

# THE ROLE OF DIRECT NUMERICAL SIMULATIONS IN VALIDATION AND VERIFICATION

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## Abstract

The role of direct numerical simulations (DNS) of multiphase flows, where all continuum length and time scales are fully resolved, in validation and verification of models for the average flow, is discussed. Although DNS are usually limited to relatively small problems and are generally impractical for predictions of full-scale multiphase systems, DNS offer unprecedented data and insight. Indeed, if correctly done, DNS provide an essentially exact solution for the system under study. With the growing ability to conduct DNS of increasingly larger and more complex multiphase systems, they are bound to play a major and critical role in the development and validation of models designed for the predictions of the average or large-scale behaviour of industrial flows. Methods designed for DNS of multiphase flows are briefly discussed and two examples where DNS have led to fundamentally new insight are reviewed. In the conclusion we look at the immediate needs for further development of multiphase DNS and how such development will impact multiphase flow modelling.

## 1. INTRODUCTION

Numerical modelling of practical problems usually requires the inclusion of many different processes, taking place over a wide range of time and length scales. Accounting for everything that matters, on computers that exist, and in a time that is realistic, has traditionally required considerable tradeoffs in terms of details that can be included in a model. The challenges to the modeller are of two major types:

- Often the governing equations are not completely known, or include processes only poorly understood, and
- frequently the range of scales is so large that even when the governing equations are known it is not practical to resolve all time and length scales fully.

This does not, of course, eliminate modelling as a viable prediction tool. Equations for the average large-scale behaviour of systems ranging from turbulence in pipes to the evolution of the climate are routinely solved and used to predict industrial and natural processes. To account for unknown processes and unresolved behaviour we resort to phenomenological modelling. For unknown physics, experimental correlations of observable quantities substitute for our lack of understanding of the underlying processes. For unresolved but known physics, such as the unsteady motion in turbulent flows, direct numerical simulations (DNS) are increasingly providing an alternative to experimental measurements. In DNS the conservation continuum equations with the appropriate constitutive material models are solved on a grid that is sufficiently fine to resolve every space and length scale for a system that is sufficiently small so this is feasible, yet sufficiently large so that non-trivial scale interactions take place. The simulations are generally run for long enough times that well converged average and statistical information can be collected. DNS of turbulence go back over a quarter century and in the last decade and a half, DNS of multiphase flows have become increasingly common. The availability of DNS results where every flow variable is available for realistic—although small—systems, is already changing how we obtain closure for the average descriptions.

Attempts to follow the unsteady motion of multiphase systems go back to the very beginning of computations fluid dynamics. Much of the early effort at the Los Alamos National Laboratory was, for example, directed at free surface or multiphase flows (Harlow and Welch, 1965). Although the literature in the seventies and eighties contains many examples of impressive—for the time—multiphase flow computations done by the early MAC method or early versions of the VOF method, significant progress had to wait for faster computers and improved algorithms. The early nineties saw the emergence of a number of new algorithmic ideas that although building firmly on the approach

taken by earlier researchers, nevertheless marked the beginning of significant progress. The new methods include new advection schemes for sharp interfaces and new strategies for computing surface tension in improved VOF methods, level set methods and new front tracking methods (Brackbill, Kothe and Zemach, 1992; Osher and Sethian, 1988; Unverdi and Tryggvason, 1992). All these methods are based on solving the so-called one-fluid form of the Navier-Stokes equations on regular structured Cartesian grids.

DNS of larger and more complex systems will be emerging rapidly over the next few years and with new results come new opportunities for modelling. The development of new models and new ways to use the massive amount of data provided by DNS may well turn out to be the biggest obstacle to progress. However, it seems unlikely that a significant progress can be made in the development of fully validated models without the data provided by DNS. Here we review briefly methods designed for DNS of multiphase flows and then discuss two examples where DNS has lead to fundamentally new insights. In the last section we examine the immediate outlook for further development of multiphase DNS and how DNS can impact multiphase flow modelling in the near future.

