A generalized continuous surface tension force formulation for phase-field models for multi-component immiscible fluid flows

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Abstract

We present a new phase-field method for modeling surface tension effects on multi-component immiscible fluid flows. Interfaces between fluids having different properties are represented as transition regions of finite thickness across which the phase-field varies continuously. At each point in the transition region, we define a force density which is proportional to the curvature of the interface times a smoothed Dirac delta function. We consider a vector valued phase-field, the velocity, and pressure fields which are governed by multi-component advective Cahn-Hilliard and modified Navier-Stokes equations. The new formulation makes it possible to model any combination of interfaces without any additional decision criteria. It is general, therefore it can be applied to any number of fluid components. We give computational results for the four component fluid flows to illustrate the properties of the method. The capabilities of the method are computationally demonstrated with phase separations via a spinodal decomposition in a four-component mixture, pressure field distribution for three stationary drops, and the dynamics of two droplets inside another drop embedded in the ambient liquid.

Key words: Continuum surface tension, phase-field model, Navier-Stokes equation, multi-component Cahn-Hilliard equation, interfacial tension, nonlinear multigrid method

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1 Introduction

The interfacial hydrodynamics of a mixture of different fluids plays an increasingly important role in many current scientific and bio-medical engineering applications [28]. Examples include extractors, separators, reactors, sprays, polymer blends, and microfluidic technology [29,30]. A fluid-fluid interface is in a state of tension, as

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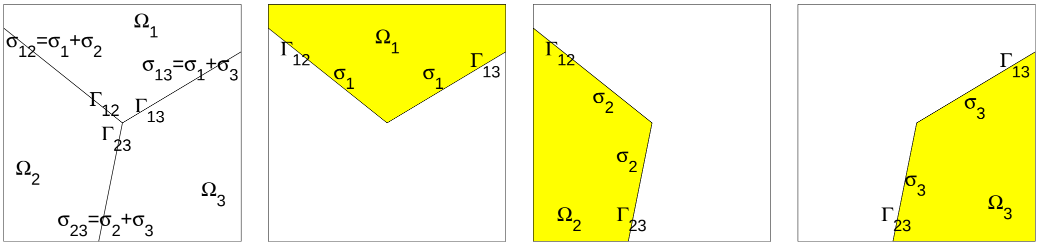
though interfaces have an elastic skin, because fluid molecules at or near the interface experience uneven molecular forces of attraction [31]. Due to the inherent nonlinearities, topological changes, and the complexity of dealing with the unknown, active, and moving surfaces, multiphase flows are challenging. Much effort has been put into studying such flows through analysis, asymptotics, and numerical simulation.

There are many ways to characterize and model moving interfaces. The two main approaches to simulating multiphase and multicomponent flows are interface tracking and interface capturing. In interface tracking methods (examples include volume-of-fluid [12,33], which tracks the volume of the fluid in each cell; front-tracking [41], immersed boundary [44], and immersed interface [26]), Lagrangian (or semi-Lagrangian) particles are used to track the interfaces. In interface capturing methods such as level-set [8,32,37,38] and phase-field methods [9,20,45], the interface is implicitly captured by a contour of a particular scalar function (for example, a signed distance function in a level-set method and mass concentration in a phase-field method). Readers can review a recent review paper [24] for details of the two-phase flow models.

However, compared to the large body of research on two-phase [2,8,9,12,13,35,36,42] and three-phase [5,21,23,40] fluid flows, there have been few theoretical and numerical studies of flows containing four (or more) liquid components with a surface tension effect. The basic idea underlying all continuum surface tension models is the representation of surface tension as a continuous force per unit volume that acts in a neighborhood of the interface. Previous methods have suffered, however, from difficulties in modeling more than three component fluid flows with surface tension. One of the greatest difficulties in modeling four immiscible fluid flows is modeling surface tension effects.



(a) (b) (c) (d)

Fig. 1. Schematic of domain. (a) σ_{ij} denotes the surface tension coefficient of the interface Γ_{ij} of fluids Ω_i and Ω_j. (b) Phase specific surface tension coefficient, σ_1, on interfaces, Γ_{12} and Γ_{13}. (c) and (d) are similarly defined.

In three component fluids [5,21,23,40], the phase specific decomposition surface forces are used. We decompose the given physical surface tension coefficients, σ_{ij}, of the interface Γ_{ij} between fluid $i(\Omega_i)$ and fluid $j(\Omega_j)$ (see Fig. 1(a)) into the phase specific surface tension coefficients $\sigma_1,\ \sigma_2$, and σ_3 such that:

$$\sigma_{12} = \sigma_1 + \sigma_2,\ \sigma_{13} = \sigma_1 + \sigma_3,\ \sigma_{23} = \sigma_2 + \sigma_3. \tag{1}$$

The decomposition is uniquely defined as $\sigma_1 = (\sigma_{12} - \sigma_{23} + \sigma_{13})/2$, $\sigma_2 = (\sigma_{12} + \sigma_{23} - \sigma_{13})/2$, and $\sigma_3 = (-\sigma_{12} + \sigma_{23} + \sigma_{13})/2$ (see Fig. 1(b), (c), and (d)). Then the continuous surface tension force is defined as

$$\mathbf{SF} = \sum_{k=1}^{3} \mathbf{SF}_k = \sum_{k=1}^{3} \sigma_k \kappa(c_k)\mathbf{n}(c_k)\delta(c_k), \tag{2}$$

where $\kappa(c_k)$, $\mathbf{n}(c_k)$, and $\delta(c_k)$ are the total curvature, the unit normal vector, and the smoothed Dirac delta function of the k-th fluid interface, respectively. c_k is the phase variable to be defined.

