

DNS FOR MULTIPHASE FLOW MODEL GENERATION AND VALIDATION

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Abstract

The modeling of averaged properties of multiphase flows has traditionally suffered from the lack of detailed and reliable data against which closure models can be validated. Direct Numerical Simulations (DNS) have now advanced to the point that they are able to provide such data for relatively complex systems such as hundreds of bubbles in turbulent flows. Here we discuss recent DNS results for bubbly flows in vertical channels and how these results are impacting our understanding of such flows. We also discuss briefly simulations of boiling flows and the challenges in conduction DNS of complex nucleate boiling.

Introduction

Exact solutions of analytical models of physical processes have played a key role in establishing our current understanding of innumerable problems. For multiphase flows such solutions are, however, few and far between. Direct numerical simulations (DNS), where all continuum time and length scales are fully resolved, can provide what is essentially an exact solution to a mathematical description of a fully characterized system. Such solutions are especially important for computational modelling of industrial multiphase flows where it is impractical to resolve all scales and we must resort to equations describing the average or large scale flows. The unresolved processes are represented by closure laws and exact solutions (analytical or from fully resolved simulations) can provide the insight and data needed for the development of closure laws. For turbulent flows of single-phase fluids, DNS are increasingly providing an alternative to experimental measurements for obtaining the data needed for closure laws. Similarly, although DNS of multiphase flows are far behind what can be done for single-phase flows, we are starting to see the impact of DNS on modelling. Here we review the results of DNS of the flow of buoyant bubbles in vertical channels where simulations have provided insight that allow many aspects of the problem to be predicted analytically. The result showed that for nearly spherical bubbles the lateral migration of the bubbles due to lift results in two regions: A core where the void fraction is such that the weight of the liquid/bubble mixture balances the imposed pressure gradient (and the velocity is therefore constant) and a wall-layer that is free of bubbles for downflow and bubble-rich for upflow. Deformable bubbles, on the other hand, generally do not migrate to the walls. The status of simulations of more complex flows such as nucleate boiling is also discussed briefly. While DNS results are critical for the development of closure relations for unresolved processes for multiphase flows, their utility is likely to go far beyond that. We should, in particular, be able to use such simulations to explore the sensitivity and stability of flow configurations and therefore help us assess the expected uncertainty of models based on long time averages.

1. Numerical Approach

The need for Direct Numerical Simulations of multiphase flows has been understood for a long time. Indeed, some of the very earliest computations of the unsteady Navier-Stokes equations 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 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, [1,2]), 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 solutions 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 for 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 [3]. 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, we advect the interface and reconstruct a marker function from the interface location. The interface is identified by connected marker points that are moved with the fluid velocity, interpolated from the fixed fluid grid. Once the marker points have been advected, a marker function is constructed from the new location. 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 [4,5].

2. DNS of Bubbly Flows

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. The modeling of industrial size multiphase flow systems must by necessity rely on models of the average flow. The averaging introduces terms that must be modeled and the representation of those terms, describing the effect of the fluctuations in the liquid and the gas velocity on the average motion, as well as the forces between the phases, remains the major challenge in numerical modeling of large-scale industrial systems. Descriptions of the most commonly used models, including the two-fluid model where separate conservation equations are written for the gas and the liquid, can be found in [6-8], for example.

