Multiphase Flows, Models, Current Status, and Future Needs

Type of multiphase flow and physics	Description	Applications	Current Modeling approaches	What can be modeled with confidence	Level of validation	Further development needs
Gas-liquid flow	General gas-liquid contact reactors or equipment, usually with packing material to increase contact surface area.	Absorbers, scrubbers, acid gas removal (AGR) equipment in CO2 capture, Trickle bed reactors, Taylor flow in micro reactor channels, bubble columns, spray towers, liquid fuel combustors	VOF, dispersed phase model, Eulerian multiphase, population density model, mixture model	Packing element level small scale models to understand physics; dilute liquid phase with DPM; dilute gas phase with DPM		Bubble breakup and coalescence, slug formation and breakup
Liquid-solid flow	Slurries	Coal slurry feeder, gravity assisted filtration system with fixed bed,	Single phase approximation with non-Newtonian properties, Eulerian multiphase, DPM			Sedimentation and agglomeration
Gas-liquid-solid flows	Three phase flow reactors	Slurry bubble column reactors, bio digesters, hydrogenators, Fisher Tropsch reactors, oil sand processors	Eulerian multiphase, Two-phase approximation (gas liquid, or liquid solid)			
Gas-solid flow	Fixed bed flows and granular flows	Adsorbers, air-lift reactors, pneumatic transporters, Cyclone separators, fluidized beds, solid fuel combustors	Porous medium model, dispersed phase model if applicable, Eulerian multiphase, detailed element level model	Fixed bed reactors and adsorbers, dilute solid phase with DPM		Agglomeration,
Liquid-liquid flows	Immiscible liquids	Oil-water flows,	VOF, mixture model, Eulerian model			

General challenges for all multiphase flows:

1. Solution speed up with code optimization and algorithm improvement to bring turn-around time to practical level for the inherently time dependent problems in multiphase flows.
2. Fundamental understanding on interface mass and momentum transfer and its impact on turbulence and flow.
3. Solid and liquid fuel combustions are unique multiphase flows where the dispersed phase model has been successful due to the dilute nature of the dense phase.
4. Industry has solutions for most problems with a combination of experimental and theoretical approaches. But there is a general reluctance of sharing the knowledge.

Fundamental Questions:

1. Academic research in Eulerian multi-fluid models has focused on the **laminar** transport equations. By laminar we mean flows for which large-scale turbulent structures are not explicitly modeled. Grid-independent solutions to such equations require fine grids and time-dependent flow solvers (just as in direct numerical simulation (DNS) of single-phase flows.) The latter is rarely achieved in reported studies in the literature; hence, such studies might be best thought of as under-resolved DNS or "uncontrolled" large-eddy simulations (LES). This state of affairs raises a number of significant questions:
    a. Are the constitutive models used to close the laminar transport equations valid over a wide range of hold up (dilute to dense) and flow regimes (homogeneous to turbulent)?
    b. What is the "minimal" model needed to predict flow transitions (with fully resolved simulations)?
    c. How do we reconcile the fact that the laminar transport equations that are currently used for gas-liquid flows are unstable (i.e., have only time-dependent solutions) with the experimental observation that homogeneous flow is statistically stationary? Are we missing important physics?
    d. If we increase the flow Reynolds number (e.g., by increasing the gassing rate in a bubble column) the laminar two-fluid model will generate large-scale turbulent flow (i.e., buoyancy-driven turbulence). Do the flow statistics of the "numerical" turbulence agree with experimental measurements? In other words, can we (as is done in single-phase flows) use these numerical simulations to validate multiphase turbulence models?
    e. Once the flow becomes turbulent, can it be described by statistical quantities such as mean holdup, mean velocities, Reynolds stresses? Do we have sufficient experimental data to show that this is (or is not) the case?

f. Is high-Reynolds number multiphase turbulent flow independent of the "molecular-scale" transport coefficients (as is the case in single-phase flows)? In other words, are flow statistics determined by the convective terms and isotropic stress terms (i.e., with energy-containing and inertial range scaling independent of viscosity?)

