MULTISCALE ISSUES IN DNS OF MULTIPHASE FLOW

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ABSTRACT

Direct Numerical Simulations (DNS) of bubbly flows are rapidly allowing studies of systems containing hundreds of deformable bubbles in turbulent flows. Such simulations have already suggested that bubbly flows in vertical channels exhibit a particularly simple structure dominated by the direction of lift forces acting on the bubbles. The lift depends on the flow direction and the deformability of the bubbles and while the resulting structures and the flow rate depends strongly on the governing parameters, the underlying physics is relatively simple. Extracting how the small-scale processes produce a simpler average or large-scale structure is a classical example of multiscale analysis. Multi-phase flows, however, also often exhibit another type of multiscale processes, where "features" such as thin films that are much smaller than the "dominant" flow scales, appear. The flow and the geometry of these features are usually simple, since they are dominated by surface tension and viscosity. In isolation these features are therefore often well-described by analytical or semi-analytical models. Recent efforts to capture thin films using classical thin film theory, and to compute mass transfer in high Schmidt number flows using boundary layer approximations, in combination with DNS of the rest of the flow, are described.

1. INTRODUCTION

Many multiphase flows exhibit what we might call a "dominant scale." In bubbly flows this is the average bubble size, in atomization it is the average drop size, and so on. The dominant scale is set by the appropriate nondimensional numbers being O(1), and in direct numerical simulations (DNS) of multiphase flows the dominant scale generally sets the resolution requirement. In traditional DNS the goal is to examine the flow over a sufficiently large range of scales so that it is possible to infer how the collective motion of well-resolves bubbles or drops determine the motion at larger scale. Such simulations have been carried out for a number of relatively simple systems, including bubbles in fully periodic domains and vertical channels. The results show that in some cases the collective motion leads to unexpected simplifications that are unlikely to emerge from studies focusing on only a few bubbles. Here, we first review simulations of bubbly flows in vertical channels briefly, where the flow direction, as well as the bubble deformability, has profound implications for the flow structure and the total flow rate. Results obtained so far are summarized and open questions identified.The text margins are to be set so that the text body is within the dimensions of 1-inch margins top, bottom, left and right.

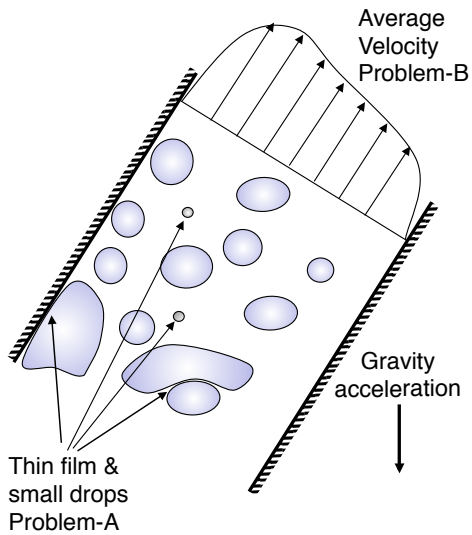

Figure 1. A schematic of multiscale modeling of bubbly flow in an inclined channel, showing where "A" and "B" type problems arise.

Multiphase flows also often exhibit another type of multiscale behavior. Frequently scales much smaller than the dominant length scale are present, either as a spontaneous feature of the evolution, usually manifesting itself as a thin film, thread, or a tiny drop, or due to the presence of additional physical processes that operate on a very different time scale than the fluid flow. The presence of these small-scale features demands considerable and often excessive resolution from conventional numerical approaches. However, at small flow scales the effects of surface tension are generally strong so the interface geometry is simple and viscous forces dominate the flow and keep it simple also. These are exactly the conditions under which analytical models can be used and we will discuss efforts to combine a semi-analytical description for the small-scale processes with a fully resolved simulation of the rest of the flow. For the film between a droplet falling onto a wall we have shown that a simple film model, where the pressure from the fully resolved simulations drive the flow in a thin film, which then provides shear boundary conditions to the large scale flow, greatly reduces the resolution required for a given accuracy. Similarly, we have developed a method to capture the mass transfer from bubbles in liquids where the diffusion of mass is much slower than the diffusion of momentum. This results in very thin mass-boundary layers that are difficult to resolve, but the new approach allows us to simulate the mass transfer from many freely evolving bubbles and examine the effect of the interactions of the bubbles with each other and the flow.

