Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2023-0295

Vol. **36**, No. 1, pp. 104-132
July 2024

Modeling Two-Phase System in Complex Domains Based on Phase-Field Approach with Interfacial Correction

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Received 14 November 2023; Accepted (in revised version) 24 April 2024

Abstract. We introduce a novel phase-field model designed for ternary Cahn-Hilliard (CH) dynamics, incorporating contact angle boundary conditions within complex domains. In this model, we utilize a fixed phase field variable to accurately represent intricate domains within the ternary CH system. Simultaneously, the remaining two phase field variables are employed to simulate CH dynamics effectively. The contact angle term is derived from Young's equality and the hyperbolic tangent profile of the equilibrium interface. To ensure compliance with the hyperbolic tangent property at the interface, a fidelity term is incorporated into the original CH model. This addition reduces mass loss for each phase and improves the accuracy of the contact angle effect. Moreover, we implement a finite difference scheme along with a nonlinear multigrid method to solve the corrected ternary CH model. A series of numerical experiments is conducted in both two- and three-dimensional spaces to demonstrate the efficiency and robustness of the proposed model.

AMS subject classifications: 35K55, 35J60, 65M06

Key words: Ternary Cahn–Hilliard system, complex domains, hyperbolic tangent property, multigrid method.

1 Introduction

The Cahn-Hilliard (CH) equation, originally formulated by Cahn and Hilliard [1], represents a fundamental phase-field model utilized to describe the mass-conserved spinodal

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decomposition observed in binary alloys. In the CH equation, an order parameter, referred to as the phase-field variable, is introduced to characterize the physical state of the system. Notably, this phase-field variable assumes distinct values within each phase, with, for instance, -1 representing the liquid phase and 1 representing the solid phase. The interface separating these phases is characterized by a continuous and finite transition layer, and its position can be defined as a level set of the phase-field function. This unique formulation allows implicit capture of topological changes in the interface during the solution process. Moreover, it is worth noting that the CH equation naturally satisfies mass conservation when either periodic or homogeneous Neumann boundary conditions are applied. The CH equation, governing the behavior of the phase-field variable, adheres to the H^{-1}-gradient flow principle of the total free energy. Through appropriate modifications, the original CH equation has found wide-ranging applications in modeling diverse physical phenomena, including but not limited to diblock copolymer dynamics [2–4], surfactant behavior [5–7], contact angle and wetting phenomena [8, 9], the dynamics of gravity and capillary waves [10], solid tumor growth [11, 12], as well as applications in topology optimization and image processing [13, 14], etc..

Many real-world physical phenomena and natural processes, such as the formation of double emulsions in micro-fluidic devices [15, 16], the behavior of hydrocarbon fluids in the petroleum industry [17], the intricate dynamics of water-oil-surfactant mixtures [18, 19], and multi-component chemo-mechanics [20], etc., inherently involve more than two components, including substances like water, surfactants, alcohols, and other immiscible materials. Researchers, such as Fontaine [21] and Morral and Cahn [22], have extended the CH model to address multi-component systems, enabling the modeling of the dynamic behavior of materials featuring multiple phases within their microstructures. In the multi-component CH phase-field model, tailored for systems involving more than two components, a minimum of three phase-field variables is employed, with each variable representing an individual component. For instance, a value of 1 signifies the presence of the respective component, while 0 indicates its absence. This multi-component CH model has found widespread application in fluid simulations. For instance, Kim [23] introduced a generalized continuous surface tension force model to account for surface tension effects in multi-component fluid flow. Lee and Kim [24] conducted a numerical investigation into buoyancy-driven mixing of incompressible immiscible fluids, involving multi-component CH equations, within two-dimensional tilted channels. Additionally, Zhang et al. [25] delved into the ramifications of droplet inertia and interfaces, utilizing an incompressible fluid flow-coupled ternary CH model to analyze the flow dynamics during the collision of two immiscible droplets. This allowed them to evaluate factors such as film thickness, maximal spreading time, and deformation, with a particular focus on the liquid-liquid interface. Furthermore, Kalantarpour et al. [26] constructed a ternary phase-field Lattice Boltzmann model to explore scenarios involving high-density ratios and total spreading within three incompressible and immiscible fluids. Their work showcased the utilization of multi-component CH equations to monitor the phasic evolution of the system. The simulation results in the context