## 2. NUMERICAL METHODS FOR DNS OF MULTIPHASE FLOWS

The numerical methods responsible for the progress in DNS of multiphase flows over the last decade and a half all rely on the so-called ‘one-fluid’ form of the Navier-Stokes equations, solved on regular structured Cartesian grids. This approach was already used in the Marker-and-Cell (MAC) method and early VOF methods, but more accurate advection and surface tension computations—along with more powerful computers—opened up new possibilities.

The Navier-Stokes equations for the simultaneous flow of many fluids and phases, separated by a sharp interface, can be written for the whole computational domain by allowing for variable material properties and adding singular terms to account for surface tension. The 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. For incompressible flows, for example, the ‘one-fluid’ Navier-Stokes equations are:

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

Here,  $\mathbf{u}$  is the velocity,  $P$  is the pressure, and  $\rho$  and  $\mu$  are the discontinuous density and viscosity fields, respectively.  $\delta$  is a three-dimensional delta-function constructed by repeated multiplication of one-dimensional delta functions.  $\kappa$  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. In most cases the flow is assumed to be incompressible so equation (1) is supplemented by

$$\nabla \cdot \mathbf{u} = 0. \quad (2)$$

When combined with the momentum equation, equation (2) leads to a non-separable elliptic equation for the pressure. For non-isothermal flows the energy equation needs to be solved also and for mass transfer and reactions we need to add equations for species conservation. The one fluid formulation naturally incorporates the correct mass, momentum and energy balances across the interface, yielding the standard jump conditions if we integrate the governing equations across the interface. Equations (1) and (2) can be solved by essentially any method designed for homogeneous flows and in most implementations a relatively conventional projection method is used. The key challenges are advection as the Reynolds number gets larger and the solution of the pressure equation. The main different between the various methods are the way the interface is advected and surface tension is computed.

The Navier-Stokes equations are usually solved by a second-order accurate projection method on a fixed, staggered grid. The interface can be advanced in many different ways but in our approach we track the fluid interface by connected marker points (the "front"), in order to keep the boundary between the phases sharp and to accurately compute the surface tension. The front points are advected by the flow velocity, interpolated from the fixed grid. The surface tension is represented by a distribution of singularities (delta-functions) located at the front. The gradients of the density and viscosity become delta functions 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 to impose a divergence-free velocity field. For a detailed description of the original method and various verification tests, see Unverdi and Tryggvason (1992), Tryggvason *et al.* (2001), Esmarelli and Tryggvason (1999) and Tryggvason, Scardovelli and Zaleski (2010). For high Reynolds number flows we usually use the QUICK or the ENO schemes for the advection terms. For the pressure equation we originally used a multigrid method but more recently we have used a Krylov method (BiCGSTAB) to give us better robustness for large density differences across the interface. For large-scale simulations we use a version of the code that has been fully parallelized, using MPI.

The purpose of tracking the front is to advect a marker function (and compute surface tension) that is used to set the density and other material properties used when solving the Navier-Stokes equations. Instead of generating the marker function from the location of the front at every time-step, most other approaches to multiphase flow simulations are based on advecting a marker function on the grid used for the fluid solver. The Volume of Fluid (VOF) and the level set methods are the best-known 'front capturing' methods, although other ways to advect the marker function certainly exist (Takewaki, Nishiguchi and Yabe, 1985; Jacqmin, 1999). In the VOF method the marker function is advected directly and special strategies are used to keep the edge of the marker function confined to just one grid cell. In the level set method a smooth function is advected and the interface identified with the zero contour. The marker function is then generated from the level set function.

