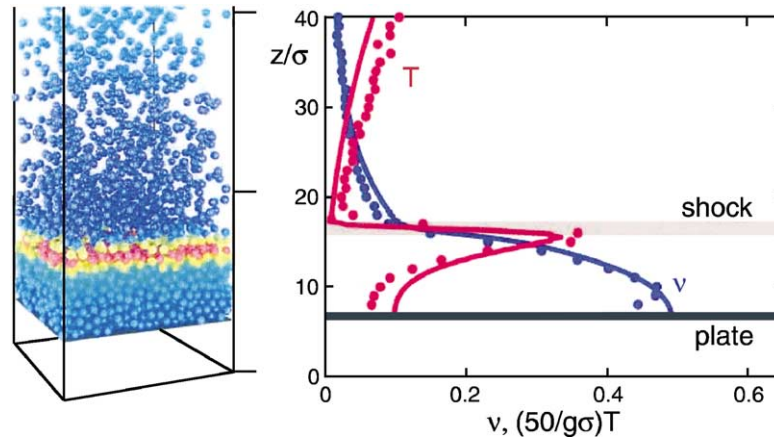


Fig. 4. The picture on the left shows results from a particle dynamics simulation of a granular layer in a vertically oscillating container, at a time that is 22% of a cycle past the time when the container was at its lowest point. The particles are color coded according to the granular temperature, T : high T in red, low T in blue. The graph on the right compares results from the particles dynamics simulation (dots) and a simulation of continuum equations (continuity, momentum and granular energy balance equations) for the horizontally averaged volume fraction v (blue) and temperature T (red), as functions of z (ordinate). The horizontal axis label is correct for v ; T is shown in units of $gd/50$, where d is particle diameter. The good agreement suggests that continuum equations are able to capture the simulations (source: Bougie et al., 2002).

relative to a gas or liquid phase (fluidized bed) or a bubble phase rising through a liquid (bubble column) is almost always unstable and gives way to non-uniform structures spanning a wide range of length and time scales (Lammers and Biesheuvel, 1996; Agrawal et al., 2001; Sundaresan, 2003). It is known that rapid shear flow of granular materials is unstable for sufficiently large gap thickness (Nott et al., 1999). Although stability analysis has not been performed for bubble suspension and gas–solid suspensions subject to simple shear flow, similar instabilities may be anticipated. Bidisperse suspensions also undergo instabilities that are driven by the interactions between the various particle species. It is likely that additional mechanisms of instability remain to be discovered.

To obtain a proper understanding of these instabilities, it would be valuable to directly extract evidence of the instabilities from particle-scale numerical simulations and compare the results directly with analysis of the averaged equations of motion. These comparisons should include testing theoretical predictions for the conditions of marginal stability and comparing simulated inhomogeneous flows to the solutions obtained from averaged equations (e.g., see study on sedimenting bidisperse gas–solid suspensions by Valiveti and Koch (1999)). Such comparisons will serve as stringent tests of the averaged equations.

In addition to understanding the marginal conditions for instability and having a mechanistic understanding of the instabilities, it is important to be able to model flow behavior of suspensions that are unstable. Usually, the typical length scale of the dominant mode through which a homogeneous state of a concentrated suspension loses stability is quite small (only a few particle or bubble diameters) and inhomogeneous suspension flows often manifest structures ranging from the size of the device down to the length scale of the dominant primary instability. First, the validity of the averaged equations when gradients arise on such short length scales is not clear.