The two multiscale aspects discussed above can be put into a broader context by considering the classification of E and Enquist [1] who divide multiscale problems into two broad categories:

- Type A Problems: Dealing with Isolated Defects
- Type B Problems: Constitutive Modeling Based on the Microscopic Models

Figure 1 shows the issues schematically for bubbly flow in an inclined channel. Problem B is the classical averaging encountered in turbulence and multiphase flow modeling and Problem A is the accurate computation of the evolution of thin films, fine threads and small drops/bubbles.

Below we address both aspects. After reviewing briefly our computational approach, we first discuss recent results for flows in vertical channels, where simulations have helped us get an improved understanding of the dynamics of the flow, and then discuss efforts aimed at modeling thin mass-transfer boundary layers in simulations of bubbly flows, where the Schmidt number is generally very high and the mass transfer usually requires very fine grids.

2. NUMERICAL APPROACH

The need for Direct Numerical Simulations of multiphase flows has been understood for a long time and some of the earliest fluid flow computations focused on multiphase flow. The MAC (Marker-And-Cell) method was explicitly designed for free-surface and interface flows and early simulations using the method included gravity currents, the Rayleigh-Taylor instability and splatting drops. The MAC method was soon replaced by the VOF (Volume Of Fluid) method, where a marker function replaced the discrete markers to identify the different fluids. Although both the MAC and the early VOF methods produced some very impressive results (see, for example, [2,3]), difficulties with including surface tension and maintaining the integrity of the interface limited their usefulness. In the very late eighties and early nineties several developments took place that gradually allowed reliable and accurate simulations of a relatively large range of multifluid problems. Those developments included the introduction of level-sets methods to track fluid interfaces, improved interface tracking and a technique to include surface tension in VOF methods, and the introduction of a front-tracking method specifically designed for multifluid flows. These new methods have now made simulations a standard tool to examine the evolution of fairly complex flows.

All of our own simulations have been done using a finite-volume/front tracking method originally described in [4]. The Navier-Stokes equations are solved using the “one-fluid” formulation where a single set of equations is solved on a regular structured grid covering the entire computational domain. The equations govern the motion of all the fluids involved and different constituents are identified by a difference in the material properties. Surface tension is added as a smoothed body force at the interface separating the different fluids. This formulation is the foundation for most other methods that have been used for DNS of multiphase flows, such as VOF and level-set methods. To identify the different fluids a marker function is usually advected directly on the fluid grid. In the front-tracking method, on the other hand, the interface is marked by connected marker points that are moved with the fluid velocity, interpolated from the fixed fluid grid. The marker function is then reconstructed from the new location of the interface. The front is also used to compute surface tension, which is then smoothed on to the fluid grid and added to the discrete Navier-Stokes equations. In addition to the computation of the surface tension and the construction of the marker function, the chief challenges in front-tracking is the dynamic updating of the front, where marker points are added or deleted to maintain the point density needed to fully resolve the interface. Discussions of various improvements and refinements of the original method, along with a discussion of various verification studies can be found in [5,6].

3. DNS OF BUBBLY FLOWS

The conventional argument for DNS of fluid flows is that the results provide us with a complete insight into the dynamics and all the quantitative information that we might need and that if this does not help us develop models of the large scale flow, nothing will. This is certainly true and DNS of multiphase flows are rapidly providing insight, understanding and data that cannot be obtained in any other way. While a number of multiphase flows have been examined by DNS, bubbly flows have perhaps received most attention and here we will focus on recent work that we have been engaged in.

For DNS bubbly flows, our group has been one of the main contributors. For early work on bubbles in fully periodic domains, see [7-11], for example. More recently we have been examining considerably more complex systems [12-14]. In a study of nearly spherical buoyant bubbles in vertical channels, we found that the insight provided by the DNS allowed us to essentially solve for some aspects of the problem analytically. The main results are that for sufficiently large number of bubbles in upflow and downflow, independently of whether the flow is laminar or initially turbulent, the middle region is in hydrostatic balance where the weight of the mixture is such that it balances exactly the imposed pressure gradient. This observation allows us to write down a very simple analytical expression for what the void fraction in the center should be, given the imposed pressure gradient and the average void fraction. For upflow, the void fraction in the core is lower than the average, and knowing that we can predict how many bubbles move to the wall. For downflow the void fraction must increase and the number of bubbles that must be taken from the wall region determines its thickness, which again, is given by a simple, formula. For downflow the velocity in the wall region is given either by a parabolic velocity profile in the laminar case or by the law-of-the-wall for the turbulent case. Since the velocity in the center is controlled by what happens in the wall-layer, the total flow rate is thus easily predicted. For upflow the velocity in the wall-layer is not as easily predicted due to the presence of bubbles, but the simplicity of the layer suggests several possible approximations. Although considerable information was available for these flows experimentally, the DNS study provided both additional information and helped us bring it all together in ways not possible before.