Simulations of bubbly flows are a good example of the opportunities and challenges in applying DNS to understand complex multiphase flows. Problems in Nature tend to have large range of scales, and material properties can vary greatly. On the computer, however, it is easiest to work with problems where the range of scales is modest 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). For bubbly flows the limitations are many. First of all is system size. Real industrial systems often involve a large number (hundreds and thousands) of bubbles interacting with complex flow structures. Second is viscosity. We are often interested in air bubbles in water and even for small bubbles, the rise Reynolds number is in the hundreds. System size and Reynolds number are closely related. As the Reynolds number increases, the number of grid points needed to resolve the flow around each bubble increases and fewer bubbles can therefore be included if the Reynolds number is high. Of considerably lesser practical importance—but often of a major significance when talking with our experimental colleagues—is the density difference between the bubbles and the air and the surface tension for very small bubbles. For air bubbles in water the density ratio is about 800 at normal temperature and pressure. Using this ratio in a computation generally is difficult. Some methods simply will not work and for other the solution of the pressure equation takes a long time, compared with cases where the density difference is smaller. The density inside the bubble affects the evolution of the flow in two ways. First of all, the buoyancy force is directly proportional to the density difference times the gravity acceleration and secondly, the inertia of each bubble is determined by its density. Of those, the first one is more important. In many cases the buoyancy force is what drives the fluid (bubble and liquid) motion and getting it right affects rise velocity. The bubble inertia is only important for unsteady bubble motion and usually it is the inertia of the surrounding fluid that is much more important than the inertia of the bubble itself. For a spherical bubble the inertia force is given by the sum of the “added mass” and the mass of the bubble. Although at a first glance it might seem that the importance of the density ratio on the total mass is larger than for the buoyancy force, one has to remember that the total mass multiplies the acceleration, which itself depends on the density ratio. Thus, buoyancy is what drives the system and the inertia is a second order effect. These arguments are somewhat similar to those made for the Boussinesq approximation for low density differences, where the full difference is included for the buoyancy term but the inertial terms are computed using the average density. Surface tension can also cause somewhat similar difficulties since very high values can cause parasitic currents that dominate the flow. Often, however, it is not necessary to set the surface tension as high as it should be. For very small bubbles, surface tension keeps the bubbles completely spherical. For high Reynolds number flows the bubbles are essentially spherical once the Eotvos number is about 0.1 and increasing the surface tension further (lowering the Eo) causes no changes. Thus, once the surface tension is sufficiently high so the bubbles stay spherical, the flow is independent of the exact value of the surface tension and there is no need to increase it further. It is important to stress that the validity of these approximations are specific to bubbly flows and other systems will in general require different considerations.

In spite of the challenges, DNS offers unprecedented opportunities to learn about the behavior and properties of bubbly flows. As with other computational studies we have, first of all, access to the complete data, and secondly, we have complete control over the setup that we wish to study. These two aspects set DNS studies apart from experimental investigations where neither is generally true and, indeed, the main challenges are precisely measurements and control. Thus, experiments and DNS should be viewed as complementary approaches where one provides the ability to examine the overall behavior of a large systems with the right physical properties and the other allows us to obtain detailed data for well controlled systems. DNS allows us to control the exact size distribution

of bubbles, their deformability, whether they coalesce or not, and the exact flow conditions. From the data we can gather information about how the bubbles move, how they organize themselves with respect to each other and the flow structures, and how the bubbles modify the flow. Given these details, we can answer questions such as: do the bubbles tend to cluster and if they do, what is the structure of the clusters. Many bubbles forming horizontal “rafts” will generally rise slower than uniformly distributed bubbles and bubbles forming vertical “chimneys” will rise faster, for example. We can also address how the bubbles interact with the flow. Lateral lift force on bubbles in wall-bounded flows can push the bubbles either to the walls or away from the walls and the flow can change in fundamental ways, depending on where the bubbles end up. The location of the bubbles can have decisive impact on the flow rate as well as the transfer of heat and mass and predicting accurately how the behavior depends on bubble size, void fraction, and the flow rate can mean the difference between a successful design and one that does not work. In many cases the effects that govern the behavior are subtle and cannot be properly understood unless we have the ability to control the setup in great detail. Thus, while experiments may show overall behavior and trends as the controlling parameters are changed, it is often difficult to isolate specific relations. We cannot, for example, isolate the effect of bubble size in a situation where there are many sizes present and coalescence and breakup can take place. Similarly, uncontrolled contamination and the presence of surfactants can leave doubt as to what is really the cause of an observed behavior.

2.1 Bubbly flows in unbounded domains

We have been examining bubbly flows using DNS for some time. The interactions of two bubbles was examined briefly in [3] and the motion of many nearly spherical bubbles at moderate Reynolds numbers was studied in [9], for a case where the average rise Reynolds number of the bubbles remained relatively small (1-2). In [10] we looked at another case where the Reynolds number was higher (20-30). A much larger number of three-dimensional bubbles, using a parallel version of the method, was simulated in [11], where our largest simulation followed the motion of over two hundred three-dimensional buoyant bubbles per periodic domain, for a relatively long time. The effect of deformability was studied in [12], where we found that relatively modest deformability could lead to a streaming state where the bubbles gathered in a stream or a chimney. This investigation was extended to higher bubble Reynolds numbers in [13], where the bubbles rise unsteadily (wobbling). We showed again the importance of bubble deformability, but did not find streaming. These simulations allowed us to determine how the bubble rise velocity depends on the void fraction, the basic bubble-bubble interaction mechanisms and how they depend on the deformability of the bubbles, how the bubble motion generates velocity fluctuations in the liquid (pseudo-turbulence), how the bubble velocity fluctuates and the bubbles disperse, how the bubbles form small-scale structures and the stability of these structures, and many other aspects of the flow behaviour.

