Topical:
Predictive Capabilities for Multiphase Flows in Extreme Environments

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Broad Background

Humans live where air meets liquid water and multiphase systems are central to human life on Earth. As humans spend more time in space, and settle the Moon and March, they will increasingly have to rely on multiphase systems. On Earth, buoyancy often determines the behavior of such systems, making it challenging to use what we currently know in environments with different or zero gravity. Thus, developing the capabilities to model and design multiphase systems and accurately predict their behavior is a go/no-go mission-critical challenge.

Importance

Phase change is by far the most efficient mechanism to transport heat and thus plays a dominant role in power generation, refrigeration and air conditioning on Earth. Similarly, bubble columns are one of the key equipment for a large variety of chemical processes, essential for both reuse and processing of important materials. Scavenging hydrophobic particles out of a slurry consisting of many different materials by froth flotation is one of the most widely used process to extract minerals and it is increasingly being used for recycling. Flotation is going to be essential for mineral extraction on extra-terrestrial bodies and recycling of materials on long space missions. The relative motion of the phases is a critical part of the operation of such systems and in reduced or zero gravity we are deprived of one of the main mechanics to control the locations of the different phases, or to move bubbles or drops relative to the continuous phase. We will also almost certainly want to make objects in space by 3D printing and must understand how the absence of gravity affects the laying down of polymer filaments.

We are rapidly learning that we can affect the behavior of fluids in multitude of ways. It has been understood for a long time that acoustic forcing can be used to influence bubble motions but we now know that oscillations of incompressible flows can also rearrange bubbles in various ways, depending on the frequency and amplitude. Similarly, temperature gradient can provide the needed driving force and coalescence can produce the needed momentum to move one of the phases, such as when coalescing drops “jump” away from walls. And forced flow will become increasingly important when gravity is not there, or does not play as significant role as on Earth.

State of the Art

Our ability to numerically simulate multiphase flow dynamics has come a long way in the last couple of decades. It is now possible to accurately simulate fairly complex systems containing spatial and temporal scales spanning several orders of magnitude. We can follow the motion of hundreds of bubbles or drops in turbulent flows for a long enough time so that converged statistical information can be collected; simulate the breakup of phase boundaries as in atomization and wave breaking; reproduce homogeneous, film and nucleate boiling in both initially quiescent and forced flow; follow the thermocapillary motion of bubbles and drops; study electrohydrodynamic effects on bubble and drop suspensions; compute the solidification of materials and how flow effects the growth of microstructure; study cavitation involving many interacting bubbles; reproduce non-Newtonian flow and solidification of polymer filaments in 3D printing; simulate mass transfer and reactions in bubble columns, and in general compute the dynamics of many complex multiphase problems.

Numerical simulations are possible for large systems and the size increases every year. Yet, a fully resolved simulation requires resolution of all relevant scales and in natural systems the range of scales, even staying within the continuum assumption, can be very large. For such systems, we need coarse grained or reduced order models. While such models can be validated against fully resolved simulations, experiments are sometimes needed because the scale range is too large. Furthermore, since the goal of models is to predict the behavior of physical systems, validations against experiments are often required to establish trust in their predictions. We often also come up against situations where "almost" all of the flow is easily resolved, but thin films, filaments or droplets, or thin mass boundary layer in high Schmidt number flows or thin reaction zones, require much finer local resolution. While adaptive grid refinement is possible, the increase in number of grid points often make that strategy impractical and other multiscale strategies, such as using embedded models, are needed.

Advances in numerical modeling are making experiments more important than ever. Numerical simulations can only reproduce the physics that is prescribed as equations or parameters and to uncover new physics or determine specific material parameters, we must do experiments. We now understand however that modeling and experiments must be tightly integrated to make any advances and any experimental campaign must be designed to provide input to models or to directly validate predetermined modeling issues. Experiments without a clear connection to modeling often results in information that are not very relevant, either because they do not address open modeling questions or do not provide all the necessary boundary and initial conditions. Experiments without modeling connections only provide results for a given situation, rather than improving our general predictive capabilities.

Near Term Needs

We have come a long way in the development of numerical strategies to predict the behavior of multiphase flows, but more is needed. Some of the more immediat tasks are:

- Coarse grained models for large scale systems. Such models already exist for disperse flows of drops, bubbles and solid particles, where point particle approximations have been combined with large eddy simulations (or rather LES-like approaches since the range of unresolved scales is often larger than in "true" LES), but little is available for more complex high volume fraction flows, particularly with complex physics.

- Increasingly we are seeing the applications of various "data" strategies for the development of coarse models. Finding ways to integrate what we already know (conservation laws, symmetries, scaling laws) and data driven approaches is already starting to take place but much more needs to be done, particularly for complex systems.