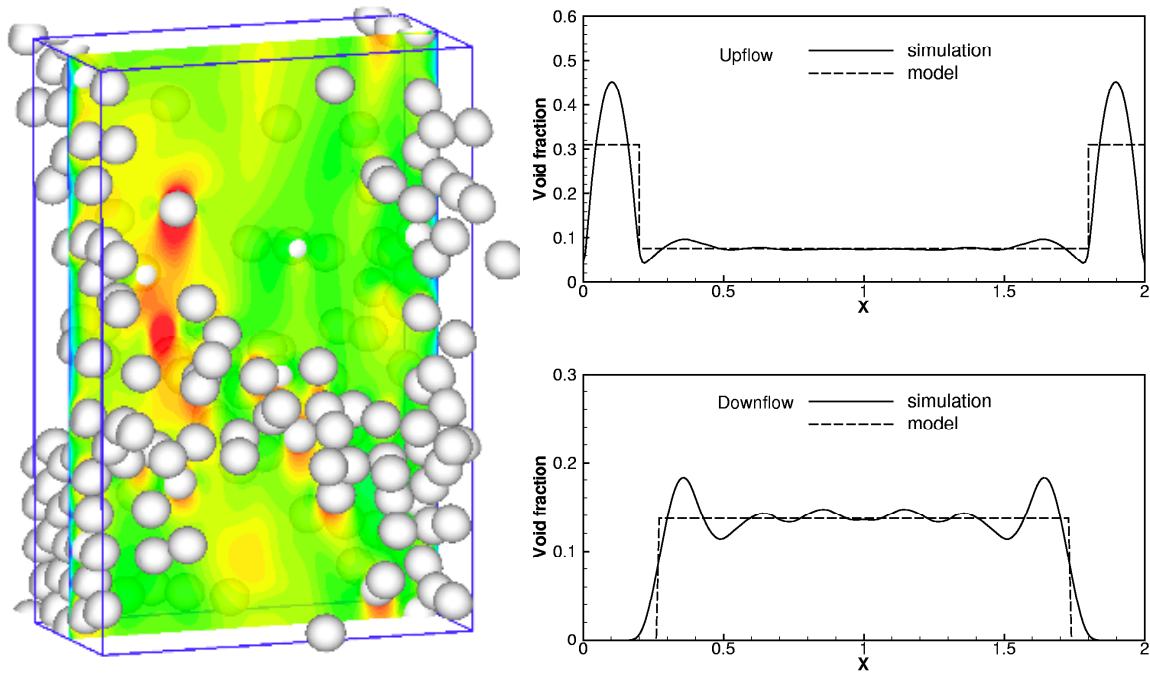
### 3. EXAMPLES OF DNS OF BUBBLY FLOWS

A large number of DNS studies have focused on bubbly flows. Bubbly flows are found in an extraordinary number of natural and industrial processes, ranging from explosive volcanic eruptions and the mass transfer between the ocean and the atmosphere to boiling heat transfer, the stirring of metal melts and suspensions of cells in bioreactors. Here we review briefly two DNS studies of bubbly flows.

#### 3.1 Bubbly Flows in Vertical Channels

Bubbly flows in vertical channels are found in a large number of practical applications and several researchers have examined such flows experimentally, see, for example, Serizawa, Kataoka and Michiyoshi (1975); Wang, Lee, Jones and Lahey (1987); Liu and Bankoff (1993); Liu (1997); Kashinsky and Randin (1999); and Matos, Rosa and Franca (2004). These experiments show that nearly spherical bubbles in upflow result in a wall-peaking of the void fraction but a bubble free wall-layer for downflow. The velocity in the core of the channel is nearly uniform in both cases. Experiments of laminar upflow include Song, Luo, Yang, and Wang (2001) who studied flows with both uniform and nonuniform distribution of bubble sizes and Lou, Pan, and Yang (2003) who examined the motion of light particles. Wall peaking was found in both cases. Modeling of bubbly flows in channels has generally treated the mixture using the two-fluid model where separate equations are written down for the motion of the liquid and the gas. Such models for turbulent flows can be found in, for example, Lopez De Bertodano, Lahey, and Jones (1994), Kuo, Pan, and Chieng (1997), and Guet, Ooms and Oliemans (2005). A two fluid model for laminar flow was developed by Antal, Lahey and Flaherty (1991).