2.2 Bubbles in vertical channels

Many of our recent studies of bubbly flows have focused on wall-bounded flows. For nearly spherical buoyant bubbles in vertical channels, our results show that at steady state the flow is relatively simple. For laminar bubbly flow in vertical channels, both for upflow and downflow, we see two well-defined regions: Thin wall-layers and a homogeneous region, 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, in upflow a bubble near the wall 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 due to a velocity gradient. For upflow the mixture, on the average, must be sufficiently light so the imposed pressure gradient can push it upward. As bubbles are moved from the core to the walls, the average density in the core region increases 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 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. This 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. Similarly, 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. Since the velocity increase across the wall-layer determines the liquid velocity in the core of the channel, it is critical for predicting the total flow rate. For the most part the bubbles in the wall-layer interact only weakly with the bubbles in the core region and as a first approximation it seems that they can be neglected, as long as the fluid there is in hydrostatic equilibrium and the shear is zero. We have therefore looked at the dynamics of a bubbly wall-layer, neglecting the bubbles in the core region but eliminating any shear there, by applying a body force adjusted to balance the pressure gradient there. For modest Reynolds numbers we have found that the contribution to the shear in the wall-layer from the Reynolds stress terms is insignificant, but the bubble deformation plays a very significant role. While we do not fully understand yet how to predict the bubble deformation, we find that if we take information about the deformation from the computations and use them in a very simple model for flow, then we predict the velocity increase across the wall-layer fairly accurately. For a detailed description of our studies of laminar bubbly flows in vertical channels, see [14].

Simulations of bubbly flows in turbulent channels suggest a similar picture. For the downflow case the lift force drives nearly spherical bubbles away from the walls, as for the laminar flow case. The velocity in the bubble free wall-layer is therefore given by the standard law of the wall. The main complication is that if the wall-layer is too thin, the presence of the bubbles may prevent the growth of turbulence structures near the wall and if the wall-layer is too thick, the core may meander in an unsteady way. The results suggest that even for a very thin wall-layer (less than fifty wall units thick) the turbulence is sustained but that for thick wall-layers the boundaries may vary in time due to meandering of the bubbly core. For turbulent flow the velocity in the middle of the channel is relatively uniform in the absence of bubbles and since the main effect of the presence of the bubbles is to make the velocity there completely uniform, adding the bubbles causes surprisingly little change in the velocity. The main increase in velocity takes place in the bubble free wall-layer where the velocity profile remains nearly the same and while the turbulent velocity profile without bubbles is not completely flat as it is after adding the bubbles, the differences are small. Since the flow in the

core of the channel is uniform, the turbulent Reynolds stresses there are zero and in the buffer layer these are reduced. The slow growth of the velocity in the buffer layer and the wall region is also cut short at the outer edge of the wall-layer and replaced by the uniform velocity characterizing the bubbly core. In addition to examining the effect of the void fraction (by changing the number of bubbles), we have also examined the effect of the bubbles size [15, 16]. Those tend to be relatively minor.

For turbulent upflow, we have examined the effect of the deformability of the bubbles in [17]. The results showed that nearly spherical bubbles behaved very much like the laminar ones, forming a wall-layer and a hydrostatic core. As the bubbles became deformable, however, the bubbles no longer drifted to the wall but stayed in the middle of the channel. The flow rate was reduced significantly when the bubbles drifted to the wall, but this reduction was not seen for the deformable bubbles.

