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GEORGE YADIGAROGLU*

Application of cascades of CFD methods to two-phase flow problems

Swiss Federal Institute of Technology-Zurich (ETHZ), Nuclear Eng. Laboratory, ETH-Zentrum, CLT, CH-8044 Zurich, Switzerland

Abstract

Although traditionally two-phase flow problems have been treated with the interpenetrating media (two-fluid) approach, certain situations require application of new techniques, including interface tracking methods such as Volume of Fluid (VOF); methods considering the effects of turbulence on the dispersed phase (with classical Reynolds-averaged type turbulent flow models or Large Eddy Simulation, LES); etc. Often such methods need to be applied in a sequential or "cascade" form to achieve final resolution and closure of the problem. The condensation of large bubbles injected in a pool and bubble plumes are considered as case studies.

Keywords: Two-phase CFD; Large bubbles; Bubble plumes; Condensation; VOF; LES

1 Introduction

Computational fluid dynamics (CFD) methods are being applied with increasing success to a variety of problems. The flows of industrial interest are most of the time turbulent. For turbulent single-phase (gas or liquid) flows, solutions of the well established governing "exact" Navier-Stokes equations can be obtained with sufficient temporal and spatial resolution only in some very simple cases (we speak in this case of Direct Numerical Simulation, DNS). For practical applications, the equations are written in various simplified, averaged or "modelled-turbulence" forms and solved in a relatively coarse mesh using a variety of numerical techniques. Although several research groups or industries have developed their own specialised tools and solvers for this purpose, today

*E-mail address: yadi@ethz.ch

there are also a few general-purpose codes that are commercially available and used worldwide.

In the past, two- or multiphase flows have been treated most of the time in one dimension, ignoring the effects of turbulence, and resorting to a number of specialised or simplified approaches: for example, *ad hoc* two-phase models take into account the topological distribution of phases – the flow regime – and describe the interactions between the phases accordingly. The interpenetrating media approach has been used to describe the interactions between the phases assuming that these (as the name implies) co-exist with a certain probability – the phase fraction – at every point. The interpenetrating media approach and the resulting "two-fluid" or "six equation" model of two-phase flow has been successfully applied to a variety of nuclear safety and design problems, as well as in other industries such as the chemical industry, the transport of hydrocarbons in pipelines, etc. In the nuclear as well as the oil and gas industries, large "system" codes based on the two-fluid model are used to predict complex flow motion transients in large systems, e.g., accidents in water-cooled reactors or transients in pipelines. Although tremendous developments and successes have been achieved with such system codes, there are clearly cases beyond their reach; new, alternative approaches are needed then.

CFD-based approaches to multi-phase flow problems and applications are relatively very recent. The development of such approaches for multiphase flows is one of the challenges facing CFD. The author and his collaborators have been motivated by the need to better understand a family of safety problems that appear in proposed advanced, passive Light Water Reactor designs to tackle a number of such techniques and explore their applicability. This paper reviews some of the experiences made and results obtained.

Avenues alternative to the ones discussed here are investigated presently in a number of European projects. For example, the 5^{th} Framework Programme project EUROFASTNET related to the French FASTNET initiative [1] will provide a general survey of improved analytical tools and development of new codes, and the ASTAR project will contribute to the development of new 3D two-phase tools [2].

Addressing the problems at a multiplicity of scales

Some times one attempts to fully understand a situation by considering a "cascade" of problems at various scales with a corresponding panoply of tools. For the nuclear systems, that motivated this work, the behaviour of the entire system is typically obtained using a system code based on the two-fluid approach and operating at scales comparable to the dimensions of the system. Local phenomena, or the behaviour of parts of the system, may need then to be addressed at the meso-scale level, with tools considering smaller scales. Finally one may need to obtain wall and interfacial momentum, heat and mass transfer laws by performing studies at the smallest possible scale via DNS; such level of spatial resolution is indeed needed to resolve the gradients determining transfers at the interfaces; an example of such an approach will be given below.