For turbulent upflow, we have examined the effect of the deformability of the bubbles in reference [15]. The results showed that as the bubbles became deformable, the bubbles no longer drift to the wall but stay in the middle of the channel. The flow rate is reduced significantly when the bubbles drift to the wall, but this reduction is not seen for the deformable bubbles. Most recently we have done a series of simulations where only the deformability of the bubbles is changed (by changing surface tension) and this study shows that the flow is relatively insensitive to the exact value of the surface tension as long as the bubbles remain nearly spherical and there was a well-defined bubble-rich wall-layer. As the deformability increased, the flow then abruptly transitions to a very different state where the bubbles do not accumulate near the walls, but remain in the middle of the channel. In this new state the main effect of the bubbles is to make the mixture lighter than single-phase liquid and once the pressure gradient is adjusted to account for the weight of the mixture, the flow structure is remarkably similar to what is seen for single-phase flow. Changing the deformability of the bubbles in this new state had little effect on the liquid flow rate and other characteristics of the flow, as long as the bubbles did not break up. We have also examined the formation of the wall-layer and whether it is sensitive to the size of the

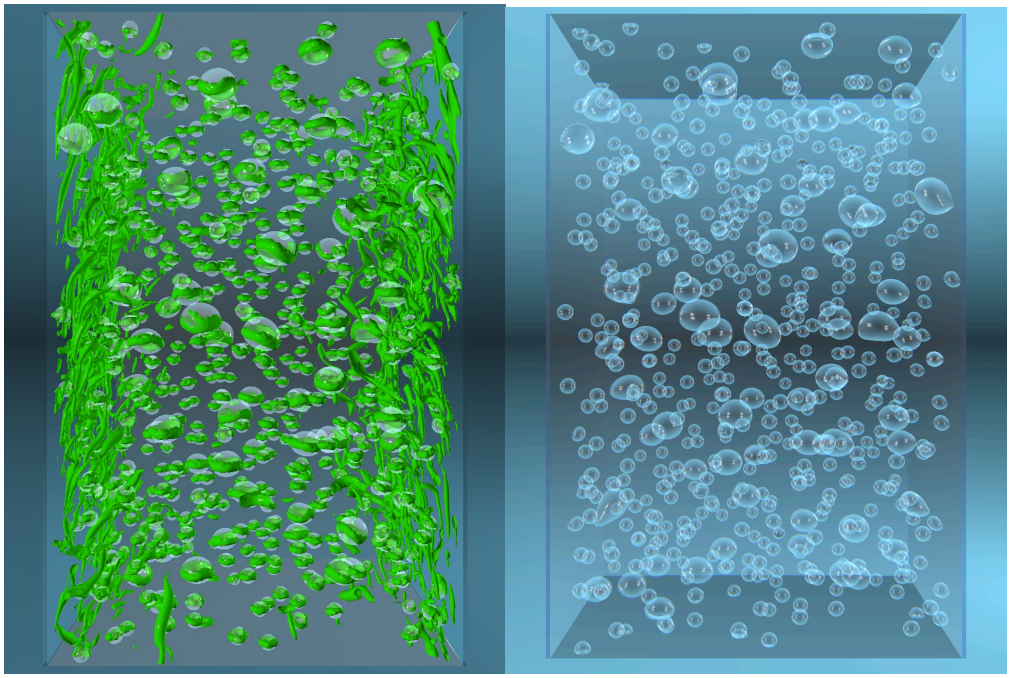

Figure 2. Results from a simulation of several hundred bubbles of different sizes in turbulent up flow in a vertical channel at an early time when the small bubbles have not moved to the wall. In the right frame only the bubbles are shown but in the frame on the left the vortical structures, visualized by the lambda-2 method are shown also.

system and the Reynolds number. So far, the results suggest that this is not the case. However, it is possible that if the Reynolds number is sufficiently high, turbulent dispersion may prevent the accumulation of bubbles on the wall. This remains to be examined.