Just as for DNS of turbulent flow of a single phase fluid, for multifluid flows it is generally desirable to examine as large system as possible, at as high Reynolds number as possible. While the ability to simulate hundreds of bubbles using grids with billion of more grid points is likely to be feasible on modern day computers, we have elected to take a more gradual approach, examining a successive collection of cases of increasing size. The arguments are, of course, that since very large runs are very expensive, it is desirable to build up our experience so that we are able to design our largest simulations in such a way that they yield maximum information. In figure 1 we show two frames from a simulation of 119 small bubbles and one large bubble in a turbulent upflow in a vertical channel with an initial friction Reynolds number of 250 and a channel Reynolds number of 4000. The flow is driven by an imposed pressure gradient, yielding the desired friction Reynolds number. The size of the domain is π by 2 by $\pi/2$ units and the left and the right boundaries are rigid no-slip walls. In the streamwise and spanwise direction we use periodic boundary conditions. The domain is resolved by 512 by 384 by 256 grid point in the spanwise, streamwise and wall-normal direction, respectively, or about 50 million grid points total, and the simulations have been carried out using 192 processors at the Centre for Research Computing at the University of Notre Dame. Since the flow takes a fairly long time to reach an approximate steady state, we initially ran the simulation on a coarser grid (256 by 192 by 128) until time about 100 (in computational units) and then refined the grid. The initial velocity field was taken from simulations of single phase fully turbulent flow, but relatively early in the simulation we also adjusted the fluid velocity by reducing the streamwise velocity by a constant fraction, since adding the bubbles reduces the flow rate. The results from the fine grid are shown, at time 414. In frame (a) we plot the bubbles and the turbulent structures as identified by the lambda-2 method. In frame (b) we show the bubble distribution looking parallel to the walls, perpendicular to the flow. The results show the bubble distribution that we expect. The majority of the small bubbles slide along the walls, while the large bubble, along with some of the smaller bubbles rise in the middle of the domain. These results are consistent with what we saw in [17]. What was not as visible there, however, due to the much smaller number of bubbles is the clustering of the bubbles on the wall. On both walls the small bubbles rise in very tight groups, leaving large fraction of the walls without bubbles. It is clear from the vortical structures that the large bubble has significant impact on the flow by stirring up the flow and depositing significant amount of wake vortices into the flow.

Although it is important to examine both the steady-state and the transient evolution of the flow, we would like to initially focus on the former. Thus, we have simulated the behaviour of the present system for a reasonably long time, taking the steps outlined above to accelerate the convergence to steady-state. In spite of these steps and the total time simulated, the system has not completely