Pushing the computations and the scales considered to the infinitesimal level, Molecular Dynamics is the ultimate tool if one tries to understand phase change phenomena. We will only mention here the possibility of investigating phenomena such as the vaporisation of an ultra-thin liquid layer on a hot metallic surface by molecular dynamics simulations [3]. In this case, the forces acting between all combinations of pairs of wall and fluid molecules are modelled and the evolution of the system is simulated numerically; the results show resemblance to our knowledge of the vaporisation of a similar macroscopic system.

2 Beyond the capabilities of the classical multi-field models: "multiphase CFD"

Two case studies are briefly described below; they were both motivated by the need to understand certain phenomena taking place in passive Boiling Water Reactor (BWR) containments. In the first case, we consider the condensation of large bubbles injected into a pool of water from a large vent. The second case deals with steam/air mixture injections from an immersed sparger; small-bubble plumes are created in this case.

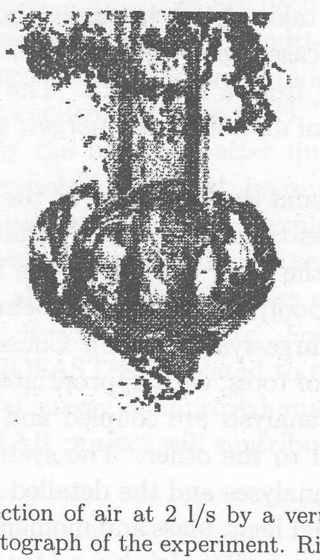
In both cases, it is necessary to understand the behaviour at the microscopic interfacial scale (momentum, heat and mass transfer at the interface), the local (or mesoscale) level (predict the shape of the large bubbles or the behaviour of the bubble plume, including mixing of the pool), and finally the behaviour of the entire containment system (the integral or large-system scale). Consequently, the analysis must be conducted with a variety of tools, each appropriate to a certain scale or level. Clearly, the three levels of analysis are coupled and information must be fed back and forth from one level to the other. The system code will provide boundary conditions for the local analyses and the detailed microscopic-level investigations will provide the interfacial heat, mass and momentum transfer laws needed to close the problem at the intermediate level.

3 Tracking of interfaces

The two-fluid or, more generally, the multi-field approach is based on an interpenetrating media formulation: all phases are present everywhere in the domain with a certain volume fraction (or probability of appearance) and the interfaces are not specifically located or their shape computed. Problems where the development of large-scale interfaces is important are not well treated, or cannot be treated at all by this method. Tracking of the interfaces separating the phases by Lagrangian markers, by the Volume-of-Fluid (VOF) [4], or Level Sets [5] Methods, or by Embedded Interface Methods (e.g., [6]) is needed. The description of these methods is beyond the scope of this paper; a recent review can be found in [7]. In essence, the interface tracking methods provide means for following the development of the interfaces separating the phases and computing the flows on both sides of the interface.

Condensation of large bubbles in a pool of water

The formation of large bubbles at the exit of a vertical, downwards-pointing vent injecting a mixture of steam and non-condensables (say air) into a water pool is the problem considered here. The evolution, condensation and break-up of the air/steam volumes (large bubbles) are to be investigated; in particular to find out whether the bubbles could emerge not-fully condensed from a relatively shallow vent immersion depth.



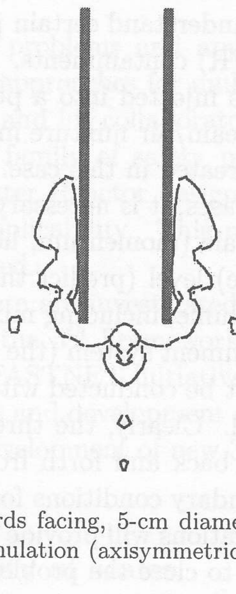


Figure 1. Injection of air at 2 l/s by a vertical downwards facing, 5-cm diameter vent. Left: photograph of the experiment. Right: VOF simulation (axisymmetric) [8].