Our examinations of bubbles in laminar and turbulent flows in vertical channels have already lead to considerable insight into relatively simple flows where the bubbles are all of the same size. These results should eventually lead to improved models that can be used to make industrial scale prediction of multiphase flows. In [17] we compared flow in laminar channels with the model presented by [18] and analysed further by [19]. While we found that upflow was very sensitive to the tuneable parameters of the model, for downflow the model predictions were very robust. In [20] we examined the transient motion of a cluster of bubbles across a horizontal channel and showed that the void fraction evolution is accurately described by a simple drift-flux-like model.

In real systems the bubbles usually come in a variety of sizes and most recently we have started to look at the effect of a distribution of sizes. Figure 2 shows one frame from a simulation with 504 bubbles of four sizes in a turbulent flow with a shear Reynolds number of 500. The domain is resolve by $1024 \times 768 \times 512$ grid points, uniformly distributed in the streamwise and spanwise direction but stretched in the wall-normal direction to allow a finer resolution at the walls. The frame is from an early time, before any small bubbles have migrated to the wall.

4. EMBEDDED ANALYTICAL DESCRIPTION FOR UNRESOLVED-SCALES

In direct numerical simulations of multiphase flows, all scales are fully resolved. When we use analytical or semi-analytical models to capture small-scale motion in isolated regions of the flow, we also attempt to resolve everything. However, instead of using a single approach, we use different approaches for the different scales. Most of the flow is resolved in standard ways, where each term in the governing equations is approximated using a finite difference or a finite volume technique. To resolve certain small scale features, however, such as thin films and threads, thin boundary/reaction layers, and small drops and bubbles, we take advantage of the fact that these features often have a relatively simple structure and can be described accurately using analytical or quasi-analytical theories. Given a simple description (which may have to be solved numerically) of a feature not resolved on the fluid grid, the challenges are to identify when and where the small scale description should be used and how to pass information between the numerically computed flow and the small-scale description. Obviously, we have to introduce new computational objects to capture the small-scale features. In our front tracking method those already exist and while the front was originally introduced to describe the fluid interface, the general data structure is generally well suited for the inclusion of models for analytical models for the small scales.

Our first attempt to use embedded analytical descriptions of small scale processes is described in reference [21], where we used it to capture the thin film between a sloping wall and a drop falling on it, and the subsequent sliding of the drop down the wall. Most of the flow was well resolved, but a thin film model was used to describe the flow in the film between the drop and the sloping wall. Outside the film we applied the usual no-slip boundary conditions when computing the flow field, but where the film was, the wall shear stress, as found from the film model, was prescribed. Although the film description was very simple, it allowed us to simulate the motion relatively accurately on a grid where the film was not fully resolved. To assess the accuracy of the approach, we compared the results with results from simulations using very fine grids where the film was fully resolved. While the results showed minor differences, the agreement was generally good, and much better than results from the coarse grid where the analytical description was not used. Although this study focused on a relatively simple problem, where the location of the film was easily identified, we believe that the general approach should work also for more complex problems such as collisions of freely moving drops. In any case, the study allowed us to identify the main aspects needed for the use of embedded analytical descriptions in DNS, such as the challenges of identifying where the models should be used and how information about the resolved flow (such as pressure gradient and strain-rate) must be interpolated from the fixed grid, as well as how information are passed back, from the small-scale description to the flow grid.

To examine the use of embedded analytical descriptions for a very different problem, we have more recently studied mass transfer from bubbles, where the large discrepancy in the diffusivity of mass and momentum leads to very thin mass boundary layers. The physics is actually rather simple. Mass diffuses from the bubble surface and is then swept by the flow toward the back where it is carried away as the flow separates. For high Schmidt numbers (where the diffusion of mass is much slower than the diffusion of momentum), the mass boundary layer is thin and can be difficult to resolve numerically. To derive a description to capture the mass transfer in a boundary layer that is too thin to be resolved, we decompose the scalar field into two fields, one