We have recently examined bubbly flows in vertical channels in a series of paper. In Lu, Biswas and Tryggvason (2006) we simulated the motion of several nearly spherical bubbles in a laminar flow in a vertical channel, both for upflow and downflow, fully resolving all flow scales. The simulations showed that in both cases the flow consists of two well-defined regions: A thin wall-layer and a homogeneous core, occupying most of the channel. The formation of these regions is due to lift induced lateral motion of the bubbles. For a nearly spherical bubble rising due to buoyancy in a vertical shear, it is well known that the lift force pushes the bubble toward the side where the liquid is moving faster with respect to the bubble. Thus, a bubble near the wall in upflow is pushed toward the wall and in downflow the bubble is pushed away from the wall. The weight of the bubble/liquid mixture and the imposed pressure gradient must be balanced by a shear stress induced by a velocity



**Figure 1.** The bubble distribution at one time for upflow in a vertical channel is shown on the left and the void fraction profiles for both upflow (top) and downflow (bottom) on the right. The analytical prediction for the average void fraction is shown by a dashed line.

gradient. For upflow the mixture, on the average, must be sufficiently light so the imposed pressure gradient can push it upward. As bubbles are removed from the core, its average density decreases until the weight is balanced exactly by the pressure gradient. The shear is then zero and the migration of the bubbles to the wall stops. For downflow the opposite happens. Bubbles move into the core and make it more buoyant, until its weight is balanced by the pressure gradient and further lateral migration is stopped. Thus, in both cases the core is in hydrostatic equilibrium and it is only in the wall-layer where there is a non-zero velocity gradient. For upflow where the weight of the mixture in the core is increased by pushing bubbles to the wall, the light, bubble rich mixture in the wall-layer is driven upward by the imposed pressure gradient. For downflow, on the other hand, bubbles must be drawn away from the wall to decrease the weight of the mixture in the core and the dense bubble-free wall-layer is driven downward by its weight and the imposed pressure gradient. The distribution is stable in the sense that if too many bubbles end up in the wall layer for upflow, the core slows down with respect to the wall layer, thus generating shear that will drive the bubbles out of the wall-layer. Similar if too many bubbles end up in the core for downflow, its velocity is reduced and bubbles are driven back to the wall. For downflow, where the wall-layer is bubble free, the velocity profile is easily found by integrating the Navier-Stokes equations for steady laminar parallel flow and the flow rate can be predicted analytically, with a fair degree of accuracy. For upflow, on the other hand, the presence of the bubbles makes the situation more complex and the velocity profile is not as easily found. Figure 1 shows the bubble distribution for upflow at one time, as well as a comparison of the computed void fraction distribution for both up and down flow and an analytical model based on the considerations described above.

For turbulent flow we have examined the effect of both bubble size (Lu and Tryggvason 2007) and void fraction (Lu and Tryggvason, 2008) in some detail. The overall conclusions are the same as for laminar flow. There is a bubble free wall-layer whose thickness is determined by how many bubbles are needed to reduce the average density of the core layer to the hydrostatic value and the flow in the wall-layer can be predicted by the law-of-the-wall. The velocity in the core layer is constant and determined by the velocity increase in the wall-layer, just as for the laminar flow but since the velocity profile in a turbulent channel flows without bubbles is nearly flat, the changes in the flow rate are not as dramatic as for laminar flow.

