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An efficient numerical method for simulating multiphase flows using a diffuse interface model

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HIGHLIGHTS

- A new diffuse interface model for multiphase flows is presented.
- Surface tension and buoyancy effects on multiphase flows are studied.
- We employ a new chemical potential that can eliminate spurious phase-field profiles.
- We consider a variable mobility to investigate the effect of the mobility on the fluid dynamics.
- We significantly improve the computational efficiency of the numerical algorithm.

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ABSTRACT

This paper presents a new diffuse interface model for multiphase incompressible immiscible fluid flows with surface tension and buoyancy effects. In the new model, we employ a new chemical potential that can eliminate spurious phases at binary interfaces, and consider a phase-dependent variable mobility to investigate the effect of the mobility on the fluid dynamics. We also significantly improve the computational efficiency of the numerical algorithm by adapting the recently developed scheme for the multiphase-field equation. To illustrate the robustness and accuracy of the diffuse interface model for surface tension- and buoyancy-dominant multi-component fluid flows, we perform numerical experiments, such as equilibrium phase-field profiles, the deformation of drops in shear flow, a pressure field distribution, the efficiency of the proposed scheme, a buoyancy-driven bubble in ambient fluids, and the mixing of a six-component mixture in a gravitational field. The numerical result obtained by the present model and solution algorithm is in good agreement with the analytical solution and, furthermore, we not only remove the spurious phase-field profiles, but also improve the computational efficiency of the numerical solver.

1. Introduction

Multiphase flows play an important role in many scientific and engineering applications, such as extractors [1], polymer blends [2], reactors [3], separators [4], sprays [5], and microfluidic technology [6,7]. For example, emulsification is one of the most common techniques used to produce micro- or nano-scale droplets. However, conventional emulsification techniques, which use inhomogeneous extensional and shear flows to rupture droplets, generate polydisperse emulsions

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with a wide distribution of droplet sizes. Microfluidic technology offers the capability to precisely handle small volumes of fluids and produces almost monodisperse emulsions of immiscible fluids [8]. The composition, shape, and size of emulsions are influenced by the geometry and wettability of channels, and the physical properties (e.g., density, surface tension, and viscosity) of fluids [9]. Another example from nuclear safety concerns a hypothetical severe accident in a reactor. In such a scenario, the degradation of the core can produce multiphase flows in which interfaces undergo extreme topological changes such as breakup or coalescence [10].

Various numerical methods are used for simulating multiphase flows, such as the front-tracking [11,12], immersed boundary [13], volume-of-fluid [14,15], lattice Boltzmann [16,17], level-set [18–20], and diffuse interface [10,21–32] techniques. Because of its advantage in capturing interfaces implicitly, the diffuse interface method has gained considerable attention in recent years. This method replaces sharp interfaces by thin but nonzero thickness transition regions in which the interfacial forces are smoothly distributed [33]. The basic idea is to introduce an order parameter that varies continuously over thin interfacial layers and is mostly uniform in the bulk phases. The temporal evolution of the order parameter is governed by the Cahn–Hilliard equation [34,35]. Here, we view the diffuse interface method as a computational tool, and use the surface tension force derived from the geometry of the interface.

There are numerous numerical studies on two-phase [21–23,26,29,36–44] and three-phase [10,24,25,27,28,45] fluid flows. Recently, Kim [30] proposed a generalized continuous surface tension force formulation for the phase-field model for any number of fluids. To the author's knowledge, this work was the first attempt to model surface tension effects on four-component (or more) fluid flows. A critical feature of the formulation is the incorporation of a scaled delta function $\delta(c_i, c_j) = 5c_ic_j$, where c_i and c_j are the phase variables of fluids i and j, respectively, which is the simplest form and combines two different fluids. This formulation makes it possible to model any combination of interfaces without any additional decision criteria. And, Lee and Kim [31] employed this formulation to study the effect of the surface tension parameter on the mixing dynamics of multi-component fluids in a tilted channel and found that the surface tension parameter makes the flow structures more and more coherent with increase in its value.

The purpose of this paper is to extend the previous works of Kim [30] and of Lee and Kim [31] in three important ways. First, the chemical potentials used in Refs. [30,31] generate additional spurious phases at binary interfaces. Thus, we employ a new chemical potential that can eliminate spurious phases. Second, in Refs. [30,31], the constant mobility case was only considered. Thus, we consider here a phase-dependent variable mobility to investigate the effect of the mobility on the fluid dynamics. Finally, the numerical scheme used in Ref. [30] is not practical for simulating a large number of fluid components, because the calculation of a nonlinear discrete system becomes complicated when the number of components is increased. Thus, we significantly improve the computational efficiency of the numerical solution algorithm by adapting the recently developed scheme for the multiphase-field equation [46].

This paper is organized as follows. In Section 2, we present a new diffuse interface model for the mixture of N incompressible immiscible fluids. In Section 3, a numerical solution is given. We perform some characteristic numerical experiments for multi-component fluid flows in Section 4. Conclusions are drawn in Section 5. In the Appendix, we describe a nonlinear multigrid method used to solve the nonlinear discrete system at the implicit time level.

2. A diffuse interface model for the mixture of N incompressible immiscible fluids

We consider the flow of N incompressible immiscible fluids. Let $\mathbf{c} = (c_1, c_2, \ldots, c_N)$ be a vector-valued phase-field. Each order parameter c_i is the concentration of each component in the mixture. Thus, admissible states will belong to the Gibbs N-simplex

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

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

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

where Ω is a bounded open subset of $\mathbb{R}^d$ ($d = 1, 2, 3$) occupied by the system, $F(\mathbf{c}) = 0.25 \sum_{i=1}^{N} c_i^2 (1 - c_i)^2$, and $\epsilon > 0$ is the gradient energy coefficient. The time evolution of $\mathbf{c}$ is governed by the gradient of the energy with respect to the $\dot{H}^{-1}$ inner product under the additional constraint (1). This constraint has to hold everywhere at all times. In order to ensure the last constraint, we use a Lagrange multiplier β_i [27,30,31,46–54]:

$$\frac{\partial c_i}{\partial t} = \nabla \cdot \left[M(\mathbf{c}) \nabla \frac{\delta}{\delta c_i} \left(\mathcal{F}(\mathbf{c}) + \beta_i \mathcal{G}(\mathbf{c}) \right) \right], \tag{2}$$

where $M(\mathbf{c})$ is a diffusional mobility and $\mathcal{G}(\mathbf{c}) = \int_{\Omega} \left(\sum_{j=1}^{N} c_j - 1 \right) \mathrm{d}\mathbf{x}$. By treating the N phases independent [48,51], Eq. (2) can be reduced to

$$\frac{\partial c_i}{\partial t} = \nabla \cdot \left[M(\mathbf{c}) \nabla \left(\frac{\delta \mathcal{F}(\mathbf{c})}{\delta c_i} + \beta_i \right) \right].$$