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A New Multi-Component Diffuse Interface Model with Peng-Robinson Equation of State and its Scalar Auxiliary Variable (SAV) Approach

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Abstract. A new multi-component diffuse interface model with the Peng-Robinson equation of state is developed. Initial values of mixtures are given through the NVT flash calculation. This model is physically consistent with constant diffusion parameters, which allows us to use fast solvers in the numerical simulation. In this paper, we employ the scalar auxiliary variable (SAV) approach to design numerical schemes. It reformulates the proposed model into a decoupled linear system with constant coefficients that can be solved fast by using fast Fourier transform. Energy stability is obtained in the sense that the modified discrete energy is non-increasing in time. The calculated interface tension agrees well with laboratory experimental data.

AMS subject classifications: 65N06, 65B99

Key words: Peng-Robinson equation of state, multi-component diffuse interface model, scalar auxiliary variable approach, energy stable scheme.

1 Introduction

In reservoir engineering and chemical flows, multi-component and multi-phase fluid systems are unneglectable with important roles in the thorough and accurate understanding of flow behaviors in a large range of applications [2–4, 6, 15, 17, 22]. In numerical

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simulations, it is a key effort to determine whether the studied fluid mixtures remain in one single phase or split into multiple phases including oil phase, water phase, gas phase, etc. Thermodynamic equilibrium conditions are the basic rule to control physical properties of the mixture fluid flow, such as composition and density of each phase if split, and whether the phase split occurs at all. Recently, realistic equations of state (EOS) (e.g. Peng-Robinson EOS [18]) have attracted more and more attention in the multi-component multi-phase flow simulation, which is very useful in the study of thermodynamic mechanism. It can be applied in many areas, especially in the pore scale modeling of subsurface fluid flow [7–9, 11]. The main cause of capillarity, a major immiscible two-phase flow mechanism for systems with a strong wettability preference, is often attributed to the interface tension, which is mainly determined by phase behaviors of multi-component fluids. In order to capture the phase properties and behaviors better, diffuse interface models based on Peng-Robinson EOS have been widely studied in recent years [6, 11].

While modeling the multi-component system, the mobility tensor is a significant element to be considered. Mobility, which is a variable defined in diffuse interface models, plays an essential role to keep the developed model consistent with thermodynamic laws. The mobility matrix M shall be symmetric and positive semi-definite so that Onsager's reciprocal principle and the second law of thermodynamics are satisfied. Different methods have been proposed to model the mobility tensor, which could be summarized into three types. The first one is to define mobility as a diagonal matrix with positive diagonal elements, which satisfies the aforementioned two principles and is convenient to implement. Only the diffusivity of each component is considered, so that the mobility tensor could be represented simply as: M_{ii}. The second one is to take mobility matrix as a full matrix, and namely we have two tensors M_{ii} and M_{ij}. It should be noted that the mole mean diffusivity matrix $D_{ii}=0$ but $D_{ij}>0$. The third one is to use mass mean diffusivity instead of mole mean diffusivity. More details on the modeling of the mobility tensor could be found in [13] and references therein. In this paper, inspiring from the first choice of mobility, we propose a new multi-component two phase diffuse interface model in order to use certain fast calculation approaches.

How to select the initial value of multi-component mixture becomes an important modeling issue when the realistic equation of state (EOS) is involved. To handle this, we need to consider a phase splitting problem. The NPT flash calculation (temperature T, pressure P and composition N) and the NVT flash calculation (temperature T, volume V and composition N) are two common phase splitting approaches. As discussed in [21], classical coupled schemes based on the NPT flash calculation suffer from a few essential limitations, such as the requirement of constructing a pressure equation as there is no intrinsic pressure equation. An alternative modeling framework, based on the NVT flash calculation with moles, volume and temperature as the primal state variables, has been actively studied very recently [7, 8]. It allows us to get the molar density of gas and liquid of a specific substance when the phase transition occurs, and is better posed than the NPT flash calculation. The obtained solution can be used as the initial value of the