Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. **14**, No. 2, pp. 494-527

DOI: 10.4208/aamm.OA-2021-0008
April 2022

Exponential Time Differencing Schemes for the Peng-Robinson Equation of State with Preservation of Maximum Bound Principle

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Received 10 January 2021; Accepted (in revised version) 9 June 2021

Abstract. The Peng-Robison equation of state, one of the most extensively applied equations of state in the petroleum industry and chemical engineering, has an excellent appearance in predicting the thermodynamic properties of a wide variety of materials. It has been a great challenge on how to design numerical schemes with preservation of mass conservation and energy dissipation law. Based on the exponential time difference combined with the stabilizing technique and added Lagrange multiplier enforcing the mass conservation, we develop the efficient first- and second-order numerical schemes with preservation of maximum bound principle (MBP) to solve the single-component two-phase diffuse interface model with Peng-Robison equation of state. Convergence analyses as well as energy stability are also proven. Several two-dimensional and three-dimensional experiments are performed to verify these theoretical results.

AMS subject classifications: 35B50, 35K55, 65M12

Key words: Peng-Robinson equation of state, diffuse interface model, maximum bound principle, exponential time differencing, Lagrange multiplier.

1 Introduction

Equations of state (EOS) modeling are widely used for predicting the fluids phase properties [35, 36]. As one of the most prominent methods, the Peng-Robinson equation of

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state [38] has been widely studied and applied for describing the thermodynamic properties of fluids in chemical engineering and petroleum industry, such as phase equilibria calculations [24–26] and prediction of surface tension between gas and liquid [27, 30]. Among various EOS models, the Peng-Robinson EOS is considered as one of the best two constants third-degree equations of the state applicable to vapor-liquid equilibria, and volumetric and thermodynamic properties calculations for pure substances and mixtures. Based on thermodynamic principles [1], the well-known model is established by Van der Waals [43] and is then extended by Cahn and Hilliard [6, 7]. To describe the initial value of multi-component mixture when the Peng-Robinson EOS is involved, the NVT flash calculation (temperature T, volume V, and composition N) is a common phase splitting approach, which is based on calculation with moles, volume, and temperature as the primal state variables. It allows us to get the molar density of gas and liquid of a specific substance when the phase transition occur. The total Helmholtz free energy based on the well-accepted second thermodynamic law often consists of the homogeneous part of pure phase for substance and the gradient part determined by the density variation at the interface for the phase-field model. Thus we can use the functional to approximate the total energy, such as the double-well potential [20, 21], the molecular beam epitaxy model with [42] or without slope selection [10, 11], the phase field crystal energy functional [2, 23] and so on. The Peng-Robinson EOS is more commonly used than other cubic equation of state models because it can better predict fluid density and obtain reliable results near the critical region.

Since the structure of its energy functional is highly nonlinear and more complicated than many conventional phase field models of the diffuse interface model, it is desired to design an accurate and efficient energy stable numerical method for the Peng-Robinson EOS. One numerical method is the convex splitting scheme inheriting the discrete energy dissipation law which have been extensively used in recent works, we refer to [16, 26, 39, 40, 46]. The convex splitting approach can be proved to be unconditionally energy stable. However, it produces stiff nonlinear systems that demand the complicated implement of efficient nonlinear iterative solvers and cost expensively at each time step. The invariant energy quadratization (IEQ) approach [51–53] is a novel method and has been intensively applied to many phase field models for gradient flow models which generalizes the Lagrange multiplier approach proposed in [17]. The essential idea of IEQ is to transform the bulk free energy into a quadratic form through introducing a set of new variables which still retains a similar energy dissipation law. The scalar auxiliary variable (SAV) approach [44, 45] is inspired by the IEQ approach but improves most of its shortcomings. It only the convex splitting needs to solve the linear, decoupled systems with constant coefficients at each time steps and leads to the second-order unconditional stablility. There has been many researches related to IEQ and SAV approaches for solving the Peng-Robinson EOS. For example, Li et al. [32, 54] designed first order and second order schemes for temporal discretization of the diffusive interface model with the Peng-Robinson EOS based on the IEQ approach for the single-component two-phase fluid system and the multi-component two-phase fluid system. Qiao et al. [41] employed SAV nu-