2. Industrial applications of multiphase flows are most always in the turbulent regime. The CFD vendors offer multiphase turbulence models based on simple extensions of models for single-phase flows with additional terms to describe turbulence generation by momentum transfer between phases. As with single-phase flows, industrial users are interested in the steady-state flow statistics and thus they assume that these multiphase turbulence models have steady-state solutions. In single-phase turbulence models, grid-independent steady-state solutions are attained by having a sufficiently large "turbulent" viscosity to stabilize the flow. The Eulerian multi-fluid models (even with terms added for turbulent transport) can be unstable under many flow conditions. Indeed, some researchers have attempted to model the homogeneous to heterogeneous flow transition in bubble columns using multiphase turbulence models, even though experimentally we know that homogeneous flow is not turbulent in the "classical" sense. Industrial users rely on steady-state, coarse-grid solutions for design of industrial equipment. It is very likely that if a finer grid were employed with a time-dependent solver, the grid-independent results would be very different (e.g., they will not be stationary.) These observations raise a number of important questions:
   a. Is multiphase turbulence "universal" (as is the case for single-phase turbulent) so that quantities such as turbulent viscosity, turbulent diffusivity, etc. can be defined in a consistent manner?
   b. What is the "minimal" multiphase turbulence model that yields grid-independent, steady-state solutions with the correct flow statistics at high Reynolds numbers?
   c. Can we trust steady-state solutions found from current multiphase turbulence models on coarse grids?
   d. Do we have the experimental data for high Reynolds number multiphase flow statistics that will be needed to validate multiphase turbulence models? What are the technical limitations that must be overcome to get such data?
   e. Do the interphase momentum transfer terms in the Eulerian multi-fluid models have a significant effect on the turbulence statistics?
   f. Should academic research be refocused on development of multiphase turbulence models (with the expected properties at high Reynolds numbers) instead of testing various formulations of laminar models (and other low Reynolds number effects)?

3. Turbulent gas-liquid flows have a number of "complicating" factors such as bubble coalescence and breakage (to name just one), which are important in industrial applications. The existing multi-fluid models can be used to model coalescence and breakage by adding more fluid phases (e.g., to represent multiple bubble sizes). Phenomenological models are then required to describe the

coalescence and breakage dynamics in terms of local turbulence quantities (which, as noted earlier, cannot currently be measured experimentally.) Because the effective "bubble diameter" enters the drag law (and hence affects the turbulence statistics and hold up), there is a strong coupling between the mass and momentum balances. Experimental validation of the model predictions is complicated by the fact that we currently do not have data for local bubble size distributions and turbulence statistics. Instead, a model is assumed to be "accurate" if it does a reasonable job of predicting the average local hold up (which itself is not easy to measure accurately.) To complicate matters more, existing literature studies rely on unvalidated multiphase turbulence models, often solved on coarse grids with steady-state solvers. Ideally, one could proceed in steps: first, develop and validate models with a uniform "bubble" size (buoyant particles?) over a wide range of sizes and hold up, then study bubble size distributions with no coalescence nor breakage, then finally investigate systems with coalescence and breakage. Such a comprehensive research project would require long-term funding (and would not address industrial cases in the short term), but is probably the only way to proceed towards addressing these important questions.

4. In the short and medium term, there are a number of computational and numerical issues that arise when using current commercial CFD codes for industrial problems that can be addressed. For example, when using the steady-state solver in a widely used CFD code to find the hold up in gas-liquid (or fluid-solid) flows, the mass balance for each phase is not conserved during iterations from the starting guess. This is observed in closed systems (i.e., a stirred tank with solids in a liquid) and requires the users to make repeated initial guesses in order to get the correct total solid mass. Other issues such as grid dependence and the adequacy of the governing equations for predicting steady-state solutions have already been mentioned. Finally, convergence to the steady-state solutions is often extremely slow (compared to single-phase flow) with current iterative solvers in commercial CFD codes. This situation limits the usefulness of CFD in the industrial setting for equipment design and scale up.