

# Linear and Unconditionally Energy Stable Schemes for the Multi-Component Two-Phase Diffuse Interface Model with Peng-Robinson Equation of State

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**Abstract.** In this paper we consider numerical solutions of the diffuse interface model with Peng-Robinson equation of state for the multi-component two-phase fluid system, which describes real states of hydrocarbon fluids in petroleum industry. A major challenge is to develop appropriate temporal discretizations to overcome the strong nonlinearity of the source term and preserve the energy dissipation law in the discrete sense. Efficient first and second order time stepping schemes are designed based on the “Invariant Energy Quadratization” approach and the stabilized method. The resulting temporal semi-discretizations by both schemes lead to linear systems that are symmetric and positive definite at each time step, and their unconditional energy stabilities are rigorously proven. Numerical experiments are presented to demonstrate accuracy and stability of the proposed schemes.

**AMS subject classifications:** 65M12, 65M06, 65M15

**Key words:** Diffuse interface model, Peng-Robinson equation of state, linear scheme, Invariant Energy Quadratization, energy stability.

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## 1 Introduction

Many problems in the fields of science and engineering, particularly in materials science and fluid dynamics, involve flows with multiple constitutive components [11, 22, 28, 29]. A typical well-known application is the subsurface gas and oil reservoir, which contains

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gas phase, oil phase and water phase, together with the solid phase [9]. From mathematical modeling and numerical algorithmic points of view, it is a challenge to perform numerical simulations of multiphase flows and study interfaces between phases, due to inherent nonlinearities, topological changes, and complexities of dealing with unknown moving interfaces.

There are many approaches to categorize the moving interfaces. The first method to simulate multiphase and multi-component flows is interface tracking (sharp interface modeling [24], front-tracking [10], immersed boundary [27]), and the interface is described as a zero-thickness two-dimensional entity. This approach can successfully predict the shape and dynamics of the interface, assuming that the interface tension is given. However, it can not provide information within the interface itself. The second method is the phase field model (interface capturing, diffuse interface theory) to simulate multiphase and multi-component flows [1,2,4,5,21,23], which is an increasingly popular choice for modeling the motion of multiphase and multi-component fluids. In the phase field model, a conserved order parameter such as a mass concentration that varies continuously over thin interfacial layers is introduced, and the order parameter is mostly uniform in the bulk phases. Based on this idea, sharp fluid interfaces are replaced by thin but nonzero thickness transition regions where the interfacial forces are smoothly distributed. The free interface can be automatically tracked without imposing any mathematical conditions on the moving interface. One advantage of the phase field model is that the governing system of equations in the model can be derived from the variational principle. Moreover, the phase field model usually leads to well-posed nonlinear systems that satisfy the energy dissipation law. Therefore, this model has become a well-known simulation tool to resolve the motion of free interfaces in multiple components, and has also been successfully applied to many problems in the fields of science and industry (see [12,13,30,31] and the references cited therein).

In order to study the interface between phases, the development of energy stable schemes for phase field model is an important issue. There are several popular numerical approaches to construct energy stable schemes. The first approach is the convex splitting method, which is introduced by Elliott and Stuart [3,6] and popularized by Eyre [7]. The main idea is assuming the free energy density can be split as the difference of two convex functions, where the convex part is treated implicitly and the concave part is treated explicitly. Although the convex splitting method is unconditionally energy stable and uniquely solvable, it reduces to a nonlinear system at each time step and the implementation is complicated and the computational cost is high. The second widely used approach is the stabilized method which treats the nonlinear terms explicitly, and adds an artificial stabilization term to overcome strict temporal step constraint [39,40]. This method is also energy stable and produces a linear system at each time step which is easy to implement. However, it is not easy to find the stabilization term for all problems, and it can not be unconditionally energy stable for second order scheme.

In this paper, we focus on the diffuse interface modeling of multi-component and multiphase fluid systems, and consider the energy stable schemes for a more realistic