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Mass and Volume Conservation in Phase Field Models for Binary Fluids

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Abstract. The commonly used incompressible phase field models for non-reactive, binary fluids, in which the Cahn-Hilliard equation is used for the transport of phase variables (volume fractions), conserve the total volume of each phase as well as the material volume, but do not conserve the mass of the fluid mixture when densities of two components are different. In this paper, we formulate the phase field theory for mixtures of two incompressible fluids, consistent with the quasi-compressible theory [28], to ensure conservation of mass and momentum for the fluid mixture in addition to conservation of volume for each fluid phase. In this formulation, the mass-average velocity is no longer divergence-free (solenoidal) when densities of two components in the mixture are not equal, making it a compressible model subject to an internal constraint. In one formulation of the compressible models with internal constraints (model 2), energy dissipation can be clearly established. An efficient numerical method is then devised to enforce this compressible internal constraint. Numerical simulations in confined geometries for both compressible and the incompressible models are carried out using spatially high order spectral methods to contrast the model predictions. Numerical comparisons show that (a) predictions by the two models agree qualitatively in the situation where the interfacial mixing layer is thin; and (b) predictions differ significantly in binary fluid mixtures undergoing mixing with a large mixing zone. The numerical study delineates the limitation of the commonly used incompressible phase field model using volume fractions and thereby cautions its predictive value in simulating well-mixed binary fluids.

AMS subject classifications: 65M70, 76M22, 76T99

Key words: Phase field model, compressibility, multiphase fluid flows, spectral methods.

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1 Introduction

Phase field models have been used successfully to study a variety of interfacial phenomena like equilibrium shapes of vesicle membranes [12–16, 35], blends of polymeric liquids [17, 36–38], multiphase fluid flows [19, 23–25, 28, 40–45], dentritic growth in solidification, microstructure evolution [21, 22, 29], grain growth [8], crack propagation [9], morphological pattern formation in thin films and on surfaces [26, 30], self-assembly dynamics of two-phase monolayer on an elastic substrate [27], a wide variety of diffusive and diffusion-less solid-state phase transitions [10, 39], dislocation modeling in microstructure, electro-migration and multiscale modeling [34]. Multiple phase-field methods can be devised to study multiphase materials [40]. Recently, phase field models are applied to study liquid crystal drop deformation in another fluid, liquid films, polymer nanocomposites, and biofilms [5, 18, 19, 23–25, 28, 40–44, 46].

Comparing to other mathematical and computational technologies available for studying multi-phase materials, the phase-field approach exhibits a clear advantage in its simplicity in model formulation, ease of numerical implementation, and the ability to explore essential interfacial physics at the interfacial regions etc. Computing the interface without explicitly tracking the interface is the most attractive numerical feature of this modeling and computational technology. Since the pioneering work of Cahn and Hilliard in the 50's of the last century, the Cahn-Hilliard equation has been the foundation for various phase field models [6, 7]. It arises naturally as a model for multiphase fluid mixtures should the entropic and mixing energy of the mixture system be known. For immiscible binary fluid mixtures, one commonly uses a labeling or a phase variable (also known as a volume fraction or an order parameter) ϕ to distinguish between distinct fluid phases. For instance $\phi=1$ indicates one fluid phase while $\phi=0$ denotes the other fluid phase in an immiscible binary mixture. The interfacial region is tracked by $0<\phi<1$. Given the historical reason, most mixing energies are calculated in terms of the volume fraction instead of the mass fraction in the literature [11, 20]. Consequently, the system free energy including the entropic and mixing contribution has been formulated in the volume fraction as well, especially for polymeric systems [11, 20]. We acknowledge the existence of diffuse interface models derived using mass fractions [28], which do not belong to the class of phase field models we are addressing in this paper. We denote the system free energy for the material system to be modeled by $F(\phi, \nabla\phi, \cdots)$. A transport equation for the volume fraction ϕ along with the conservation equation of momentum and continuity equation constitutes the essential part of the governing system of equations for the binary fluid mixture. The volume fraction serves as an interval variable for the fluid mixture.

In the literature on immiscible binary mixtures of incompressible fluids, one uses the concept of chemical potential to formulate the transport equation for the volume fractions of the fluids ϕ_1 and ϕ_2. In this formulation, the material incompressibility is on the one hand modeled by the continuity equation

$$\nabla\cdot\mathbf{v}=0, \tag{1.1}$$