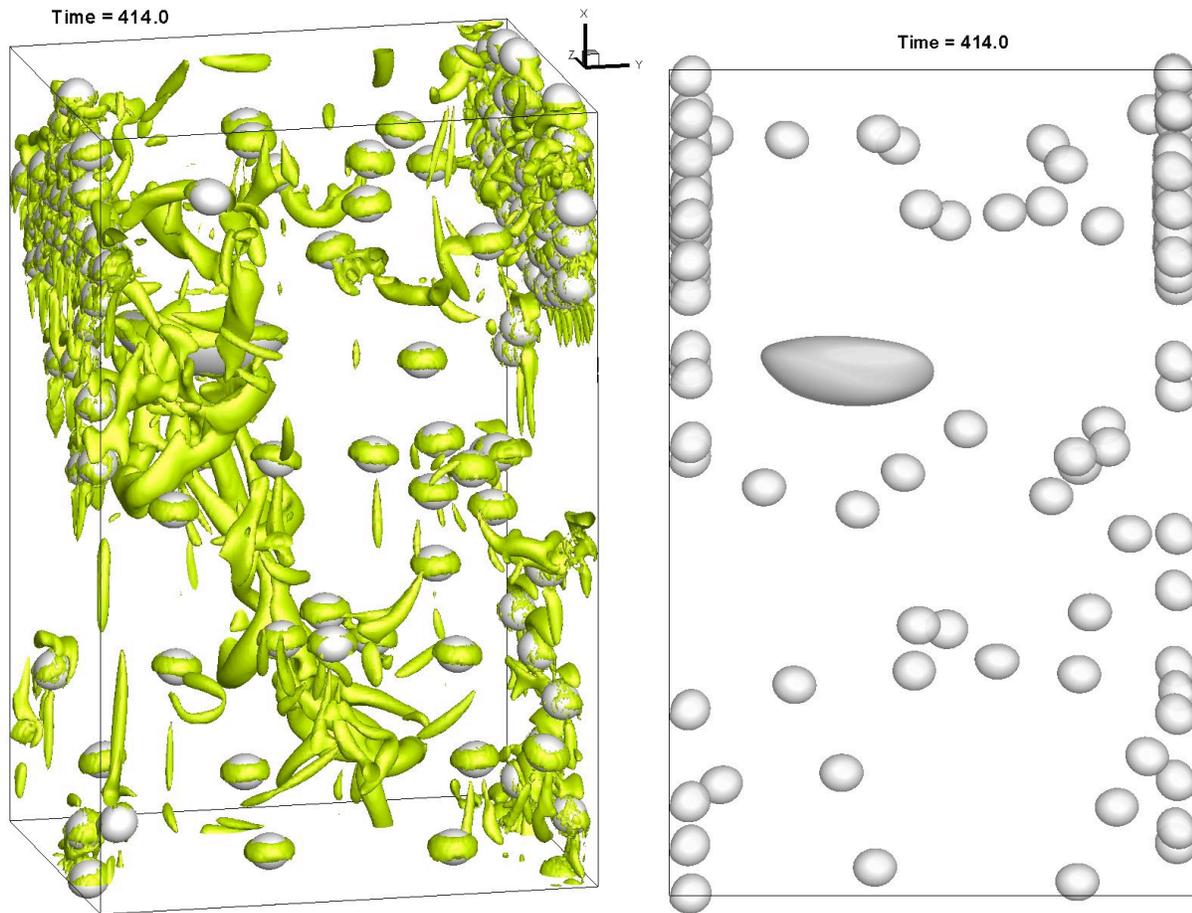


Figure 1 The results from a simulation of 119 small and one large buoyant bubble rising in a turbulent upflow in a vertical channel at time 178. The bubbles and the vortical structures, visualized using the lambda-2 method are shown on the left. On the right, only the bubbles are shown in a plane perpendicular to the walls.

reached a statistically steady state. In figure 2(a) we show the wall shear as a function of time and in figure 2(b) we show the total flow rate versus time. The plot shows the evolution from the time when we interpolated the results from the coarser grid run. Initially we continued the coarser grid run also but as it resulted in a slightly higher flow rate than the fine grid run, we eventually terminated it. At steady state the wall shear must match the pressure gradient and the weight of the mixture and we see that we have not completely reached that state yet. Similarly, the flow rate shows a slow decrease (consistent with the higher wall shear), also indicating that we have not reached a completely steady state. In spite of that, we have started to examine the properties of the flow and in figure 3 we plot the average velocity, the void fraction distribution, and average cross velocity component of the Reynolds stresses versus the wall-normal coordinate for two times (equal to 178 and 414 computational units). The clear asymmetry of the flow, visible in figure 1, is reflected in these quantities. The void fraction at the right wall is, in particular, significantly higher than at the left wall, although the difference is less at the later time. We have also plotted the void fraction as predicted by the hydrostatic model introduced in [14]. This model is based on the observation that nearly spherical bubbles in upflow move toward the walls until the void fraction in

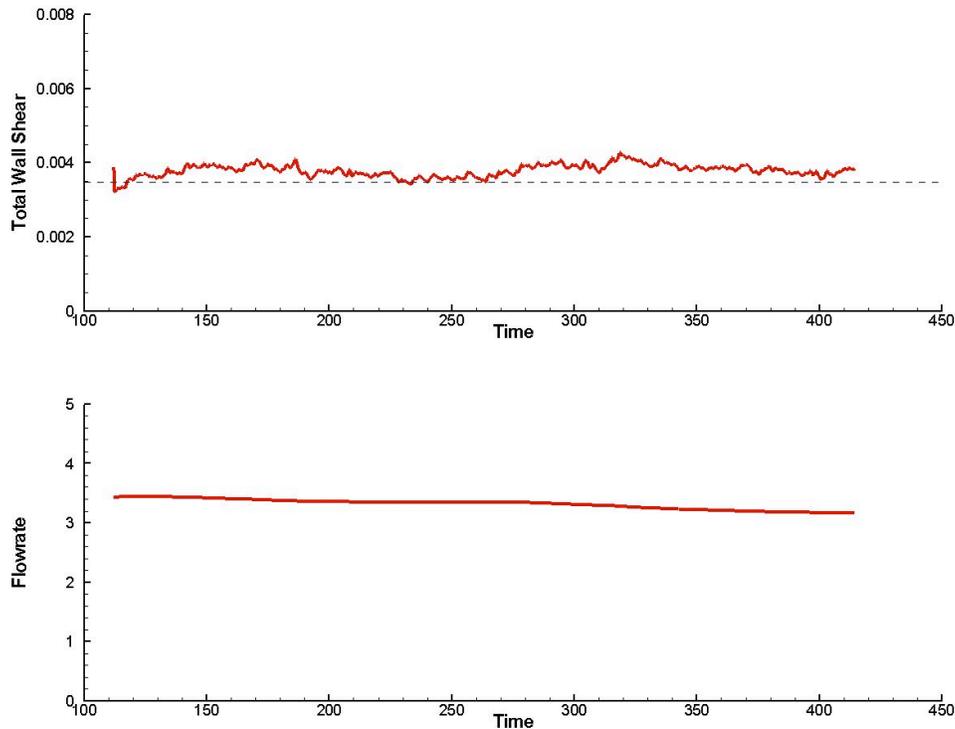


Figure 2 The wall shear (top) and the flow rate (bottom) for the simulation shown in figure 1. Results for both a high and low resolution simulation are shown.

