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Energy Stable Linear Schemes for Mass-Conserved Gradient Flows with Peng-Robinson Equation of State

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Abstract. First and second order numerical schemes for the fourth order parabolic equation with Peng-Robinson equation of state, which are based on recently proposed invariant energy quadratisation method are developed. Both schemes are linear, unconditionally energy stable and uniquely solvable. The reduced linear systems are symmetric and positive definite, so that their solutions can be efficiently found. Numerical results demonstrate the good performance of the schemes, consistent with experimental data.

AMS subject classifications: 65N30, 65N50, 49S05

Key words: Conservative gradient flow, Peng-Robinson equation of state, invariant energy quadratisation, unconditional energy stability.

1. Introduction

Modeling and simulation of the multi-phase hydrocarbon systems of the oil-exploitation processes are popular in engineering practice [17]. The subsurface crude oil reservoirs often contain small amounts of nitrogen, carbon dioxide and hydrocarbons from methane through C_{30+} in both vapor phase and liquid phase together with solid phase (rock or soil) and water phase [29,41]. The anisotropic forces at the surface or interface between immiscible and/or partially miscible fluids at pore-scale yield the surface tension. The capillary effect at Darcy-scale and the resultant capillary pressure caused by the surface tension is one of the major forces in fluid flow and transport in subsurface reservoirs. It is also the leading mechanism in oil recovery from fractured oil reservoirs [29]. In addition, the surface tension influences the relative permeability and residual saturation in porous medium

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processes and thus influences the flow and the transport of the vapor and liquid phases on the pore scale. Therefore, appropriate mathematical models play an important role in simulation and prediction of interface phenomena and in the calculation of important interface parameters connected with different phases of oil mixture.

There are at least three main approaches to the study of interface phenomena. The first one is carried out either by molecular Monte Carlo simulations or molecular dynamics simulation with an intermolecular potential function [12,38]. The second approach is known as sharp interface modeling. In this case, the interface is considered as a zero-thickness two-dimensional entity, where density experiences a big jump [23,28,38]. Although it can predict the shape and the dynamics of the interface with a given interface tension, the interface details can not be derived. The third one is the phase field model [44], gradient theory [4], diffuse interface model [33]. The density is constant for homogeneous phase and experiences continuous variation at the interface.

In our simulations of the interface phenomena, the phase field model is selected. This well-known model was established by Van der Waals [42] in his work on the interface predictions based on thermodynamic principles [1], and extended by Cahn and Hilliard [5–7]. To describe the final steady state of a system based on the well accepted second thermodynamic law, the Helmholtz free energy is usually used as starting point. According to the phase field model, the total Helmholtz free energy often consists of the homogeneous part of pure phase for substance and the gradient part determined by the density variation at the interface. Thus the total energy can be approximated by a functional, describing the phenomenological characters of the investigated system — e.g. by the double-well potential [21,22], the molecular beam epitaxy model with [39] or without [8,9,40] slope selection, the Ericksen-Leslie model for nematic liquid crystal flows [13], the phase field crystal energy functional [2,24], the energy of polymer hydrogels [37,50] and so on. On the other hand, to provide reliable predictions for all thermodynamic properties, the total Helmholtz free energy has been obtained from the equation of state for a real substance. To derive the corresponding free energy expressions, serious efforts are needed. In particular, for every substance of interest at each development step, some practical laboratory experiments should be carried out along with the study of the interaction of different components or different phases for real mixture. The Peng-Robinson equation of state model is used more often than other cubic equations of the state due to better prediction of fluid densities and reliable results in the vicinity of critical regions [34,41].

These energy functionals are used to derive the Euler-Lagrange equation for the system equilibrium. The popular Allen-Cahn and Cahn-Hilliard equations are typical examples of such flows. A variety of numerical schemes for parabolic equations are based on these energy functionals. Note that the main concern for these methods is the energy stability and, excluding the approach [40], there are four ways to guarantee this. The first one, relying on the addition to discrete equation of a stabilised term of order $\mathcal{O}(\Delta t)$ or higher, is called the stabilised method [44,51]. The stabilised parameter should be expedient to balance the stability and convergence of the scheme [31]. The second one is the convex-splitting scheme proposed by Eyre [15] for the Cahn-Hilliard equation. The basic idea of this method is that if the total energy could be represented as the difference of two con-