The averaged equations, as derived, are of limited value in solving many engineering problems involving large process vessels, as the resolution required to capture all the spatiotemporal structures is prohibitive (Sundaresan, 2000). It would be desirable to develop more manageable models that are useful for probing macro-scale flow after averaging over both the statistics associated with individual particle motion and the statistics of the unstable particulate flow structures (Agrawal et al., 2001; Zhang and VanderHeyden, 2002). The latter averaging may be performed at all scales (analogous to the RANS approach in single phase flow) (Hrenya and Sinclair, 1997) or over a limited scale as in large-eddy simulations. One strategy for developing such models is to obtain solutions of the averaged equations of motion (obtained by averaging over the statistics associated with individual particle motion) for unstable situations and gather the requisite statistics (Agrawal et al., 2001) (see Fig. 5). Only a few computations of this kind have been performed so far, and they suggest that fluctuations associated with the unstable

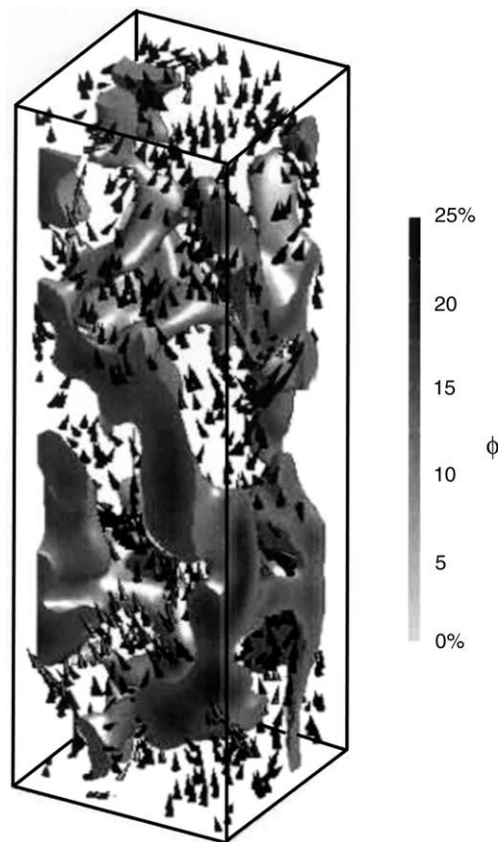


Fig. 5. Snapshot of solids volume fraction and gas velocity fields in a 3D simulation. Cones represent gas velocity, with orientation and length indicating direction and magnitude, respectively. A contour plot of the surface in the interior of the domain where particle volume fraction is 0.05 is shown. The solids volume fraction at points on the faces is as indicated in the grayscale (provided it exceeds 0.05). The mean solids volume fraction in the domain is 0.05. Simulations were performed in a periodic box using continuum balance equations. The mean pressure gradient in the vertical direction balanced the weight of the suspension per unit volume. An initially uniform state gave way to a time-dependent structure, and the figure shows an instantaneous snapshot of the time-dependent solution (source: Agrawal et al., 2001).

structures very quickly overwhelm those at the level of the individual particles (Agrawal et al., 2001), so accounting for the former is crucial. It should be noted, however, that the validity of the averaged equations in such calculations is not clear, as sharp gradients will be on short length scales, which are invariably not considered in the formulation of the averaged equations. Therefore, it is important to validate this approach by comparing with particle-scale simulations (which would be restricted to smaller flow domains) and experiments.

Very little is known about the fluctuation statistics in such unstable flows. It appears that, to a large extent, the energy is extracted from mean flow by interphase drag, giving rise to small-scale structures, which interact with each other yielding larger scale fluctuations. Unlike single phase flow, macro-scale shear plays only a secondary role in these multiphase flows (Agrawal et al., 2001). Indeed, there is little reason to believe that the models for unresolved turbulence developed for single phase flow are even qualitatively correct for this class of multiphase flow problems. It now appears that coarse-grid simulations of multiphase flows should include the effects of unresolved structures via time-averaged and stochastic forcing terms (Loezos and Sundaresan, 2001). Physical and computational experiments probing the fluctuation statistics are needed. Physical experiments involving intrusive measurements may end up perturbing the local instability associated with the relative motion between the continuous and dispersed phases. Nevertheless, such measurements may yield useful information on structures arising from instabilities that were initiated elsewhere in the vessel and transported to the probe location (Zenit et al., 2001). Non-intrusive measurement techniques, which can provide sufficiently fine spatial and temporal resolutions, should be developed and deployed.

