Phase Field Model of Thermo-Induced Marangoni Effects in the Mixtures and its Numerical Simulations with Mixed Finite Element Method

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Received 29 October 2008; Accepted (in revised version) 30 March 2009
Communicated by Pingwen Zhang
Available online 14 May 2009

Abstract. In this paper, we study the Marangoni effects in the mixture of two Newtonian fluids due to the thermo-induced surface tension heterogeneity on the interface. We employ an energetic variational phase field model to describe its physical phenomena, and obtain the corresponding governing equations defined by a modified Navier-Stokes equations coupled with phase field and energy transport. A mixed Taylor-Hood finite element discretization together with full Newton’s method are applied to this strongly nonlinear phase field model on a specific domain. Under different boundary conditions of temperature, the resulting numerical solutions illustrate that the thermal energy plays a fundamental role in the interfacial dynamics of two-phase flows. In particular, it gives rise to a dynamic interfacial tension that depends on the direction of temperature gradient, determining the movement of the interface along a sine/cosine-like curve.

Key words: Phase field, Navier-Stokes equations, Marangoni effects, temperature dependent surface tension, mixed Taylor-Hood finite element, Newton’s method.

1 Introduction

Phase field models are an increasingly popular choice for modeling the motion of multiphase fluids (see [3] for a recent review). In the phase-field model, sharp fluid interfaces
are replaced by thin but nonzero thickness transition regions where the interfacial forces are smoothly distributed [9]. The basic idea is to introduce a conserved order parameter (e.g., mass concentration) that varies continuously over thin interfacial layers and is mostly uniform in the bulk phases. These models allow topological changes of the interface [6, 18, 19, 25] and have many advantages in numerical simulations of the interfacial motion [12]. Thus, it is also known as the diffuse-interface model. More precisely, in this work, a phase-field variable \( \phi \) is introduced, which can be thought of as the volume fraction, to demarcate the two species and indicate the location of the interface. A mixing energy is defined based on \( \phi \) which, through a convection-diffusion equation, governs the evolution of the interfacial profile. The phase-field method can be viewed as a physically motivated level-set method, and Lowengrub and Truskinovsky [25] have argued for the advantage of using a physically determined \( \phi \) profile instead of an artificial smoothing function for the interface. When the thickness of the interface approaches zero, the diffuse-interface model becomes asymptotically identical to a sharp-interface level-set formulation. It also reduces properly to the classical sharp-interface model in general. Recently many researchers have employed the phase field approach for various fluid models [2, 4–6, 13–15, 18–20, 24, 26, 29, 33]. Based on an energetic variational formulation, Liu and Shen [22] employed a phase field model to describe the mixture of two incompressible Newtonian fluids. The mixing energy studied is related to the usual Ginzburg-Laudau model for phase evolutions.

The study of the evolution of the free interfaces is one of the most important fundamental area in the theory of hydrodynamics and rheology. The analytical and numerical analysis of these problems has attracted attention for more than one hundred years, where the Marangoni effect is a typical model. Marangoni effects [35, 36] are due to the inhomogeneity of the interfacial properties. The effects can be attributed to either the non-uniform distributions of particles (surfactants) or the distribution of temperatures which is the case we will study in this paper. This ubiquitous phenomena (such as wine tears) had been studied for more than 150 years since James Thomson, Carlo Marangoni and Willard Gibbs. It is involved in almost all studies of free interface and interface properties. The Marangoni-Benard convection is one of the most fascinating phenomenon in fluids. It has becoming more and more important in the application of non-Newtonian fluids and ocean-geophysical dynamics.

The conventional Marangoni-Benard convection is described by the following two phase fluids with a sharp interface, involving the Boussinesq approximation

\[
\rho(u_t + (u \cdot \nabla)u) + \nabla p - \nu \text{div} D(u) = -\rho_\theta g, \quad (1.1) \\
\nabla \cdot u = 0, \quad (1.2) \\
\theta_t + u \cdot \nabla \theta = k \Delta \theta, \quad (1.3)
\]

where \( u, p \) and \( \theta \) stand for the fluid velocity, pressure, and temperature, respectively. \( \rho \) is the density of fluid mixture, \( \rho_\theta \) is the temperature-dependent density defined as

\[
\rho_\theta = \rho \left[ 1 - \alpha(\theta - \theta_0) \right], \quad (1.4)
\]