Meier et al. [8] produced VOF simulations for the injection of air bubbles into water; these mimicked well experimental findings (Fig. 1). In particular, the characteristic frequency of appearance of bubbles at the exit of the vent could be reproduced, as well as the shape of these bubbles and their way of break-up. Meier could not compute the behaviour of bubbles containing also steam for lack of a condensation heat and mass transfer law. The ultimate goal, namely to capture the geometry of the interfaces and to resolve sufficiently well the region near the interface, so that heat and mass transfer could be computed is much more elusive. Indeed, there are difficulties inherent to the physics of the problem itself: for Prandtl and Schmidt numbers typical of this application, the thickness of the regions over which the vapour concentration and temperature gradients are significant is a fraction of a millimetre [9] and resolution of the corresponding boundary layers is not possible at the scale at which the VOF simulations are performed. Other ways must be found for determining the interfacial exchange laws and incorporating them into the VOF simulation.

Measurements of the rate of condensation at the surface of large bubbles are quasi-impossible. In the absence of experimental information, the last resort is to rely on DNS of the flow, including the effects of turbulence, to elucidate the fundamental laws of condensation. As a first step in this direction, DNS computations can be performed in an idealised configuration, in which steam or a steam/air mixture flows over a liquid surface. First, one has to compute and describe the flow and turbulence structure in the thin diffusive layers on either side of the interface; then to arrive via the collected information at a correct parameterisation of turbulence in terms of, for example, a turbulence length scale; the ultimate finding should be the interfacial exchange laws. These final steps are underway as a doctoral dissertation at ETH [10]: a DNS of counter-current air/steam-water flow with a free deformable interface will provide guidance for modelling heat and mass exchanges at the interface of the large condensing bubble.

This example illustrates well what we have referred to as a "cascade" of methods. To deal with the venting of the steam/air mixtures, we had to address the problem at various scales with a variety of tools: system behaviour (in the example cited here, the flow rate and the composition of the mixture entering the vent) with a system code; large bubble behaviour with VOF; finally, the direct-contact condensation heat transfer law via DNS.

4 Bubble plumes

The motivation for the second case study presented here was the need to develop a better understanding of the behaviour of bubble plumes in liquid pools. Bubble-induced mixing in liquid pools occurs in a number of situations of interest in energy technology, process engineering, etc., as well as in BWR containment pools, where such plumes are created by injection of gases from spargers. In this case, as the bubbles are relatively small and there is no need to consider each one individually, an interpenetrating media (two-fluid) approach is possible and in practice the only feasible one. Instead of locating the exact position of each bubble and its interface, one is satisfied with computing the distribution of void fraction in the pool, in addition to the average flow fields of the two phases. It would have been prohibitively expensive to track the interfaces of a large number of bubbles (although this has been done in simpler situations [6]).

Using the interpenetrating media formalism, separate conservation equations are written for each phase. The interfacial exchange laws (the average effect of the forces acting on the bubbles) are obtained from known descriptions of these forces in idealised configurations; the bubbles are most often considered as spherical objects. It is imperative to include in this case the effects of turbulence in the two-fluid model since turbulence plays a key role as a phase distribution mechanism for such bubbly plumes. The classical $k-\varepsilon$ model has been used for this purpose by a number of authors. The approach has been tested in a limited number of cases with some success [11,12] but considerable development effort is still required for reliable two-phase simulations. This is because the correlations for interfacial transfer of mass, momentum and energy are not yet fully established, and, most important, turbulence models usable under two-phase flow conditions are needed. For bubbly flows, the turbulence in the liquid has been until now modelled as the superposition of a conventional liquid shear-induced turbulence term and an additional, new term describing the effect of the bubbles on liquid-phase turbulence. A high degree of empiricism remains in such turbulence models and the success of the method most often relies on some tuning of the coefficients of the turbulence models and/or of the interfacial exchange laws.

