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A diffuse interface model with immiscibility preservation

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ABSTRACT

A new, simple, and computationally efficient interface capturing scheme based on a diffuse interface approach is presented for simulation of compressible multiphase flows. Multi-fluid interfaces are represented using field variables (interface functions) with associated transport equations that are augmented, with respect to an established formulation, to enforce a selected interface thickness. The resulting interface region can be set just thick enough to be resolved by the underlying mesh and numerical method, yet thin enough to provide an efficient model for dynamics of well-resolved scales. A key advance in the present method is that the interface regularization is asymptotically compatible with the thermodynamic mixture laws of the mixture model upon which it is constructed. It incorporates first-order pressure and velocity non-equilibrium effects while preserving interface conditions for equilibrium flows, even within the thin diffused mixture region. We first quantify the improved convergence of this formulation in some widely used one-dimensional configurations, then show that it enables fundamentally better simulations of bubble dynamics. Demonstrations include both a spherical-bubble collapse, which is shown to maintain excellent symmetry despite the Cartesian mesh, and a jetting bubble collapse adjacent a wall. Comparisons show that without the new formulation the jet is suppressed by numerical diffusion leading to qualitatively incorrect results.

1. Introduction

Aspherical-bubble dynamics has been studied extensively using boundary integral numerical method [1–9]. Since this formulation is for incompressible fluids, it must therefore be supplemented, when feasible, with additional models whenever compressibility effects are important. For example, in violent collapses, artificial energy extraction is needed to account for the substantial energy lost to acoustic emission [9]. In bubble-cluster collapse, it is known that these same pressure pulses affect the dynamics of nearby bubbles [10,11]. This limitation motivates the development of methods that explicitly include compressibility. Unfortunately, it is often difficult for compressible flow formulations to ensure that the interface between the liquid and the gas remains realistically sharp, especially given the dissipation inherent in shock-capturing schemes. A challenge in any multiphase compressible numerical method is the simultaneous and faithful representation of both shocks and interfaces.

One class of compressible multiphase flow approaches is Lagrangian, which includes arbitrary Lagrangian–Eulerian [12], free-Lagrange [13,14], and front tracking methods [15–18]. These maintain sharp interfaces via explicit representation, but they introduce geometric complexity for large deformations and topological changes. A level-set [19,20] based Eulerian approach coupled with the ghost fluid technique mitigates topological difficulties [21,22]. However, the method requires special

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thermodynamic management at the interface for flows with high density or pressure ratios [23–31]. Another way to cope with the geometric challenges of Lagrangian tracking is to allow the interface to artificially diffuse into thin zones where multiple fluids overlap, forming in effect a mixture region. Multiphase flow theory is invoked to define thermodynamic variables in these mixture zones [32–42]. To be consistent with the nominally discontinuous interface of an actual immiscible fluid, these zones should be thinner than the features of the flow. In the well-known "single-fluid" model, this description is implemented by augmenting the Euler equations with equations that describe the evolution of smooth functions that mark different fluids [43–49].