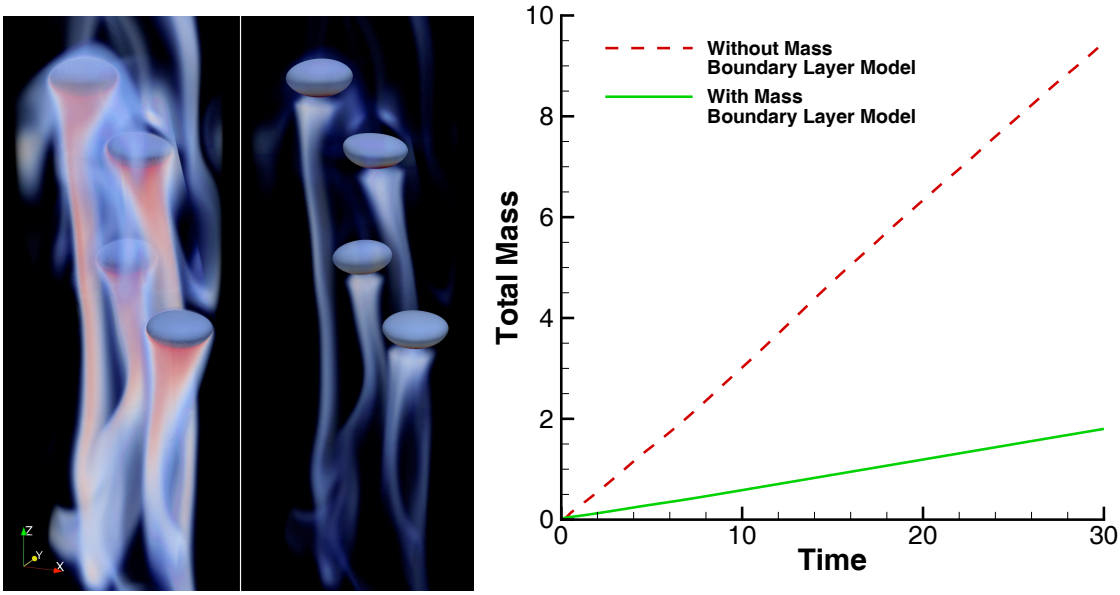

Figure 3. The two frames on the left show the scalar field around a few freely rising bubbles at one time. In the first frame the mass transfer is computed on the same grid as the fluid flow and the mass transfer is over-predicted. In the other frame the mass transfer is computed using the multiscale approach described in the text. In the graph on the right the total scalar released from the bubbles is plotted versus time for both simulations. The green line is for the multiscale approach and the red (dashed) line is when no multiscale approach is used.

resolved on the grid and the other captured by the boundary layer description. Since the advection-diffusion equation is linear, in principle these two fields can evolve independently. Where the boundary layer remains thin, the boundary layer accounts for all the mass that diffuses out from the bubble and the mass field resolved on the grid does not "know" about the mass coming from the bubble. There is, in particular, no flux of mass from the bubble to the grid-mass field. For those parts of the bubble surface where the boundary layer is thick, we transfer the mass from the boundary layer and follow it using advection resolved on the grid. We note that mass is taken away from the boundary layer and given to the grid but not the other way around and that while mass diffuses from the bubble into the boundary layer along its entire length, mass only leaves where the boundary layer is "thick." In general, we may have several thick segments of the boundary layer along the bubble surface and this results in several coupling points. The basic formulation of this approach, along with results for two-dimensional flow has been described in [22], where we demonstrated the accuracy of the model by comparing with calculations on fine grids where the mass transfer is fully resolved.

More recently, we have been conducting comparisons for fully three-dimensional flows with experimental results and, again, generally find good agreement. In figure 3, we show results from two simulations of fully three-dimensional flows for Schmidt number of 120 and an average bubble rise Reynolds number of 91, resolved on a $64 \times 64 \times 256$ uniformly spaced grid points. The fluid flow is fully resolved and both results are for the same time. In the first frame the boundary layer model is used to find the mass transfer but in the second frame the mass transfer is computed on the fluid grid. Obviously there is a big difference. This difference is also seen in

the graph on the right, where the total mass transferred from the bubble to the liquid is plotted versus time. The results for the simulation without a model are not surprising, since while the flow is fully resolved, the mass transfer is not and the low resolution leads to significant over prediction of the diffusion.

5. CONCLUSION

Direct numerical simulations of multiphase flow have now reached the point where we can use them to examine fairly complex two-fluid systems, such as the motion of hundreds of buoyant bubbles in vertical channels. In some cases the results show that the collective interactions of many bubbles lead to surprising simplifications that are unlikely to be found by examining only a few bubbles.

In general, multiphase flows of practical interest are not just multiscale but multiphysics as well. Often, new physics introduces new length and time scales that must be resolved along with the fluid flow. In some cases the structure of the new processes is relatively simple and we have recently been experimenting with using embedded analytical descriptions, coupled with fully resolved simulations of the rest of the flow, to follow the evolution. Results obtained so far for mass transfer in gas/liquid bubbly flows suggest that in some cases this approach captures the evolution well.

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