4. Dense “solid-like” particulate systems

An important limitation of the theories noted above is that they deal only with “fluid-like” suspensions where the particles interact through the interstitial fluid and ephemeral impulsive interactions. It is important to understand the conditions leading to transition from fluid to solid like behavior, where the particles interact with each other through enduring contact between each other and boundaries, and how they depend on particle volume fraction, frictional properties of the surfaces involved, cohesive interparticle forces, dissipative collisions, etc. Such transitions are known to play a dominant role in the behavior of many granular materials and have been observed in fluidized beds. For example, defluidization experiments indicate that particle assemblies pack in a solid-like state over a range of volume fraction (ϕ_{\min} , ϕ_{\max}) (Tsinontides and Jackson, 1993; Valverde et al., 1998). Packing at higher concentrations can be achieved only by means such as tapping, flow on-off toggles or large imposed stresses. Compressive and dilational yield stress characteristics of the assemblies (at various solids volume fractions) dictate the dynamics of granular phase in this solid-like state. Theories for these stresses based on particle-level characteristics such as cohesive interparticle forces, size and shape and their distributions, frictional contact between particles, etc. must be developed, so that one can understand how to manipulate flow behavior by tailoring particle characteristics. Particle-scale simulations can shed light on conditions leading to the fluid–solid transition and the network of force chains in a solid-like state.

Our knowledge of frictional stresses in flowing granular assemblies is primitive. Quantitative modeling of the performance of many devices such as fluidized and spouted beds, standpipes,

dense phase pneumatic conveying and mixing equipment, etc. require an improved knowledge of frictional stresses. While constitutive models for quasi-static flows developed in the soil mechanics field may be good starting point, there is growing evidence that these must be modified to bring in the effect of strain rate fluctuations to transition region between quasi-static and rapid flow regimes (Savage, 1998). These should be tested with simulations and experiments.

4.1. Interaction of time scales

Transition between fluid-like to solid-like behaviors is determined by the stress relaxation time in many rheological theories for polymeric materials. While spatial correlations in dense granular flows have received much attention, relatively little has been done on temporal correlations. The magnitude of the slowest relaxation time associated with the temporal correlations of particle interactions in dense particulate systems relative to the hydrodynamic time scale is an important quantity, which determines whether viscoelastic models are needed to describe the suspension rheology or not (Zhang and Rauenzahn, 2000). The circumstances (in terms of time scales) where viscoelastic models for suspensions are essential to describe the rheology properly and the structure of such models are important frontiers.

4.2. Role of particle spin and frictional interactions with boundaries

The interaction of particles with each other and with solid boundaries involves friction and particle spin (Bizon et al., 1998; Jenkins, 1992; Louge, 1994; Jenkins and Louge, 1997). Formal theories predicting the transport of particle angular momentum near boundaries are beginning to emerge (Hayakawa, 2002). These should be extended to gas–solid flows and tested with simulations and experiments.

Solid friction is another topic that remains largely a mystery. For example, in granular flows, friction can vary with relative contact speed; it can also be hysteretic or intermittent (e.g., stick-slip). Its understanding is crucial to predict the interaction force that is tangent to a solid surface. More globally, it is important to distinguish whether particles are engaged in long-lasting frictional contact with boundaries or more ephemeral impulsive interactions. This distinction is not only crucial to gravity-driven granular flows (Louge and Keast, 2001), but also to any gas–solid flow where particles remain in contact with walls (Griffith and Louge, 1998).

