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A Convex-Splitting Scheme for a Diffuse Interface Model with Peng-Robinson Equation of State

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Abstract. We present a convex-splitting scheme for the fourth order parabolic equation derived from a diffuse interface model with Peng-Robinson equation of state for pure substance. The semi-implicit scheme is proven to be uniquely solvable, mass conservative, unconditionally energy stable and L^∞ convergent with the order of $\mathcal{O}(\Delta t + h^2)$. The numerical results verify the effectiveness of the proposed algorithm and also show good agreement of the numerical solution with laboratory experimental results.

AMS subject classifications: 65M06, 65M12, 65G99

Key words: Diffuse interface model, fourth order parabolic equation, convex-splitting scheme, convergence.

1 Introduction

Modeling and simulation of the multi-phase hydrocarbon systems involved in the oil-exploitation process are have been popular research topics in engineering practice recently [8]. The anisotropic force at the surface or an interface between two different phases at a pore scale yields the interfacial tension and consequently impacts the shape of liquid-gas interface. Moreover, the capillary effect caused by the surface tension in the Darcy-scale is usually the leading mechanism of oil recovery in fractured oil reservoirs [14]. Therefore, it is critical to simulate the interface between different phases of oil mixture and calculate the surface tension in appropriate scale.

The diffuse interface model is applied to evaluate the surface tension since it could provide more detailed description of the interface than the sharp interface model and more computational efficient than the numerical simulation conducted on the molecular scale. This theory was originally founded by van der Waals [29] to study the interface based on thermodynamic principles [1], and extended by Cahn and Hilliard [3–5]. In the

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popularly studied Allen-Cahn equation and Cahn-Hilliard equation, the total free energy with double-well potential type homogeneous density is usually employed to qualitatively predict the interface behaviors of various multi-phase fluids. However, the free energy based on a realistic equation of state is really necessary to quantitatively describe the concerning behaviors of the crude oil mixture. The Peng-Robinson equation of state is well-known for its reliability on predicting volumetric and phase behaviors of complex hydrocarbon system [20,25]. The total free energy provided by this equation of state have been applied successfully to determine the evolution process or steady state of realistic hydrocarbon species in oil-gas systems within the framework of diffuse interface model, such as the work on simulations of the surface tension of single or multi-component mixtures [12–14, 23].

The equations derived from Peng-Robinson equation of state involve high nonlinearity. It is rather challenging to design numerical scheme involve such strong nonlinearity. In addition, the energy stability is quite desirable due to its physical background. Up to now, there are two basic approaches to guarantee energy stability. The first one is called the stabilized method, where stabilized terms are added to both sides of the equations. Energy stability has been proved either under a Lipschitz assumption on the nonlinearity [27], or under a L^∞ bound assumption on the numerical solution [34]. Recently, these technical restrictions have been removed in [16, 17]. The second approach is the convex-splitting scheme which was developed by Eyer in 1998 for the Cahn-Hilliard equation [7]. By using this method, the original total energy is divided into convex part and concave part. The derivative of the convex part in the equation is treated implicitly and the derivative of the concave part is treated explicitly. This scheme is uniquely solvable due to the convexity of the modified energy expression which is also stable during the whole evolution process. So far, there are many achievements have been obtained based on this method, see e.g., [2, 6, 9–11, 26, 30–33], and the references therein.

In this paper, we investigate the fourth-order parabolic equation derived from total free energy with the Peng-Robinson equation of state [13] of particular pure substances. As mentioned in the work of Qiao et al. [23], the homogeneous energy density is almost linear, and its nonconvexity can only be detected after subtracting a linear function from its original formula. Here, a first order convex-splitting scheme is proposed to solve this fourth order equation. The theoretical analysis manifests the mass conservation, unconditional stability and L^∞ convergence of this scheme. The unboundness of the homogeneous chemical potential is the main difficulty to obtain the convergence of this scheme. To overcome this barrier, we assume the unique existence of the original fourth order parabolic equation on a close subset of of its reasonable region $(0, \frac{1}{b})$, and apply a mathematical induction method to derive the bound of the new step solution.

This paper is organized as follows. The fourth order parabolic equation and its semi-discrete convex-splitting form are presented in next section. And then some auxiliary lemmas are provided based on appropriate spaces in the third section. After that, the fully discrete version of the convex-splitting scheme for the fourth-order parabolic equation and its unique solvability, energy stability and the convergence are proved in the