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THERMODYNAMICALLY CONSISTENT MODELING AND SIMULATION OF MULTI-COMPONENT TWO-PHASE FLOW WITH PARTIAL MISCIBILITY*

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Abstract. A general diffuse interface model with a realistic equation of state (e.g. Peng-Robinson equation of state) is proposed to describe the multi-component two-phase fluid flow based on the principles of the NVT-based framework which is an attractive alternative recently over the NPT-based framework to model the realistic fluids. The proposed model uses the Helmholtz free energy rather than Gibbs free energy in the NPT-based framework. Different from the classical routines, we combine the first law of thermodynamics and related thermodynamical relations to derive the entropy balance equation, and then we derive a transport equation of the Helmholtz free energy density. Furthermore, by using the second law of thermodynamics, we derive a set of unified equations for both interfaces and bulk phases that can describe the partial miscibility of multiple fluids. A relation between the pressure gradient and chemical potential gradients is established, and this relation leads to a new formulation of the momentum balance equation, which demonstrates that chemical potential gradients become the primary driving force of fluid motion. Moreover, we prove that the proposed model satisfies the total (free) energy dissipation with time. For numerical simulation of the proposed model, the key difficulties result from the strong nonlinearity of Helmholtz free energy density and tight coupling relations between molar densities and velocity. To resolve these problems, we propose a novel convex-concave splitting of Helmholtz free energy density and deal well with the coupling relations between molar densities and velocity through very careful physical observations with a mathematical rigor. We prove that the proposed numerical scheme can preserve the discrete (free) energy dissipation. Numerical tests are carried out to verify the effectiveness of the proposed method.

Key words. Multi-component two-phase flow; Diffuse interface model; Partial miscibility; Energy dissipation; Realistic equation of state.

AMS subject classifications. 65N12; 76T10; 49S05

1. Introduction.

Modeling of multiphase fluid systems with a realistic equation of state (e.g. Peng-Robinson equation of state [39]) has become an attractive and challenging research topic in the chemical and reservoir engineering [7, 8, 13–18, 29, 30, 33, 38, 40, 42–45]. It plays very important roles in the pore scale modeling and simulation of subsurface fluid flow, especially shale gas reservoir that has become an increasingly important source of natural gas in the recent years.

Mathematical models of multiphase fluids are often formulated by a set of thermodynamic state variables and fluid velocity. In the traditional framework of modeling multiphase fluids, the thermodynamic state variables are the pressure, temperature, and chemical composition (the so-called NPT-based framework). This framework has been extensively used in many applications [4, 10, 21, 32]. However, the NPT-based framework has some essential limitations [13, 14, 29, 30, 38]. First, a realistic equation of state (e.g. Peng-Robinson equation of state) is a cubic equation with respect to the density, so the density might not be uniquely determined for the specified pressure, temperature, and molar fractions. Second, in compositional fluid simulation,

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