A generalized diffuse interface method for accurate simulations of multicomponent flows with immiscible fluids

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ABSTRACT

Flows with immiscible fluids present sharp interfaces which, in the presence of turbulence, develop complex topological changes including break-up and reconnection, along with the complicated turbulence-interface interactions. Most numerical approaches for such flows, e.g. front tracking, volume of fluid and level-set methods generally use phenomenological models for the interface physics and develop singularities. Furthermore, the equations are regularized through the numerical algorithm, which further reduces the accuracy. On the other hand, diffuse interface approaches, e.g. based on the Cahn-Hilliard (CH) equations [1], solve many of these problems, although they introduce their own specific limitations. For example, the previous CH-based approaches are derived from the incompressible binary case with Boussinesq and isothermal assumptions and the new terms are added in an ad-hoc manner.

The generalized diffuse interface method we propose is physically consistent and the formulation can be related to first principles. Thus, without assuming any "a priori" thermodynamic properties, we directly introduce the interfacial properties in a very general manner in the Helmholtz free energy. The specific terms can be obtained directly from the molecular dynamics potentials [2]. The flow equations are then derived using basic thermodynamic relations following a multicomponent generalization of Onsager reciprocal approach [3] and second law of thermodynamics, which leads to a generalized set of equations describing multicomponent ($N \geq 2$), compressible flows, with fluids having arbitrary thermodynamic properties. Next, for the first time, the incompressible generalized Cahn-Hilliard Navier-Stokes (IGCHNS) equations for fluids with any density ratios are rigorously derived following Ref. [4], which ensures full consistency between energy and species equations. It is worth pointing out that, under certain more or less severe simplifying assumptions, the well-known Stefan-Maxwell relation for pure miscible fluids and the previous CH formulations and level-set equations for immiscible fluids can be recovered from our CGCHNS and IGCHNS equations.

The newly developed generalized diffuse interface method naturally handles flows near critical conditions and, away from critical conditions, the description becomes valid when there is a large separation of scales. Thus, accurate simulations of immiscible flow problems can be performed using interface thicknesses much larger than the molecular scales, provided that the interface thickness is smaller than the flow scales. The method has been applied to various interfacial flow problems, such as immiscible Rayleigh-Taylor instability (RTI). To our knowledge, for the first time, the RTI growth rates calculated via full numerical simulations under various conditions (e.g. large range of Atwood number, surface tension, wavenumber and viscosity values) show such good agreement with those predicted by RTI linear stability analysis [5].

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