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Modelling of Compressible Multi-Component Two-Phase Flow with Multi-Component Navier Boundary Condition

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Abstract. In this paper, we derive a dimensionless model for compressible multi-component two-phase flows with Peng-Robinson equation of state (EoS), incorporated with the multi-component Navier boundary condition (MNBC). We propose three linearly decoupled and energy-stable numerical schemes for this model. These schemes are developed based on the Lagrange multiplier approach for bulk Helmholtz free energy and surface free energy. One of them is based on a component-wise approach, which requires solving a sequence of linear, separate mass balance equations and leads to an original discrete energy that unconditionally dissipates. Another numerical scheme is based on a component-separate approach, which requires solving a sequence of linear, separate mass balance equations but leads to a modified discrete energy dissipating under certain conditions. Numerical results are presented to verify the effectiveness of the proposed methods.

AMS subject classifications: 65N12, 76T10, 76N99, 49S05

Key words: Compressible, Helmholtz free energy, energy-stable, Lagrange multiplier, multi-component, Peng-Robinson EoS.

1 Introduction

Multi-component two-phase fluid systems with a realistic EoS (e.g. Van der Waals [15] and Peng-Robinson EoS [30]) are very important building blocks in many chemical and reservoir engineering [7, 9, 34, 38], especially the pore scale modelling of subsurface fluid flow. Although a lot of research work has been done on these issues in recent years, plenty of challenges remain in the understanding of liquid droplets, gas bubbles, the interface between gas-liquid phases and complex boundary conditions taking place in the multi-component two-phase fluid system. As one of the most popular methodologies to

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study two-phase interface problems, the models of incompressible two-phase flows have been widely studied [4, 18, 27], where pressure has no physics meaning which is used to impose incompressibility. In these works, a double-well potential is used, which has been qualitatively (instead of quantitatively) analyzed, this is inadequate for oil reservoir and chemical engineering practice. When a realistic model is applied for hydrocarbon mixture, the interfaces can be modeled quantitatively [8, 34]. Another important modelling framework is based on NVT, which uses the moles, volume, and temperature as the primal state variables [16,17,31,34]. Recently, in the NVT-based framework, a general multi-component two-phase compressible flow model is rigorously derived in [22,25] based on the thermodynamic laws and realistic EoS. Different from the derivation of the incompressible fluid model, in the NVT-based framework, the mathematical models of multi-phase fluids are often formulated by a set of thermodynamic state variables and fluid velocity [22]. Furthermore, a general thermodynamic pressure was proposed in NVT-based framework, which is a function of the molar density and temperature, and consequently, it is never required to construct the pressure equation. Recently, there have been many work on the machine learning and modelling in reservoir simulations [2, 39, 40, 44]. For example, the first self-adaptive deep learning algorithm in details to accelerate flash calculations is proposed in [44]. Moreover, a comprehensive review of classical reservoir simulation and a summary of recent progress in pore scale, Darcy's scale and multiscale and mesoscopic reservoir simulation, as well as some recent work in machine learning applications in reservoir simulation are provided in [39].

The problem of moving contact line, which is the problem of fluid-fluid interface intersecting the solid wall, is a classical problem that occurs in many physical phenomena. It is well known that classical hydrodynamical models with no-slip boundary conditions lead to nonphysical singularity in the vicinity of the contact line [33]. A phase field model with generalized Navier boundary condition (GNBC) is proposed in [32, 33] and widely used to resolve the issue. It is shown that the numerical results based on the GNBC can reproduce quantitatively the results from the molecular dynamics (MD) simulation [11,12,14,42]. In the work of [41], a dimensionless model for pure-component two-phase compressible flows with Van der Waals EoS and GNBC was proposed. The Van der Waals EoS has a rigorous foundation in physics, while the Peng-Robinson EoS is more accurate for hydrocarbon mixtures. In particular, the Peng-Robinson EoS is widely used in subsurface flow such as petroleum engineering modelling and subsurface CO_2 sequestration [28]. In our work, we take advantage of the Helmholtz free energy based on physical models, i.e., the Peng-Robinson EoS.

We consider a multi-component two-phase fluid system comprised of M components in a container of invariant volume V occupying a domain denoted by $\Omega \subset \mathbb{R}^d (d=1,2,3)$ at temperature Θ. For simplicity, gravity is neglected in the current paper. Let n_i be the molar density of component i, and we denote the molar density vector by $\mathbf{n}=[n_1,n_2,\cdots,n_M]^T$.

The total stress for the multi-component viscous flow can be written as [22]