There are two main challenges specific to the diffuse interface approach: (1) obtaining consistent thermodynamic laws for the mixture, and (2) preventing artificial spatial distortions of the interface functions. These two challenges are coupled as we demonstrate for the bubble collapse configuration in Section 2. The second of these challenges is the more obvious. Without correction, distortions make the interface either too sharp to be represented on the mesh or so diffuse that it is no longer thin relative to other relevant flow features. Furthermore, it is also widely recognized that inconsistent interface thermodynamics can lead to mechanical incompatibilities. Mixture models obtained by asymptotic reduction of the Baer–Nunziato non-equilibrium multiphase model [32,33] under stiff mechanical relaxation [38,40,41] provide transport of interface functions consistent with first-order pressure and velocity non-equilibrium effects. Incorporation of first-order non-equilibrium effects constitutes a significant improvement, but the interfaces can still become so diffused and distorted without proper numerical regularization that key flow features can be completely lost. We will show in Section 2 and Section 5 that this level of thermodynamic consistency alone is insufficient, particularly when strain smears the interface, as for a near-wall bubble collapse. Such distortions can be countered with specially designed terms in the governing equations that cause the interface function transition to span an approximately constant-thickness zone, as proposed recently by Shukla et al. [50] for compressible flows. Unfortunately, these source terms are not necessarily compatible with the thermodynamic mixture models in the interface zone, which can lead to accumulation of errors in space and time, even far from the interface. So et al. [51] have recently developed an anti-diffusive method to address this problem. This technique, however, is intimately tied to the underlying numerical scheme and it is therefore difficult to generalize to different discretizations, such as an increase in the order of accuracy. There is also the risk that anti-diffusive fluxes can over-sharpen the interface in flow regions already drawn thin by the resolved strain field (discussed in Section 3 and Section 5.4). Alternatively, Kokh and Lagoutière [52] have shown encouraging results with an anti-diffusive Lagrange-Remap scheme that controls numerical diffusion via limited downwind fluxes in the remap stage. The method, however, requires additional steps to compute, and remap from, Lagrangian variables, and its extension to more general interfacial mixture laws has not been explored yet.

In this paper, we present a new mixture-consistent interface regularization approach that addresses the limitations identified in the previous discussion. It maintains the integrity of the thin interface between immiscible fluids with a sharpening term, but this term is now crafted in such a way that it remains consistent with the first-order non-equilibrium mixture model. This regularization operator is incorporated into the continuum model, making the overall model independent of the numerical scheme employed. For example, it is easily demonstrated on a standard shock-tube problem in one dimension, and is also directly compatible with a multi-resolution Adaptive Mesh Refinement (AMR) implementation and a fifth-order WENO scheme we use to demonstrate its properties for three-dimensional bubble collapse.

2. Motivation: mixture-zone models and discretization

Faced with the limited availability of exact solutions that can be used for comparison and analysis of our method, we frame our initial discussion on a free-space spherical-bubble collapse in a compressible liquid. In the weak compressibility limit, this configuration has a semi-analytic solution, obtained upon solving an ordinary differential equation [53,54], which we treat as nominally "exact". Though one-dimensional in the radial coordinate, the configuration is advantageous in that it can be used to evaluate simulations on a three-dimensional mesh, and thereby illustrate key features of methods that will be important for complex-geometry applications. If a method is unable to do this, there is little hope that more complex flows can be well approximated by such a computational model. We therefore use it to motivate the development of the proposed method, which we present in detail in Section 3.

In all the simulations, water is modeled with a stiffened-gas equation of state (see (10) in Section 3 where we present the formulation in detail) using $\gamma = 4.4$ and $p^{\infty} = 600$ MPa and air is modeled as an ideal gas with $\gamma = 1.4$ ($p^{\infty} = 0$ MPa). The simulation domain is a $40 \times 40 \times 40$ mm^3 cube with a bubble of initial radius $R_0 = 1$ mm at its center. The bubble is discretized with a mesh of minimum spacing $\Delta x_{\min}$ such that $\bar{R}_{\min}/\Delta x_{\min} \approx 13.9$, where $\bar{R}_{\min}$ is its minimum radius over the entire simulated time. Details of the initial conditions are provided in Section 5.2, where we present one-dimensional (radial coordinate) simulation results for this problem. Here, we compare six approaches on the same three-dimensional mesh:

- ($\tilde{A}$) Interface capturing based upon an established equilibrium mixture model without any interface regularization [39, 46–49];
- (A) The model of Shukla et al. [50], which employs the two-fluid equilibrium model of Allaire et al. [39] and the interface regularization first proposed by Olsson and Kreiss [55] for incompressible flows;
- (B) The method of So et al. [51], which employs anti-diffusive fluxes to sharpen the interface;
- ($\tilde{B}$) Method B without the anti-diffusive fluxes;