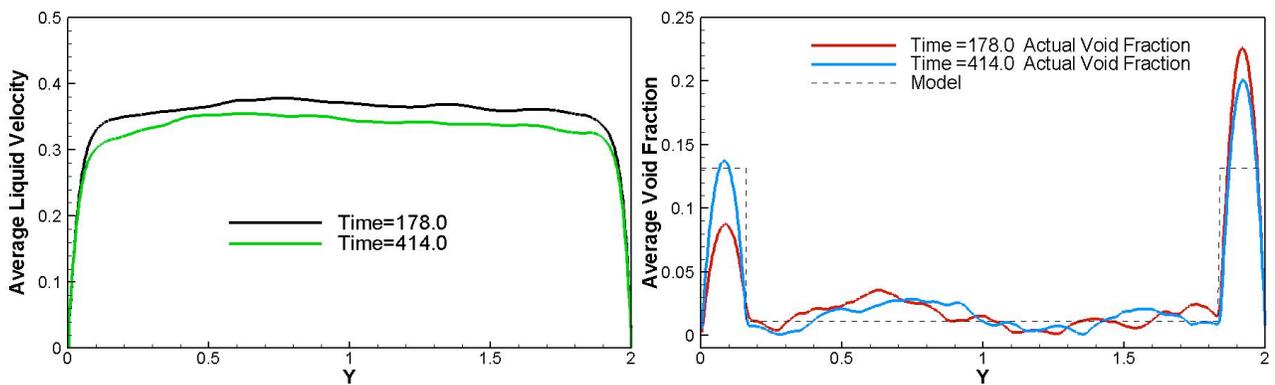


Figure 3 The average velocity (left) and the average void fraction (right) for the simulation shown in figure 1 at times 178 and 414.

the centre of the channel has been reduced sufficiently to bring the mixture in a hydrostatic equilibrium. At that point further lateral motion of the bubbles ceases (on the average). Thus, the void fraction in the centre region is given by equating the weight of the two-phase mixture with the imposed pressure gradient. Since the total void fraction is given by the initial number of bubbles, and any excess bubbles are pushed to the wall, we can compute exactly how many bubbles should be there. In spite of the asymmetry, the average of the values for the left and the right layers are clearly close to what the model predicts. We have gathered a number of other quantities for the flow, but here we only show the average Reynolds stresses in the channel, at the same time. Those

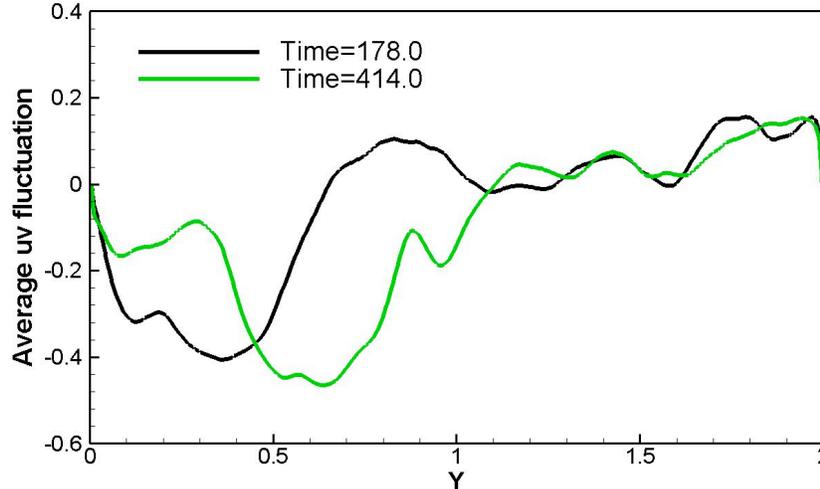


Figure 4 The turbulent Reynolds stresses for the run in figure 1, at times 178 and 414.

are plotted in figure 4, where we see that while the fluctuations in most of the channel are around zero, as we expect for flow in hydrostatic equilibrium, the large bubble causes significant negative values on the left side. We expect to continue this run for a longer time and to examine the statistical properties of the steady state in much more detail. However, it is already clear that, first of all, the bubble distribution in the wall layers tends to be fairly non-uniform, with regions of high bubble concentration accompanied by regions with hardly any bubbles. Secondly, the results indicate that the large bubble has significant impact on the statistical properties of the flow in the middle of the channel. Whether these go away at long enough times remains to be seen.