For a non-condensable gas plume in a liquid pool, turbulence in the gas phase is not important, and a turbulence model is only required for the liquid phase. Detailed description of the governing equations, and of the forces involved can be found in [13] and [14]. The forces acting on the bubbles include buoyancy, drag, lift, and virtual mass. In addition, some kind of turbulent dispersion force is needed to account for the randomness in bubble motion due to the turbulent eddies; for this purpose, the concept of a turbulent dispersion force has been advanced, [15,16]. An alternative option is to add diffusion terms to the continuity equations; see [13] for a discussion of these issues. A new approach was adopted in the work of Smith and Milelli [14], in which it is possible to dispense with artificial turbulent dispersion models by incorporating the effects of the random turbulent fluctuations in the liquid directly into the drag force term. The starting point for the resulting Random Dispersion Model (RDM) was to assume that the instantaneous liquid velocity dragging a bubble is composed of a mean and a fluctuating part; the latter is simulated in a mechanistic way to mimic to effect of eddies [14]. Although the method was fairly successful in describing the behaviour of bubble plumes, it was felt that limitations inherent to the use of the $k-\varepsilon$ model should be overcome by taking a more fundamental approach.

The next logical step was to attempt to resolve the effects of (large enough) eddies on the motion of the bubbles; the Large-Eddy Simulation (LES) technique is the natural candidate. A review of the background theory based on the "filtered multifield equations" can be found in [17]. In LES, all large-scale structures that can be resolved by the numerical method are separated from the small-scale structures (sub-grid scales or SGS) that cannot be captured on a given grid; the small-scale structures are modelled assuming homogeneity and isotropy. The main advantage of LES for modelling bubble plumes is that it inherently captures the interactions of the bubbles with the resolved large-scale structures, all the way down to scales approximately equal to the size of the computational mesh. The interaction with the sub-grid scales can be approximated by a sub-grid model. In other words, the turbulent dispersion of the bubbles is mainly due to the largest structures, which are calculated directly with LES.

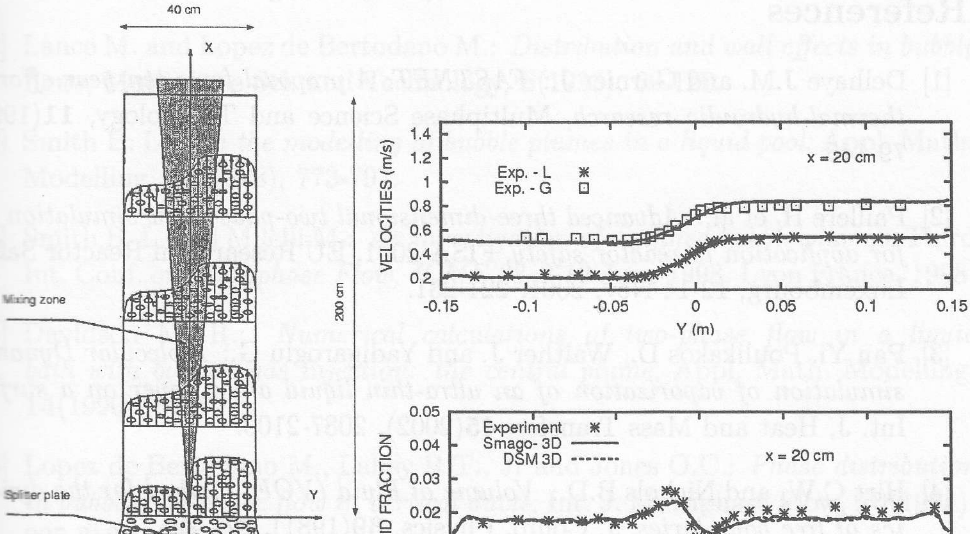


Figure 2. LES predictions [18] (right) of the void fraction and average velocity distribution measurements (at $x = 20$ cm from the bottom) from a bubbly flow experiment by Roich et al. [19] (left).

Since this is a new area of study, many open questions need to be addressed: two-phase sub-grid models do not exist, and the influence of the grid on the simulation also requires investigation, since the grid determines the turbulence scales that are going to be resolved. To pursue this approach, a LES model was implemented in the CFD code CFX-4 [18]. Test cases have been used to study the modifications induced by the bubbles on turbulence, and the effect of the filter (mesh size). LES seems to be a promising approach for describing bubble plumes. A recent result is illustrated in Fig. 2.

5 Conclusion

As noted above, multiphase CFD methods are still at an early development phase. A number of applications have appeared but lots of work remains to be done.

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