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The emptying of a bottle as a test case for assessing interfacial momentum exchange models for Euler–Euler simulations of multi-scale gas-liquid flows

Samuel Mer[a,*], Olivier Praud[a], Herve Neau[a], Nicolas Merigoux[b], Jacques Magnaudet[a], Veronique Roig[a]

[a] Institut de Mécanique des Fluides de Toulouse, IMFT, Université de Toulouse - CNRS, Toulouse, France
[b] Electricité de France R&D, 6 quai Wattier, Chatou 78401, France

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ABSTRACT

Simulating gas-liquid flows involving a wide range of spatial and temporal scales and multiple topological changes remains a major challenge nowadays, as the computational cost associated with direct numerical simulation still makes this approach unaffordable. A common alternative is the two-fluid Euler–Euler formulation that avoids solving all scales at the price of semi-empirical closures of mass, momentum and energy exchanges between the two fluids. Many of such closures are available but their performances in complex flows are still in debate. Closures considering separately large gas structures and smaller bubbles and making these two populations evolve and possibly exchange mass according to their interactions with the surrounding liquid have recently been proposed. In order to assess the validity of some of these closures, we carry out an original experiment in a simple configuration exhibiting a rich succession of hydrodynamic events, namely the emptying of a water bottle. We simulate this experiment with the NEPTUNE_CFD code, using three different closure approaches aimed at modelling interfacial momentum exchanges with various degrees of complexity. Based on experimental results, we perform a detailed analysis of global and local flow characteristics predicted by each approach to unveil its potentialities and shortcomings. Although all of them are found to predict correctly the overall features of the emptying process, striking differences are observed regarding the distribution of the dispersed phase and its consequences in terms of liquid entrainment.

1. Introduction

Gas-liquid flows involving a broad range of bubble sizes are ubiquitous in geophysical and engineering configurations and applications, such as magmatic chimneys, submarine explosions, bubble columns or nuclear safety, to mention just a few. In such situations, the gas phase frequently involves a wide range of spatial and temporal scales, from large gas pockets to small dispersed bubbles. Moreover, dramatically different flow regimes may be encountered, characterized by distinct interaction mechanisms between the gas phase and the carrying liquid. Simulating such flows remains a major challenge nowadays, although massive efforts have been devoted during the last two decades to develop modelling strategies aimed at computing multiphase flows (Prosperetti and Tryggvason, 2007).

These strategies differ according to the level of accuracy they target and the computational resources they require. A first class of numerical techniques based on Direct Numerical Simulation (DNS) of the Navier–Stokes equations shares the same main challenge consisting in precisely localizing interfaces in the flow domain and imposing the proper jump conditions across them. Three main approaches have been proposed to track interfaces, namely the Volume Of Fluid (Hirt and Nichols, 1981), Level Set (Osher and Sethian, 1988) and Front Tracking (Unverdi and Tryggvason, 1992) methods (see also Scardovelli and Zaleski, 1999; Sethian and Smereka, 2003; Tryggvason et al., 2001 for reviews). Since then, these techniques have become mature and are now widely used to get insight into detailed mechanisms governing flow configurations with increasing complexity. For bubbly flows, this may range from those involving a single bubble rising at large Reynolds number (Cano-Lozano et al., 2016) to dispersed bubbly flows with up to $\mathcal{O}(10^3)$ bubbles moving at moderate Reynolds number (Bunner and Tryggvason, 2002).

* Corresponding author.
E-mail addresses: samuel.mer@imft.fr, magnau@imft.fr (S. Mer).

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Despite the potentialities offered by these DNS approaches and their improvements associated with local grid refinement techniques (Popinet, 2009), their computational cost still makes them unable to simulate complex configurations, especially those involving multiple coalescence and break-up sequences. Such complex two-phase flows are usually computed using the much cruder Euler–Euler approach based on the so-called two-fluid model (Ishii, 1975; Ishii and Hibiki, 2006). In this framework, the governing equations are obtained after volume-averaging (or more formally ensemble-averaging) the local budgets, so that unknown terms occur at interfaces. As in any averaging scheme, closures are required to express these terms with respect to the primitive variables and their gradients. The accuracy of the simulations then depends tremendously on the validity of these closures. Many of them have been proposed for each flow configuration, e.g. separated flows, dispersed bubbly or particulate flows, etc. (see Drew and Passman, 1999 and Balachandar and Eaton, 2010 for reviews). In bubbly flows for instance, assuming non-deformable and mono-disperse bubbles, momentum interfacial exchange is usually modelled by considering drag, added-mass and shear-induced lift forces acting on individual bubbles, supplemented with turbulent diffusiophoresis and lubrification effects when the carrying flow is turbulent and walls are present, respectively. Applications of the two-fluid approach to such flows, possibly with phase change, may be found for instance in Mimouni et al. (2010, 2011a, 2011b). Similarly, specific closures with various degrees of sophistication have been developed to simulate 'slug' flow configurations (Issa and Kempf, 2003; Issa et al., 2006) and separated nearly-horizontal flows (Vallée et al., 2008).

