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# STABILITY AND CONVERGENCE ANALYSIS OF SECOND-ORDER SCHEMES FOR A DIFFUSE INTERFACE MODEL WITH PENG-ROBINSON EQUATION OF STATE*

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**Abstract**

In this paper, we present two second-order numerical schemes to solve the fourth order parabolic equation derived from a diffuse interface model with Peng-Robinson Equation of state (EOS) for pure substance. The mass conservation, energy decay property, unique solvability and $L^\infty$ convergence of these two schemes are proved. Numerical results demonstrate the good approximation of the fourth order equation and confirm reliability of these two schemes.

*Mathematics subject classification:* 65N06, 65B99.
*Key words:* Diffuse interface model, Fourth order parabolic equation, Energy stability, Convergence.

## 1. Introduction

Multi-phase fluid mixture and its behaviors play important roles in many natural and engineering systems, especially in subsurface petroleum reservoirs [5,6,30–33]. It remains a challenge to understand and to model the complex interaction between phases, namely the physically distinct, separable portions of substance. In the classical theory known as the sharp interface model [9, 27, 39], an interface between two fluids is modeled as an infinitely thin, or sharp two-dimensional entity, and it is endowed with interface properties such as surface tension. In a more detailed continuum model called as the diffuse interface model, the sharp fluid-fluid interface is replaced by a small but finite-thickness layer in which the fluids may mix. Even though the concept of a diffuse interface was originally proposed a long time ago by van der Waals [36], its numerical simulation with realistic fluids has been investigated only in recent years [20, 22]. The diffuse interface theory is also known as the gradient theory [4, 10] in the chemical society, or phase field theory [3] in the fluid dynamics society. Unlike sharp interface models where surface tension must be provided as an input parameter, diffuse interface models have been used to predict surface tension [4, 10, 18, 19]. In particular, the surface tensions of petroleum fluids have been well predicted by diffuse interface models in one spatial dimension

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together with Peng-Robinson Equation of State (EOS) [21], which is one of the most popular equations of state for hydrocarbon systems. However, little work has been carried out to investigate the numerical simulation of Peng-Robinson-EOS-equipped diffuse interface models in multiple spatial dimensions [22].

Inspired by the favorable properties of the Cahn-Hilliard equation and its derivation, we provide the fourth-order parabolic equation to describe the equilibrium state and the flow of the components in the crude oil in this article. Numerical experiments are our indispensable tools to investigate the solution to this equation. Previously proposed schemes for the Cahn-Hilliard equation [7,8,10–14,17,29,34,35,38] and other kinetics equations contain fourth order term [23,25,26,28,37] could be used as valuable references. The main contribution of this work is to develop two second-order energy stable numeircal schemes for the two-dimensional diffuse interface model with Peng-Robinson EOS of single component substance. The mass conservation and unique solvability are proved. The energy stability of these two schemes are achieved following the approach in [24]. However, it is not that smooth as we expected to obtain the $L^\infty$ convergence of these two schemes attributed to the unboundedness of the free energy density of any given substance and its first and second order derivatives respect to the molar density. Taking the work of Li et al. [15] as reference, we overcome this difficulty with a nontrivial arguments.

The rest of this paper is organized as follows. In the second section, we present the mathematical model of the diffuse interface equation derived from the Peng-Robinson EOS and the scaled fourth order equation for multi-component substances and demonstrate its energy decreasing and mass conservation characters. In the third section, we present notations on the discrete space and some auxiliary lemmas. After that, the $L^\infty$ convergence of the Crank-Nicolson scheme and the second order linearized scheme will be demonstrated in the fourth and fifth sections, respectively. And then, we provide the numerical results of these two schemes and compare them with previously published ones. The conclusion of this article will be provided in the end.

## 2. Mathematical Model of Fluid Systems with Diffuse Interface

We consider a fluid system consisting of fixed species amount on a fixed domain with spatially uniform-distributed given temperature.

### 2.1. Helmholtz free energy from Peng-Robinson EOS

Let $M$ denote the number of components in the fluid mixture, $n_i$ represent the molar concentration of the component $i$, and

$$\mathbf{n} = (n_1, n_2, \cdots, n_M)^T$$

be the molar concentrations of all components and $n = n_1 + n_2 + \cdots + n_M$ the molar density of the fluid. According to the diffuse interface model, the total Holmholtz free energy has the following form,

$$F(\mathbf{n}) = \int_\Omega f(\mathbf{n}) d\mathbf{x} = \int_\Omega f_0(\mathbf{n}) d\mathbf{x} + \int_\Omega f_\nabla(\mathbf{n}) d\mathbf{x}. \tag{2.1}$$

From Peng-Robinson EOS, the Helmholtz free energy $f_0(\mathbf{n})$ of a homogeneous fluid is given by

$$f_0(\mathbf{n}) = f_0^{\text{ideal}}(\mathbf{n}) + f_0^{\text{excess}}(\mathbf{n}),$$