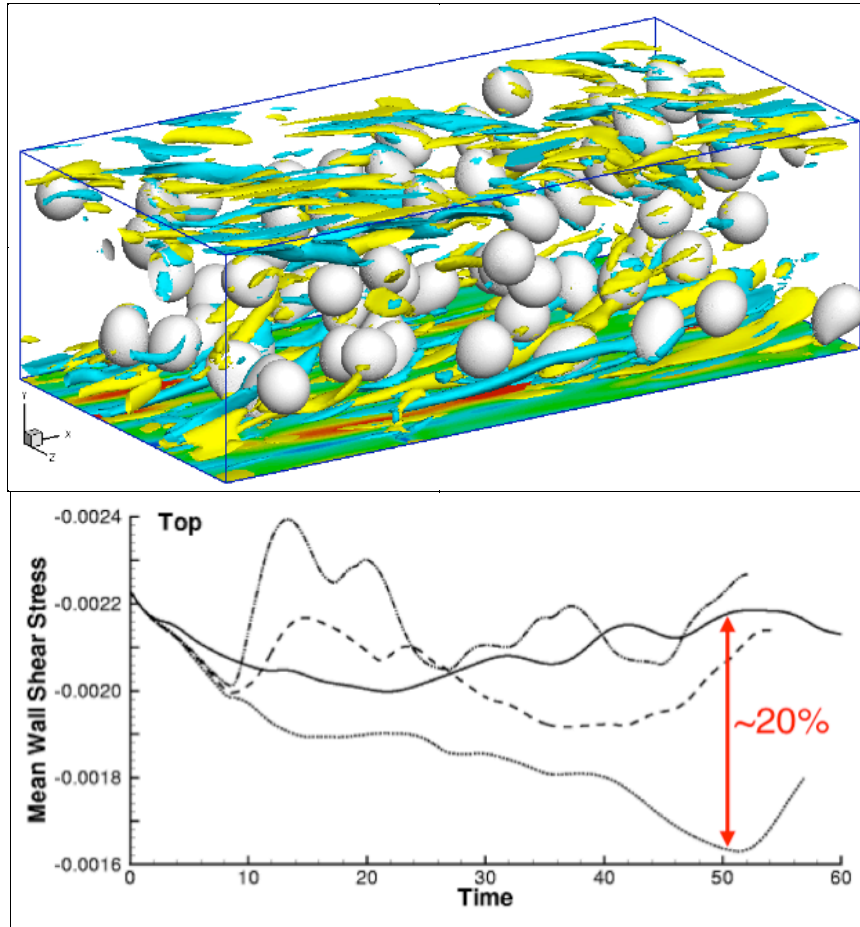
For spherical bubbles in turbulent upflow the results are also similar to the laminar cases. The void fraction consists of a wall-peak and a uniform profile in the channel core and as for the laminar flow the bubbles in the wall layer reduce the total flow rate significantly. Making the bubbles more deformable (experimentally this is usually the results of making them bigger but we isolated the effect of deformability by reducing surface tension) results in a completely different void fraction. Deformable bubbles generally experience significant less lift than spherical ones, and sometimes negative lift, so there is no force driving the bubbles to the wall. Thus, the bubbles remain in the centre of the channel and the wall region is essentially free of bubbles. The effect of the bubbles on the net flow rate is therefore relatively small. We have looked at the transition between the bubble deformability that results in wall hugging bubbles and bubbles that drift into the centre and generally find that the results are consistent with experimental observations. For details see Lu and Tryggvason (2008).

The simulations described above have shown that while averaged models capture the void fraction distribution reasonably well, particularly in the bulk away from wall, the models do very poorly in describing the velocity in the wall layer. Since the velocity in a bubbly upflow in a pipe is completely determined by what happens in the wall layer, accurate prediction of the wall layer velocity profile is obviously of major importance. We should contrast this situation with downflow, where the wall layer is generally free of bubbles and averaged models do a very good job at predicting the overall flow rate. The difficulty of accurately including the observed mechanisms in averaged models (Kunz et al., 2007) argue for the importance of examining new ways to include bubble rich wall layers. The wall layer is usually very thin and limited to about a bubble diameter (1-2 mm for air bubbles in water). For large scale simulations of industrial size systems, this layer cannot be resolved and even if it could, the evidences suggest that it needs to be treated by models that are different than those used for the flow in the bulk, such as by the introduction of a wall function, as often used in the modeling of turbulence in single phase flows.

