USING DIRECT NUMERICAL SIMULATIONS TO UNDERSTAND BUBBLY FLOW

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1. Introduction

Understanding and predicting bubbly flows is of critical importance in a large number of industrial applications, including boiling heat transfer in power plants, various metallurgical processes and in bubble columns in the chemical industry. Industrial processes depending heavily on the use of bubble columns include, for example, partial oxidation of ethylene to acetaldehyde, isobutene separation for C_4 cracking, wet oxidation of heavily polluted effluent and the production of dichloroethane (Furusaki, Fan and Garside, 2001). In bubbles columns, gas is injected at the bottom and as the bubbles rise, the gas comes in contact with the liquid or gases dissolved in the liquid and reacts. Bubbles columns ranging from tens to hundreds of cubic meters are common in the chemical industry and up to thousands of cubic meters in bioreactors where longer process times are needed. The absence of any moving parts and their relatively simple construction makes bubble columns particularly attractive for large-scale operations (Deckwer, 1992). Their operation is, however, usually dependent of the size of the vessel and the difficulty of scaling up small pilot models makes numerical predictions importance. The modelling of industrial size multiphase flow systems must by necessity rely on models of the average flow. The averaging introduces terms that must be modelled and the representation of those terms, describing both the effect of the fluctuations in both the liquid and the gas velocity on the average motion as well as the forces between the phases, remains the major challenge in numerical modelling of large scale industrial systems. The most commonly used models the two-fluid model where separate conservation equations are written for the gas and the liquid and a general descriptions can be found in Delhay (1982), Kataoka and Serizawa (1989), Zhang and Prosperetti (1994) and Drew and Passman (1999), for example.

DNS of bubbly flows, where the unsteady flow around a few moving and deforming bubbles is resolved fully, allow us to examine the unresolved terms in the equations for the average motion in great detail. Here we describe recent studies of bubbly flows.

2. Numerical Method

Numerical simulations of multiphase flows can be done using two fundamentally different methodologies. In one approach, the governing equations are written down separately for each phase and the solutions matched through jump conditions across the interface. In the other approach, a single set of governing equations is written down for all the phases involved and singular terms added to account for effects limited to the interface. While the "one-fluid" formulation was the basis of early multifluid simulations using the Marker-And-Cell (MAC) method and its successor, the Volume-Of-Fluid (VOF) method, these methods were generally

regarded as rather inaccurate and a number of authors sought to develop methods based on following the interface in such a way that the jump conditions could be implemented explicitly. This generally requires a moving grid of some sort, or extensive regridding, where the grids are adjusted to ensure that the interface coincides with a grid line. Although a number of problems have been solved successfully using this approach, it has proven to be limited to relatively simple problems and not easily extendable to three-dimensions. The "one-fluid" approach has, on the other hand, experienced a strong comeback in the front tracking method of Unverdi and Tryggvason (1992) and the level set method of Osher and collaborators. A number of authors have also developed improved VOF methods. The numerical method used for the simulations described in the next section is the finite volume/front tracking method introduced by Unverdi and Tryggvason (1992). The method has been described in detail by Tryggvason et al. (2001).

In the one-fluid formulation, a single set of equations is written for all the phases involved, and the phase boundary is treated as an imbedded interface by adding the appropriate source terms to the conservation laws. These source terms are in the form of delta-functions localized at the interface and are selected in such a way to satisfy the correct matching conditions at the phase boundary. If we assume that both the liquid and the vapor are incompressible and the only change of volume is due to the phase change at the phase boundary, the resulting "one-fluid" Navier-Stokes equations are (Unverdi and Tryggvason, 1992):

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\nabla\cdot\mathbf{uu} = -\nabla P + \nabla\cdot\mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T) + \sigma\int_F \kappa_f \mathbf{n}_f \delta(\mathbf{x}-\mathbf{x}_f)dA_f \qquad (1)$$

Here, $\mathbf{u}$ is the velocity, P is the pressure, and ρ and μ are the discontinuous density and viscosity fields, respectively. δ is a three-dimensional delta-function constructed by repeated multiplication of one-dimensional delta functions. κ is twice the mean curvature. $\mathbf{n}$ is a unit vector normal to the front. Formally, the integral is over the entire front, thereby adding the delta-functions together to create a force that is concentrated at the interface, but smooth along the front. $\mathbf{x}$ is the point at which the equation is evaluated and $\mathbf{x}_f$ is the position of the front.

For the simulations described here, these equations are solved by a finite volume/front tracking method originally developed by Unverdi and Tryggvason (1992). The Navier-Stokes equations are solved by a second-order accurate projection method, using centere-differences on a fixed, staggered grid. In order to keep the boundary between the phases sharp, to advect the density and the viscosity fields, and to accurately compute the surface tension, the phase boundary is tracked by connected marker points (the "front"). The front points, which are connected to form an unstructured surface grid, are advected by the flow velocity, interpolated from the fixed grid. As the front deforms, surface markers are dynamically added and deleted. The surface tension is represented by a distribution of singularities (delta-functions) located at the front. The gradient of the density and viscosity becomes a delta-function when the change is abrupt across the boundary. To transfer the front singularities to the fixed grid, the delta functions are approximated by smoother functions with a compact support on the fixed grid. At each time step, after the front has been advected, the density and the viscosity fields are reconstructed by integration of the smooth grid-delta function. The surface tension is then added to the nodal values of the discrete Navier-Stokes equations. Finally, an elliptic pressure equation is solved by a multigrid method to impose a divergence-