4.3. Mixing and segregation

In our discussion thus far, we were primarily concerned with flow. However, there are many systems where the mixing and segregation resulting from flow take on a greater importance than the flow itself. These arise in dry granular materials (particles surrounded by air), wet granular materials (particles in a humid environment or coated with a small amount of fluid) and slurries (dense particles completely immersed in a lighter liquid). Most common applications involve *slow flows*, where particles roll past each other and are in contact with several neighbors at the same time. This is relevant to tumbling, heaping, motions induced by moving objects, such as blades, etc. Both non-cohesive and cohesive systems are of interest. The most interesting and practically

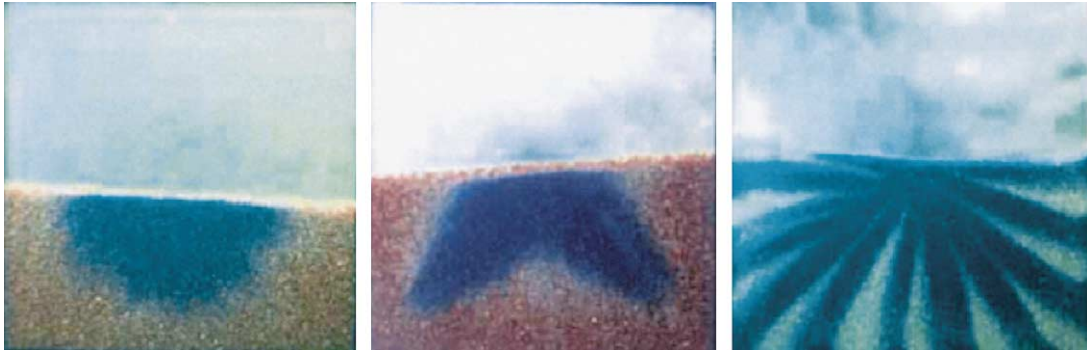


Fig. 6. Experimental results on quasi two-dimensional tumbling mixers with glass spheres of different sizes (0.8 mm blue, 1.2 mm clear, and 2.0 mm red). All three systems started well mixed and everything is equal except the degree of filling. From left to right: less than 1/2 full, 1/2 full, more than 1/2 full (source: Hill et al., 1999).

important case corresponds to bimodal populations, where the particle variation may occur in size, shape, density or surface properties.

Granular materials segregate. Small differences in size, density, surface roughness, or particle shape lead to flow-induced segregation (Ottino and Khakhar, 2000). This is a complex and imperfectly understood phenomenon. Segregation issues are, however, unavoidable in practice. Fig. 6 highlights the dramatic changes in the mixing-segregation structures caused by small changes in the operating conditions, in this case the degree of filling in a tumbler. To describe segregation, we not only need models for flow, but also constitutive models for segregation fluxes under various flow states. The bulk of the studies in the literature consider only two special cases: a mixture of particles of the same density and shape, but two different sizes, and a mixture of particles of same size and shape, but different densities. Models for combined size and density segregation remain to be developed. An even more complicated issue is particle shape. Virtually nothing is known about how to incorporate the role of cohesion. This area needs significant investments in theory and controlled experiments. In turn, experiments depend on significant advances in non-invasive techniques.

A great deal of segregation modeling work is based on particle dynamics simulations which require precise physical properties (Young modulus, restitution coefficients, Poisson ratios, etc.) (Cleary et al., 1998). Even in the case of spheres there are many important questions that need to be clarified.

- What is the parametric sensitivity of the results to the various parameters in particle dynamics models?
- How should one handle walls? How sensitive are the results to this choice?
- How can one match a real material—non-spherical, multi-sized—to input parameters?

The particle dynamics simulations can typically handle about 10^4 – 10^5 particles (Shinbrot and Muzzio, 2000), in contrast to practical systems which have $\gg 10^9$ particles and invariably require continuum modeling approach. Development of multi-scale models involving continuum and particle dynamics approaches to handle macro- and meso-scale phenomena is a scientific challenge that can be tackled within the next 5–10 years.

A possible fruitful area is control of flow and especially, mixing and segregation, via manipulation of the cohesive force. A long-range goal is to identify suitable parameters that will indicate when cohesion may either mitigate or enhance the possibility of achieving a segregated distribution of particles.