- Development of embedded multiscale strategies to handle processes taking place on small spatial scales such a thermal and mass boundary layers and thin films and small bubbles and drops.

- Development of software infrastructure that integrates the most advanced methods currently available into easily usable software suitable for complex geometries, and integrate such approaches with system level modeling software.

- Experimental studies to develop new physical models. Those include nucleation site densities and activation for boiling for a range of surfaces, material models for a range of surfactants, accurate criteria for film rupture and coalescence (particularly in the presence of surfactants), contact line dynamics (again, particularly when surfactants are present), non-Newtonian (including viscoelastic) material models, and a variety of input for models of biological fluids and solids.

- Experimental studies for system level verification of numerical models and confidence building. Nobody is going to trust numerical predictions unless they have been shown to work!

Slightly Longer Term Developments

The ultimate goal should be to have a complete model of any system that humans have built or intend to build. Such a "digital twin" allows us to design new systems, control existing systems, and diagnose systems that fail. While the short term needs described above are essential, much more is needed, including:

- Mathematical/numerical models serve many purposes and, in particular, describe processes at many different temporal and spatial scales. Our understanding of how to transition between scales and how predictivity depends on scale is currently rather rudimentary and a theoretical framework that is able to guide model selection would be most useful.

- The fundamental premise behind detailed studies is that we learn something that we can use. Often this takes the form of a correlation, a "lumped" model, or a closure model. However, it seems that our increasing ability to work with data should open up new possibilities to automatically recognize what we already know and integrate previously established knowledge into our predictions, making them both faster and more accurate.

- Increasingly experimentalists are using theory to extract complete description of flow fields from their measurements and observation, such as pressure from velocity measurements and velocity from path lines. Eventually we can imagine constructing the complete field from just a few observations. In controlled experiments we attempt to limit the variables we need to measure and the more data we extract, the less we need to control and in the limit we can imagine building mathematical models from observations of natural occurring processes rather than controlled experiments.

- The human species evolved in normal gravity and for us one direction is up and the opposite one is down. Our physiology expects this. The human body is an exceedingly complex multiphase system and while modeling of its various parts, such as the cardiovascular system, has progressed enormously in the last few decades, modeling of others, such as the digestive system, are in their infancy. An integrated human "digital twin," which is likely to rely heavily on strategies developed for "simpler" multiphase flows, is likely to be critical to assess how different individuals thrive in the new and extreme environments we are moving into.

- As we move into extreme environments where gravity plays a different role than on Earth, we are likely to have to learn to manage multiphase flows in different ways. While posing significant challenges, this also opens up opportunities. We can, for example, imagine processing chemicals in freely flying fluids blobs and making things by “sculpting” suspended material blobs. Fundamental and explorative studies of those and many other processes need to take place to both explore what is possible and to “seed” new ideas.

The focus here is on multiphase systems. However, a complete digital twin of a complete system obviously consists of other components and processes, including structures, electrical systems, computers, radiation and other environmental effects, and more. Integrating everything into a reliable model whose domain of validity and accuracy is known is obviously essential.

Discussion

Computational modeling in general, and modeling of multiphase thermal-fluid systems in particular, is at a cross road. We have become very proficient in modeling those systems that we have been focusing on for several decades, such as disperse flows of bubbles and drops, and progress has opened up new opportunities. The most obvious one is more complex systems. However, not only do many complex flows contain a very large range of scales due to either competing physical processes or topology changes, calling for novel multiscale approaches, but often the physics is much less well understood. This calls for new and integrated experiments. The other opportunity is to use our current results to increase our ability to predict. The most straightforward version of a predictive capability is closure models for coarse simulation where some scales are computed and others are parameterized in some way. However, the availability of large amount of data either from simulations or sensors, very large computers, and new tools to extract information from data are making new strategies possible. The simplest way to use data to make predictions is simply to interpolate the data. If we find a situation that looks exactly like our current situation then it is likely to evolve in the same way as the match did. But in many, if not most, cases we know the physical laws that determine (or constrain) the evolution and using that understanding is likely to greatly enhance the range of validity of our models. The value of a fully data-driven model is that it offers new ways to think about predictions but in practice an integrated approach is likely to be more useful. Finding how theory and data can be utilized in the optimal way, and how that depends of the scales we are trying to predict and how accurate our predictions needs to be is likely to be a major area of focus for computational scientists and engineers in next decade or two.

Summary

I have discussed briefly what is needed to further advance predictive capabilities for multiphase flows for reduced gravity, separating what I see as immediate needs from what has a little longer horizon. Given the rapid progress in computational modeling, the longer term developments are probably not that far off. However, we can expect it to follow a path that is different than in the past and involve a multitude of new strategies and novel ideas.

References

I have intentionally not included any references here. Many of the specific processes that I mention refer to systems that my collaborators and I have modeled and the relevant papers can be found on my Google page, for example.