### **3.2 Drag Reduction due to Bubble Injection into Turbulent Boundary Layer**

It has been known for a long time that the injection of bubbles into a turbulent boundary layer can result in drag reduction (see Merkle and Deutsch, 1990, Kato *et al.*, 1995; and Kodama *et al.*, 2002, for a review). The reason for the reduction has been essentially unknown and there has been, for example, little agreement about what size bubbles are needed. In a study described in detail in Lu, Fernandez and Tryggvason (2005) we attempted to cast some light on the mechanisms underlying drag reduction due to bubble injection and to provide data to help with the modeling of such flows. This was a fairly challenging study, in part because the need to accurately resolve both the turbulent flow and bubbles but also due to the subtlety of the interactions of the bubbles with the turbulence. Our results showed that slightly deformable bubbles can lead to significant reduction of the wall drag by sliding over streamwise vortices and forcing them toward the wall where they are cancelled by the wall bound vorticity of the opposite sign. Spherical bubbles, on the other hand, often reach into the viscous sublayer where they are slowed down and lead to a increase in drag. The results were in general agreement with experimental results obtained in the Navy's Large Cavitations Channel (Kunz et al., 2007) and small scale experiments carried out subsequently by van den Berg et al., (2005). Figure 2 shows one frame from a simulation of bubbles in a turbulent channel flow with a Reynolds number of 4000 (top). In addition to the bubbles, iso-contours of spanwise vorticity are also shown, with different shading indicating positive and negative vorticity. The wall shear on the bottom wall is also showed. The integrated wall drag is plotted versus time in the bottom frame, for simulations without bubbles (solid thick line) and bubbles of different deformability. The most deformable bubbles (thin solid line) result in significant drag reduction while the least deformable ones (dot-dashed line) increases the drag. The flow rate in these simulations is kept constant and the wall drag changes as the flow evolves, since the computational domain is relatively small. The results presented by Lu, Fernandez and Tryggvason (2005) showed that the drag reduction due to bubble injection is a subtle phenomenon that depends on a detailed understanding of how bubbles of just the right deformability interact with the vortical structure of the flow. How to account for this interaction in models of the average flow remains an open question.

“Real” problems tend to have a large range of scales, and material properties that can vary greatly. On the computer, however, it is easiest to work with problems where the range of scales is



**Figure 2.** Top: One frame from a simulation of several bubbles in a turbulent channel, showing the bubbles and the vortical structures near the wall, along with the shear stress distribution on the wall. Bottom: The integrated wall shear for both walls, from several simulations with and without bubbles.

small and the values of the material properties differ by a modest amount. Thus, a compromise is generally needed between what is desirable (real material properties and system size) versus what is practical (or possible). However, in spite of these limitations—which get less severe every year as better methods are developed and computers get faster—DNS have already shown that they will transform the way we study bubbly flows. The two examples discussed here are only meant to demonstrate what can be done. For other simulations of bubbly flows see, for example, Tomiyama et al. (1993); Takada et al., 2001; van Sint Annaland et al., 2006; and Bothe, Schmidtke and Warnecke, (2006). Similar studies have been done for flows with suspended solid particles and the reader can consult Feng, Hu, and Joseph (1994); Hu (1996); Choi and Joseph (2001) and Pan et al., (2001) for an introduction to the literature.

#### 4. OUTLOOK

DNS of multiphase flows have come a long way over the last decade and a half. We now have the ability to simulate turbulent flows containing hundreds of fully resolved bubbles, for example. While larger systems, higher Reynolds numbers and more complex situations are certainly desirable, the most urgent need for bubbly flows is actually a theoretical framework to condense the information from DNS. Simulations of turbulent flows of homogeneous fluids have lead to significant progress in theoretical modelling of turbulence, particularly for filtering as applied to large eddy simulations and the generation of subgrid models for the unresolved motion. For multiphase flows there is essentially nothing similar available yet and refinements of the two-fluid model, originally introduced in the mid

seventies (Harlow and Amsden, 1975) remains more or less the state-of-the-art. The need for a more sophisticated approach is, however, well understood and a few authors (Liovic, Lakehal, and Liow, 2004, for example) have started to examine what such models might look like.