Most simulations of turbulent bubbly flows use the point particle approximation and thus must model the interaction between the flow and the bubbles, even though the flow may be fully resolved. DNS, where the flow around each bubble is fully resolved, of many bubbles in turbulent channel flows are still relatively rare. In addition to our studies referenced above, references [18,19] contain recent results from other groups.

3. More Complex Flows

As important as simulating the motion of bubbles in turbulent flow is, it is of course only part of most industrial problems. In real flows the different fluid regions undergo topology changes where fluid masses coalesce and break apart and phase change changes the relative amount of each phase. In simulations where the interface is followed by connected marker points the topology change requires additional coding and a model to determine when topology change takes place. When the interface is captured by advecting a marker function directly on the grid, topology change takes place automatically whenever a film or a filament becomes thinner than a grid spacing. While this is very convenient—and often mimics what happens in reality—in other cases the result is a grid dependent coalescence that prevents us from obtaining a fully converged solution. When the interface is tracked by front-tracking, we have considerable more control over when coalescence takes place, but at the cost of a more complex code.

In most DNS of dispersed bubbly flows we simply start with a given bubble distribution. In reality, however, the bubbles must be injected into the flow or be generated in some other way. Often this is by boiling. We have extended the method presented in [3] to boiling flows [20,21] and used it to

examine a number of problems. Those include explosive boiling of a nucleus in an initially superheated liquid [22] and film boiling on a flat plate [23]. For the film boiling we examined, in particular, how large systems, where bubbles broke off from the vapor film at the wall, differed from systems where the bubble growth was forced to take place at the linearly most-unstable wavelength. The main question was whether subharmonic instabilities would lead to competition between waves and the formation of larger bubbles. Such mergers are seen in many other systems, but here we found that such competition was relatively weak. We also examined the effect of the wall superheat on the boiling of a finite depth pool. For low wall superheat (but high enough to prevent wetting and a transition to nucleate boiling) bubbles broke away from the vapor film. At higher superheat the vapor production was sufficiently fast so that long vapor vents formed, sometimes reaching the surface of the pool. At even higher superheat the vents became unsteady, resulting in unsteady churn-like boiling. For moderate superheat where the vapor dynamics was much faster than the total evaporation rate of the pool, the system reached a well-defined steady state, but at high superheat all the liquid quickly evaporated and no steady state emerged.

More recently we have been focusing on nucleate boiling where bubbles are generated from nucleation sites on a wall. In addition to considerable difficulties (mostly unsolved so far) associated with specifying the nucleation site distribution and activation, we need to account for the thin microlayer left behind when the vapor bubble expands. Currently we are assuming that the film is very thin and can be treated using thin film assumptions. In the simplest case we can assume that the temperature of the film surface is the saturation film temperature and that the film evaporates completely in a finite time. Assuming further that the film is short, and quasi-steady in a frame of reference moving with the apparent contact line where the bubble interface contacts the heated wall, we can derive an expression for the volume source that must be accounted for due to the evaporation of the film. While we and others ([24, 25], for example) have simulated the formation of one or more vapour bubbles, such simulations are still in their infancy and we have yet to obtain reliable results that allow us to do examine the dynamics of nucleate boiling to the same degree as we have done for bubbly flows.

4. Conclusion

Direct Numerical Simulations of multiphase flows have come a long way over the last decade and a half. We are now able to simulate relatively efficiently and accurately the evolution of turbulent flows containing hundreds of bubbles for a sufficiently long time so that we can collect meaningful and converged statistics. 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 led 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 [26] remains more or less the state-of-the-art. The need for a more sophisticated approach is, however, well understood and a few authors ([19, 27], for example) have started to examine what such models might look like.

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 contend 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, 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 may be interesting but are off the critical path. 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.

Although 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 [28]. Fully understanding how to include subgrid models of small-scale processes is likely to be particularly important for simulations of nucleate boiling.

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