It has been noted by several authors [5,23] that in the quaternary case, the use of phase specific decomposition cannot be used. This is because the decomposition generates a system of over-determined equations and a solution may not exist. In fact, in [40], "$n > 2$" only means "$n = 3$". Here n represents the number of fluid components. For example, if $n = 4$, then given the physical surface tension coefficients σ_{ij} of the interface Γ_{ij} between fluid i and fluid j, we may consider a linear system of six equations to determine the four unknowns $\sigma_1,\ \sigma_2,\ \sigma_3$, and σ_4:

$$\begin{aligned}&\sigma_{12} = \sigma_1 + \sigma_2,\ \sigma_{13} = \sigma_1 + \sigma_3,\ \sigma_{14} = \sigma_1 + \sigma_4,\\ &\sigma_{23} = \sigma_2 + \sigma_3,\ \sigma_{24} = \sigma_2 + \sigma_4,\ \sigma_{34} = \sigma_3 + \sigma_4.\end{aligned} \tag{3}$$

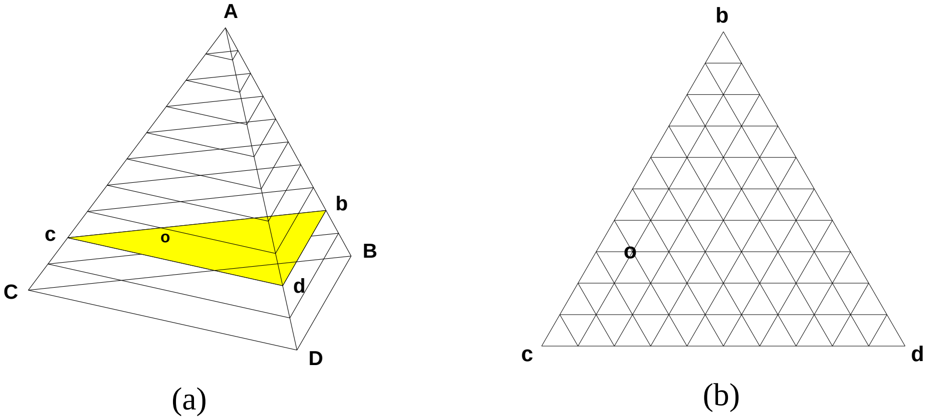
But the above systems of equations are over-determined equations; therefore, it is possible that there is no solution. In order that these equations possess a unique solution, some restrictions must be imposed on σ_{ij}. Note that, in general, for n component immiscible fluid system there are $n(n-1)/2$ possible interfaces and $n(n-1)/2 > n$ for $n \geq 4$. This implies that we have more equations than the unknowns.

To the author's knowledge, there are no four (or more) component fluid flow continuum models with surface tension effects. The main objective of this work is to develop a generalized continuous surface tension force (GCSF) formulation for phase-field models for multi-component immiscible fluid flows, having no difficulty with the over-determined system problem. Phase-field methods have become popular tools for physical modeling of multiphase systems (for a review of the development of diffuse-interface models, see [1]). Generalizations of phase-field models to any number of components without hydrodynamic surface tension effects have been recently introduced and studied in [10,11,14,15,22]. Here, we view the phase-field model as a computational method. The proposed phase-field model is a hybrid method which combines a level set type surface tension force formulation and a concentration relaxation by a phase-field model.

The outline of the paper is as follows. In Section 2, we propose a phase-field model for four immiscible fluids. In Section 3, we give an efficient and accurate numerical solution. In Section 4, we perform some characteristic numerical experiments for quaternary fluid flows. In Section 5, conclusions are drawn.

2 A phase-field model for the mixture of four component immiscible fluids

The composition of a quaternary mixture (A, B, C, and D) can be mapped onto an equilateral tetrahedron (the Gibbs simplex [34]) whose corners represent a 100% concentration of A, B, C, or D as shown in Fig. 2(a). Mixtures with components lying on planes parallel to the triangle, ΔBCD, contain the same percentage of A; those with planes parallel to the triangle, ΔCDA, have the same percentage of B concentration; analogously, for the C and the D concentrations. In Fig. 2, the mixture at the position marked '$\circ$' contains 20% A, 24% B, 48%C and 8% D.



(a) (b)

Fig. 2. (a) Gibbs tetrahedron. (b) A slice plane parallel to the BCD triangle.

Let $\mathbf{c} = (c_1, c_2, c_3, c_4)$ be the phase variables (i.e. the mole fractions of A, B, C, and D, respectively). Thus, admissible states will belong to the Gibbs tetrahedron

$$GT := \left\{ \mathbf{c} \in \mathbb{R}^4 \left| \sum_{i=1}^{4} c_i = 1,\ 0 \le c_i \le 1 \right. \right\}. \tag{4}$$

Without loss of generalities, we postulate that the free energy can be written as follows

$$\mathcal{F} = \int_\Omega \left[F(\mathbf{c}) + \frac{\epsilon^2}{2} \sum_{i=1}^{4} |\nabla c_i|^2 \right] d\mathbf{x},$$

where $F(\mathbf{c}) = 0.25 \sum_{i=1}^{4} c_i^2 (1 - c_i)^2$, ϵ is a positive constant, and Ω is an open bounded subset of $\mathbb{R}^n (n = 2, 3)$ occupied by the system. The time evolution of $\mathbf{c}$ is

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