The understanding of the competition between mixing and segregation is in its infancy. All studies to date are restricted to two dimensions and even in the classical example of axial segregation there is no agreement as to the underlying governing mechanism. A fruitful area for the next five years is the study of 3D systems. This area needs significant investments in theory and controlled experiments. Again, experiments depend on significant advances in non-invasive techniques.

It is apparent that our ability to characterize granular flows is hindered by a lack of suitable experimental techniques. The main difficulty is that granular materials are opaque; this prevents many common methods that have been successful in fluid flows. Recent developments in Magnetic Resonance Imaging (Nakagawa et al., 1993), Particle Image Velocimetry (Lueptow et al., 2000), Particle Tracking Velocimetry (Jain et al., 2002), X-ray imaging (Harwood et al., 1975) and Positron Emission Particle Tracking (Parker et al., 1997) offer tremendous opportunities in the next decade. These should be applied to the precise characterization of building block flows such as shear layers.

The goal of all the techniques above is to obtain fields; one aspect being how to construct a velocity field for the flow. Two main issues are unavoidable: The relatively low spatial resolution of the experimental measurements and the fact that for many experimental techniques (e.g. Positron Emission Particle Tracking) significant statistics is only obtained through several different experimental measurement series. Techniques must be developed to reconstruct the “true” velocity field. In particular one has to consider the possibility of very irregular, if not chaotic, flows. Such flows may not be easily distinguished in the coarse-grained velocity fields available from the experimental data.

Scale up of granular processes is notoriously difficult and there is little guidance at the present time. However, flows in granular materials are often restricted to thin regions of rapid surface flow with the rest of the material suffering only slow plastic re-arrangements. This seemingly trivial observation leads to understanding of the entire system and to the concept that an understanding of surface flows constitutes the key element for scale up of granular flow processes. However, before this becomes possible, shear flows in tumbler and heap formation need to be thoroughly characterized. The goal is to predict layer thickness and shear rates based on first principles.

5. Concluding remarks

Disperse flows are encountered in a variety of contexts: industries dealing with energy, pharmaceuticals, bulk and specialty chemicals, and consumer products, agriculture, transportation and conveying, and space exploration. They are studied, researched and applied in many academic disciplines including engineering (chemical, civil, environmental, materials science, mechanical and metallurgy), physics, atmospheric sciences (climate change, meteorology) and geosciences. Progress in this field impacts a broad range of industries and academic disciplines.

The set of challenges outlined in this report is by no means complete. It is simply a collection of some important problems which can realistically be tackled in the next decade. Resolution of these issues will lead to significant advances in our understanding and modeling capabilities.

Although this report may appear to be slightly tilted towards theory, the need for experiments and simulations cannot be over-emphasized. Model experiments which can be used to guide the development of theory and its validation are extremely important. By and large, experiments, theory and simulations are done by different research groups. It is desirable that these groups seek alliances quite early on so that experiments to probe specific aspects of theory and/or simulations will also be identified and performed.

In this report, we have outlined a number of scientific challenges which represent building blocks for comprehensive understanding and modeling of disperse flow encountered in a variety of technologies and in nature. These building blocks range from flow characteristics at the length scale of individual particles or bubbles and contact mechanics to computational and physical experiments aimed at validating models for specific aspects of multiphase physics. The importance of convergent, integrative studies which will bring together these building blocks cannot be underscored. At the same time, it is important to recognize that research on building blocks and their validation studies (such as those described in Figs. 2 and 3) need not (and should not be required to) directly address specific technological applications. Research on building blocks will be divergent, often raising more questions than answers sometimes. It is hoped that the present roadmap communicates to the reader the importance of merging integrative and divergent studies. The integrative studies are essential to understand how processes occurring over a broad range of length and time scales interact to influence multiphase flow on a large scale, while studies on building blocks will expose and resolve deficiencies in our fundamental understanding of multiphase flow fundamentals.

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