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SAV Finite Element Method for the Peng-Robinson Equation of State with Dynamic Boundary Conditions

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Abstract. In this paper, the Peng-Robinson equation of state with dynamic boundary conditions is discussed, which considers the interactions with solid walls. At first, the model is introduced and the regularization method on the nonlinear term is adopted. Next, The scalar auxiliary variable (SAV) method in temporal and finite element method in spatial are used to handle the Peng-Robinson equation of state. Then, the energy dissipation law of the numerical method is obtained. Also, we acquire the convergence of the discrete SAV finite element method (FEM). Finally, a numerical example is provided to confirm the theoretical result.

AMS subject classifications: 35K35, 35K55, 65M12, 65M60

Key words: Peng-Robinson equation of state, dynamic boundary conditions, scalar auxiliary variable, finite element method, error estimates.

1 Introduction

Hydrocarbon reservoirs engineering is a technical science which is engaged in the oilfield development design and engineering analysis method [1,2]. Its research concludes the movement law and displacement mechanism of oil, gas, and water in the development process of the reservoir (or gas reservoir). And it is also formulates corresponding engineering measures in order to improve the recovery rate and recovery factor, reasonably. The numerical simulation is a great choice to research this process. A very important research direction in hydrocarbon reservoirs engineering is using diffusion interface theory [3–5] to carry out numerical simulation of physical phenomena such as gas bubbles, droplets and capillaries pressure by the interface between phases. So, using the

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phase-field model is a general method for numerical simulation in this direction. Then, a density-dependent nonlinear system is obtained by applying the variational derivative to the Helmholtz free energy. Such a system is more consistent with the rules of energy dissipation. The Peng-Robinson equation of state is widely used phase-field model in hydrocarbon reservoirs engineering [6–12]. Compared with the two-well potential in the Allen-Cahn equation and Cahn-Hilliard equation [13–15], because of logarithmic term of the nonlinear term, the Peng-Robinson equation of state is more accurate and can reflect the real state of the fluids.

Usually, periodic boundary condition and the Neumann boundary condition are used in phase-field model [14,16]. By using these boundary conditions, the positive symmetry of the stiffness matrix can be maintained while using the finite element method, spectral method and difference method and so on, and the computational complexity of a small area on the boundary can be reduced greatly, especially for the fast algorithm FFT. Moreover, the models with classical boundary conditions leave the influence of external factors on the boundary out of consideration, which results in unsatisfactory outcomes. Recently, the dynamic boundary condition is proposed by the research [17], where the existence and uniqueness of a global weak solution are proved. According to the law of energy and the equilibrium of the system, the dynamic boundary condition is determined. The relationship between the two intersecting interfaces is better simulated, as well as, the calculation is also more complicated.

It is necessary to carry out numerical simulation of the phase-field models to describe the diffusion phenomenon, since the exact solution is difficult to confirm. Generally, the implicit scheme is applied to discrete the models in order to keep the energy unconditional stable. It is unavoidable to use the inner iteration, which increase the computational cost. For purpose of decreasing the time consumption, a lot of methods are proposed for the numerical solution of the phase-field model. The ETD methods in [18] refer to exact integration of the governing equations followed by an explicit approximation of a temporal integral relating to the nonlinear terms. Recently, the SAV method was introduced in the researches [15, 19], which can keep the energy stability of the whole system. By applying this method, we solve a constant coefficient equation at each step of the calculation. Furthermore, a new SAV method was proposed in [20] by applying the new scalar variable to make two linear equations into one linear equation, which reduce half of the time cost and keep original SAV method the other strengths. In addition, the convex splitting energy stable scheme make the equations have the property of unconditionally energy stable [11, 21]. Another interesting method is IEQ [22, 24], which discretized the nonlinear terms by the semi-explicit method. Meanwhile, the linear system is positive and the properties of the whole system are maintained.

In this paper, we mainly study the Peng-Robinson equation of state with dynamic boundary conditions and use the SAV method to keep the conservation of mass and energy dissipation in the bulk and on the surface. At the same time, we give the corresponding error analysis and a numerical example. In Section 2, we introduce the Peng-Robinson equation of state and dynamic boundary conditions. Meanwhile, we adopt the