The key limitation of the above closures is that they are specific to the configuration for which they were calibrated and are unable to properly model the interfacial exchange mechanisms at work in another type of flow. This limitation can only be overcome if the modelling approach is made able to recognize which configuration is present at a given position in space and time. Two main streams of approaches were developed during the last two decades to reach this goal. The first of them consists in switching locally from DNS (based on either the Volume Of Fluid or the Level Set approach) to the two-fluid formulation wherever interfaces exhibit a characteristic size of the order of the grid cell (Černe et al., 2001; Tomiyama et al., 2006; Yan and Che, 2010). This technique was successfully employed to compute several gas-liquid flows dominated by fragmentation, e.g. a two-phase vortex or the unstable Rayleigh-Taylor configuration. The second approach consists in extending the two-fluid model to an arbitrary number of 'fields' or 'phases', each of them corresponding to a specific flow configuration or class of two-phase entities (e.g. small bubbles, large bubbles, slugs, etc). Occurrence of each of these configurations at a given time and position has to be identified in order to evaluate the corresponding volume fraction. As each 'phase' has its own velocity field, momentum closures have to be formulated to properly account for the interaction between two of them. This approach has for instance been applied to the upward bubbly pipe flow with several widely distinct bubble sizes and possible mass exchange between them, due to phase change (Krepper et al., 2008).

Although the above methodology was initially designed to deal with dispersed flows, it may be applied to separated flows as well, provided one is able to (*i*) properly define a criterion allowing the occurrence of the 'separated' configuration to be detected, and (*ii*) derive realistic closure laws for the various separated flow regimes according to the interface roughness. This is the essence of the Large Interface Model (LIM) designed by Henriques (2006) and Coste (2013), as well as that of the Algebraic Interfacial Area Density (AIAD) model promoted by Höhne and Vallée (2010) and Deendarlianto et al. (2011). Mixed configurations in which separated and dispersed regions coexist within the flow may also be tackled within the framework of the *n*-field approach, provided the above criterion allows 'Large Interfaces' (hereinafter abbreviated as LI) corresponding to the separated configuration to be disentangled from small-scale interfaces, and distinct closure laws are employed for the dispersed and separated regions. This idea yielded several different modelling approaches, such as the Generalized Two-Phase Flow model (GENTOP, Hansch et al., 2012) or the Generalized Large Interface Model (GLIM, Merigoux et al., 2016). Examples of application of this type of approach to a gas jet impinging a free surface and a bubble column with bubbles bursting at the free surface may be found in the first reference.

Still in the context of the two-fluid and *n*-field formulations, several attempts were recently carried out to achieve a more realistic and accurate treatment of LI by taking explicitly into account surface tension effects (Bartosiewicz et al., 2008; Štrubelj et al., 2009; Gada et al., 2017). A technical difficulty arises in this type of approach, due to the natural tendency for numerical diffusion to spread stiff volume fraction gradients. Sharpening techniques have been proposed to counteract this effect and maintain well-defined separated 'phases', so that the LI may remain properly defined over time. A cutoff length must also be defined, so that interfaces with a characteristic size smaller than this critical length are no longer resolved and interactions between the corresponding dispersed phase and the continuous one are entirely modelled with the help of empirical closure laws. Last, an exchange procedure combining numerical requirements and basic physical principles has to be designed to allow a LI to break up into smaller bubbles, and such bubbles to coalesce and generate a LI. Such an approach has been implemented both in the aforementioned GENTOP formulation (Montoya et al., 2015), and in the NEPTUNE_CFD code where it is termed the Large Bubble Model (LBM, Denèfle et al., 2015; Mimouni et al., 2017). Preliminary assessment of this approach in canonical configurations, such as the Kelvin–Helmholtz and Rayleigh–Taylor instabilities, was reported by Fleau et al. (2015, 2016).

The aim of the present paper is to assess the validity of the above LIM, GLIM and LBM approaches implemented in the NEPTUNE_CFD software, by considering an academic but already significantly complex flow configuration and performing a one-to-one comparison between original experiments carried out in that flow and computations making use of the above three models. The selected two-phase configuration, namely the emptying of a water bottle, is especially relevant for checking such modelling approaches, as it exhibits a wide range of temporal and spatial scales. Large air bubbles with diameters of the order of the bottle neck are periodically generated and rise within the bottle until they burst at the free surface below the top of the bottle. While ascending, these large bubbles undergo successive break-up events, yielding swarms of smaller bubbles, part of which may coalesce again and participate into the regeneration and reconfiguration of the large bubble population.

Few computational studies have been performed so far on this flow configuration. The most noticeable is that of Geiger et al. (2012) who simulated it with the help of the OpenFoam software in the framework of a Volume Of Fluid approach. They mainly focused on the influence of geometrical parameters and bottle inclination on the emptying time. However they assumed the liquid and air phases to be both isothermal and incompressible. As we shall see later, the latter assumption is highly questionable.

The present paper is organized as follows. Section 2 introduces the multi-field formulation and details the various approaches employed to model interfacial momentum exchanges in the NEPTUNE_CFD code. The experimental and computational configurations are described in Section 3. Section 4 discusses typical results obtained through both approaches on some quantities characteriz-