Solid-fluid multiphase flows generally consist of small solid particles suspended in the fluid phases (when the solid bed is fixed we generally talk about porous media flow rather than multiphase flow). Multiphase flows of two fluid phases can often also be described as disperse flows, with one phase appearing as bubbles or drops suspended in another continuous phase. Although such flows have been studied intensively and most DNS efforts have so far been devoted to disperse flows, they are only seen under relatively restrictive conditions. In some cases the phases are better separated as in stratified and annular flows and in other cases they are more intermingled, such as in churn-turbulent flows. In many situations, including in disperse flows, the flow undergoes repeated topology changes where fluid interfaces merge and fluid masses break up. Topology changes pose a significant new set of challenges, both because we have to account for effects not included in the usual continuum description and because the rupture is preceded by the formation of very thin films and threads that are hard to resolve in a computation designed to resolve much larger flow scales. Because surface tension is high and viscosity is large on the scale of the small features, the geometry and the flow are relatively simple. Thus, it is likely that these features can be captured by semi-analytical subgrid models, building on the rich body of work that has been devoted to such problems. Relatively little has, however, been done yet in exploring the utility of such an approach. An explorative study for a thin film beneath a drop sliding down an inclined wall can be found in Thomas, Esmaeeli and Tryggvason (2010).

Closure laws for average models of multiphase flows have in the past been developed mostly using experimental data coupled with dimensional analysis, simplified analytical models, physical intuition and arm-waving. Experimental results, where available, do of course provide the “ground-truth” in the modelling of a physical process. Such results are, however, often hard to obtain and usually hard to control. For multiphase flows we often have to be content with a control of only the overall experimental conditions and the experimental results are frequently best described by ‘you get what you get.’ The size distribution of bubbles is usually determined indirectly by, for example, adjusting the flow rate of air through a nozzle and eliminating the effects of surfactants for air-water systems is next to impossible. In numerical simulations we can choose to work with bubbles of one size only and clean interfaces, for example, leading to “clean” results of the type we obtained for the bubbles in a vertical channel described above.

The use of DNS to help with the development of new models and better closures is different than simply studying interesting multiphase flows. The critical path must, in particular, include simulations of large but well-controlled and characterized systems that involve large range of scales. Although the results of such large simulations may often motivate us to examine specific aspects by looking at smaller systems, we believe that going the other way—starting with small systems of, say, one or two bubbles with the hope of eventually adding complexity—will frequently lead to efforts being diverted to problems that are not critical. Similarly, we believe that the systems simulated need to be well characterized and designed to answer specific questions. There certainly is a role for simulations where we attempt to include every process and replicate realistic systems, but for modelling those are generally less useful. If topology changes take place in an uncontrolled and poorly understood way, for example, then we no longer have results that are ‘exact.’ On the modelling side, we believe that we need to accept that there will be different models for different processes and that hoping for one universal set of equations is not realistic. For bubbly flows, for example, it is likely that bubble rich wall layers will need to be treated in a different way from the interior flow, in the same way a wall function is used for turbulent homogeneous flows. Similarly, we should expect that while small bubbles may be captured by a two-fluid like model, other aspect will need to be resolved. Models recognizing this already exists but DNS should help us take them to a new level.

While DNS of two-fluid systems, consisting of two different immiscible fluids, still provide considerable computational and theoretical challenges, the ultimate goal is, of course, to simulate much more complex flows where different physical processes are simultaneously taking place. Often such flows include other fields, such as temperature, species concentration, electric fields, that affect the interfacial forces, or a change of phase as in boiling and solidification. Adding another field usually poses little problem if the time scales are comparable, but in many cases that is not the cases.

The mass transfer from bubbles in liquid is generally much slower than the momentum transfer so mass boundary layers are much thinner than the flow scales (Radl et al., 2008) and in boiling flows the thickness of the microlayer below a growing vapour bubble is usually much smaller than the bubble size. Such small features have recently been modelled by semi-analytical subgrid models and it is likely that such models will find a much more widespread use as the complexity of problems being examined increases.

DNS of multiphase flows has been developed over the last decade and a half to the point that such computations are now routinely being used to examine the unsteady motion of mixtures of two immiscible fluids. However, their use to guide the modelling of multiphase flows and their application to flows where many complex physical processes are taking place is only beginning. The transformative impact of DNS of multiphase flows is yet to be realized but, as outlined in this paper, we can expect that to start to take place in the very near future.

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