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Entropy stable modeling of non-isothermal multi-component diffuse-interface two-phase flows with realistic equations of state[☆]

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Abstract

In this paper, we consider mathematical modeling and numerical simulation of non-isothermal compressible multi-component diffuse-interface two-phase flows with realistic equations of state. A general model with the general reference velocity is derived rigorously through thermodynamical laws and Onsager's reciprocal principle, and it is capable of characterizing compressibility and partial miscibility between multiple fluids. We prove a novel relation between the pressure, temperature and chemical potentials, which results in a new formulation of the momentum conservation equation indicating that the gradients of chemical potentials and temperature become the primary driving force of the fluid motion except for the external forces. A key challenge in numerical simulation is to develop entropy stable numerical schemes preserving the laws of thermodynamics. Based on the convex–concave splitting of Helmholtz free energy density with respect to molar densities and temperature, we propose an entropy stable numerical method, which solves the total energy balance equation directly, and thus, naturally satisfies the first law of thermodynamics. Unconditional entropy stability (the second law of thermodynamics) of the proposed method is proved by estimating the variations of Helmholtz free energy and kinetic energy with time steps. Numerical results validate the proposed method.

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Keywords: Multi-component two-phase flow; Non-isothermal flow; Entropy stability; Convex splitting

1. Introduction

Various non-isothermal multi-component two-phase flows are ubiquitous in nature and industry, and thus their research carries broad and far-reaching significance. An industrial example is the phase transition of hydrocarbon mixtures in the reservoir; at specified thermodynamical conditions, a hydrocarbon mixture may split into gas and liquid

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(oil) to stay in an equilibrium state; when the thermal enhanced oil recovery is employed, intentionally introduced heat disrupts the equilibrium states and vaporizes part of the oil, thereby changing the physical properties such that oil flows more freely through the reservoir [1,2]. Another example is the utilization of supercritical fluids as solvents in chemical analysis and synthesis [3]. In the natural world, many common phenomena, such as boiling, evaporation and condensation, are also related to physical properties and motions of non-isothermal two-phase flows [4].

For realistic fluids, the interfaces between multiple fluids always exist and play a very important role in the mass and energy transfer between different phases. Partial miscibility of multiple fluids, a common phenomenon displayed by realistic fluids in experiments and practical processes, takes place through the interfaces. Moreover, capillarity effect, a significant mechanism of flows in porous media, is also caused by the anisotropic attractive force of molecules on the interfaces [5]. To describe the gas–liquid interfaces, the diffuse-interface models for multiphase flows have been developed in the literature. The pioneering work is that the density-gradient contribution on the interfaces is introduced by van der Waals in the energy density (see [6] and the references therein), and on the base of it, the Korteweg stress formulation is induced by composition gradients (see [4,6] and the references therein). Various phase-field models for immiscible and incompressible two-phase flows have been developed and simulated in the literature, [7–22] for instance.

Modeling and simulation of compressible multi-component two-phase flows with partial miscibility and realistic equations of state (e.g. Peng–Robinson equation of state [23]) are intensively studied in recent years [24–30]. The multi-component models with realistic equations of state are traditionally applied for simulation of many problems in chemical and petroleum engineering, for example, the phase equilibria calculations [31–38] and the prediction of surface tension [5,38–40], but the fluid motion has never been considered in these applications. We note that fluid flow and transport in porous media have been well modeled, for example, in [41–51], but these studies are all at a Darcy's scale, not in a pore scale. A general diffuse interface model for compressible multi-component two-phase flows with partial miscibility is developed in [28,52] based on the thermodynamic laws and realistic equations of state. It uses molar densities as the primal state variables, and takes a general thermodynamic pressure as a function of the molar density and temperature, thereby never suffering from the difficulty of constructing the pressure equation. However, the temperature field in this model is assumed to be homogeneous and constant.

There exist many situations, such as boiling, evaporation, condensation and thermal enhanced oil recovery, in which phase transitions and fluid motions are highly influenced by an inhomogeneous and variable temperature field. In [53], the non-isothermal diffuse-interface models for the single-component and binary fluids are developed by including gradient contributions in the internal energy. In [6,54], Onuki generalizes the van der Waals theory for the single-component fluids by including gradient contributions in both the internal energy and the entropy. Subsequently, improvements and applications of the model in [6,54] are investigated in [3,4,55–59] and the other literature; especially, in [4] a continuum mechanics modeling framework for liquid–vapor flows is rigorously derived using the thermodynamical laws. The non-isothermal diffuse-interface models are extended to the compressible binary fluids in [3,60]. The aforementioned research works are done on the basis of the van der Waals equation of state, but rarely concerning the other equations of state, for example, the Peng–Robinson equation of state [23] extensively employed in petroleum and chemical industries due to its accuracy and consistency for numerous realistic gas–liquid fluids including N_2, CO_2, and hydrocarbons. It is noted that different from the single-component fluids, a reference velocity, such as mass-average velocity, molar-average velocity and so on, usually needs to be selected for multi-component fluids [61], so the models are expected to be compatible with the general reference velocity. However, up to now, the rigorous generalization of the aforementioned models to multi-component flows with the general reference velocity is still an open problem.

In this paper, we will generalize the aforementioned model; more precisely, we will derive a general non-isothermal multi-component diffuse-interface two-phase model based on the thermodynamical laws and realistic equations of state (e.g. Peng–Robinson equation of state) with mathematical rigors. A significant feature of the general model is that it has a set of unified formulations for general reference velocities and related mass diffusion fluxes. Moreover, a general thermodynamic pressure, which is a function of the molar density and temperature, is used and consequently, it is free of constructing the pressure equation.

The entropy balance equation plays a fundamental role in the derivations of diffuse interface two-phase flow models [3,4,6,53,54], by which we can apply the entropy production principle (the second law of thermodynamics) to derive the forms of thermodynamical fluxes, including the stress tensor, the mass diffusion and heat transfer fluxes. Different from the existing derivation approach using the Gibbs relation and other thermodynamical relations, we