

## 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.

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

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## 1 Introduction

Hydrocarbon reservoirs engineering is a technical science which is engaged in the oil-field 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

regularization method on the nonlinear term. In Section 3, we discretize the equations of state in space and time by using the SAV finite element method and obtain the energy dissipation law of the numerical method. In Section 4, we prove the first-order convergence of discrete Peng-Robinson equation of state. By a numerical example, we compare the difference between dynamic boundary conditions and classical boundary conditions in Section 5.

## 2 The SAV scheme of Peng-Robinson equation of state

### 2.1 The Holmholtz free energy of two-phase fluid with the dynamic boundary conditions

Let us start with some standard notations [25]. We assume that the bulk  $\Omega \in \mathbb{R}^d$  ( $d=2,3$ ) is a bounded Lipschitz domain with the boundary  $\Gamma$ . In this paper, the spaces  $W^{m,p}(\Omega)$  and  $W^{m,p}(\Gamma)$  mean the normal Sobolev spaces. Especially, the spaces  $W^{m,2}(\Omega)$  and  $W^{m,2}(\Gamma)$  are denoted by  $H^m(\Omega)$  and  $H^m(\Gamma)$ , respectively.  $(\cdot, \cdot)$  and  $\langle \cdot, \cdot \rangle$  are the inner product in the bulk and on the surface, respectively.

We focus on a two-phase fluid system at constant temperature, constant number of molecules, and a fixed domain. Then, we denote by  $u$  the molar density in the bulk. By the second law of thermodynamics, we know that the whole system is in equilibrium, when the Holmholtz free energy  $E[u]$  is at its minimum [10]. The Holmholtz free energy can contribute in two ways. One part comes from the energy produced by the homogeneous fluid, and the other part comes from the energy produced by the inhomogeneous fluid

$$E[u] = \int_{\Omega} \left( \frac{c}{2} |\nabla u|^2 + F(u) \right) dx + \hat{C},$$

where the parameter  $c$  is determined by the temperature and the molar density. While, molar density has very little effect on  $c$ . Consequently,  $c$  is a constant when the temperature  $T$  is given. And  $\hat{C}$  is a positive constant to ensure  $E[u] > 0$ .  $F(u)$  is a nonlinear function of  $u$ . We denote by  $u_{\Gamma}$  the molar density on the surface. By using the denotation in [17], the Holmholtz free energy can be divided into the bulk and the surface

$$E_{total}[u] := E_{bulk}[u] + E_{surface}[u_{\Gamma}], \quad (2.1)$$

where

$$E_{bulk}[u] = \int_{\Omega} \left( \frac{c}{2} |\nabla u|^2 + F(u) \right) dx + \hat{C}_1, \quad (2.2a)$$

$$E_{surface}[u_{\Gamma}] = \int_{\Gamma} \left( \frac{\kappa c}{2} |\nabla_{\Gamma} u_{\Gamma}|^2 + \kappa G(u_{\Gamma}) \right) ds + \hat{C}_2, \quad (2.2b)$$

with the constants  $c, \kappa > 0$ . And we can force  $G(u_\Gamma) = F(u_\Gamma)$ .  $\hat{C}_1$  and  $\hat{C}_2$  are the positive constant assuring  $E_{bulk}[u] > 0$  and  $E_{surface}[u_\Gamma] > 0$ . Then, we record

$$E_1[u] := \int_{\Omega} F(u) dx + \hat{C}_1, \quad E_2[u_\Gamma] := \int_{\Gamma} G(u_\Gamma) ds + \hat{C}_2,$$

respectively.

## 2.2 SAV Peng-Robinson equation of state

Peng-Robinson equation of state is the most common fluid model in hydrocarbon reservoirs engineering. Based on this model, the free energy of the inhomogeneous fluid is given as follows

$$\begin{aligned} F(u) &= F_1(u) + F_2(u), \\ F_1(u) &:= RTu(\ln u - 1) - RTu \ln(1 - bu), \\ F_2(u) &:= \frac{a(T)u}{2\sqrt{2}b} \ln \left( \frac{1 + (1 - \sqrt{2})bu}{1 + (1 + \sqrt{2})bu} \right), \end{aligned}$$

where  $R$  is the universal gas constant, and the energy parameter  $a(T)$  and the co-volume parameter  $b$  are related to the mixing rules of the pure fluids. Theoretically,  $u \in (0, 1/b)$ . It is easy to see that the domain of  $F_2(u)$  is  $(-\frac{\sqrt{2}-1}{b}, \infty)$ . So it is bounded at the interval  $[0, \frac{1}{b}]$ . However, when  $u=0$  and  $u=\frac{1}{b}$ ,  $F_1(u)$  is singular. In [12], based on the regularization method,  $F_1(u)$  can be given as a convex,  $C^2$  continuous, piecewise function,

$$\hat{F}_1(u) := \begin{cases} RTu \left( \ln \frac{\delta}{b} - 1 \right) - RTu \ln(1 - bu) + RT \left( \frac{bu^2}{2\delta} - \frac{\delta}{2b} \right), & \text{if } u \in \left[ 0, \frac{\delta}{b} \right), \\ RTu(\ln u - 1) - RTu \ln(1 - bu), & \text{if } u \in \left[ \frac{\delta}{b}, \frac{1-\delta}{b} \right], \\ RTu(\ln u - 1) - RTu \ln \delta \\ \quad + RT \left[ \frac{b\delta + b}{2\delta^2} \left( u - \frac{1-\delta}{b} + \frac{\delta(1-\delta)}{b(1+\delta)} \right)^2 - \frac{(1-\delta)}{2b(1+\delta)} \right], & \text{if } u \in \left( \frac{1-\delta}{b}, \frac{1}{b} \right], \end{cases} \quad (2.3)$$

where for any  $\delta > 0$ . And  $\hat{F}_1(u) \rightarrow F_1(u)$ , when  $\delta \rightarrow 0$ . So we have a nonlinear function that is bounded at the interval  $[0, \frac{1}{b}]$  and nonsingular,

$$\hat{F}(u) = \hat{F}_1(u) + F_2(u). \quad (2.4)$$

For convenience, we redefine  $\hat{F}(u)$  as  $F(u)$ .

**Lemma 2.1.** *There exists positive constants  $\bar{C}_1, \bar{C}_2$  such that*

$$-\bar{C}_1 \delta^{-1} \leq F''(u) \leq \bar{C}_2 \delta^{-2}. \quad (2.5)$$

*Proof.* Firstly, we consider the function  $F_1(u)$ . If  $u \in [\frac{\delta}{b}, \frac{1-\delta}{b}]$ , we get

$$bRT + \frac{bRT}{\delta} \leq F_1''(u) = \frac{RT}{u} + \frac{bRT(2-bu)}{(1-bu)^2} \leq \frac{bRT}{\delta} + 2bRT. \quad (2.6)$$

Next, if  $u \in [0, \frac{\delta}{b})$ , we have

$$\frac{bRT(1-b)^2}{\delta} \leq F_1''(u) = \frac{RTb[(1-bu)^2(1-b^2)+\delta]}{\delta(1-bu)^2} \leq \frac{bRT(1-b)^2}{\delta} + 1. \quad (2.7)$$

Then, if  $u \in (\frac{1-\delta}{b}, \frac{1}{b}]$ , (2.3) becomes to

$$\frac{bRT}{\delta} + bRT \leq F_1''(u) = \frac{RT}{u} + RT \frac{b(1+\delta)}{\delta^2} \leq \frac{bRT(1+\delta)}{\delta^2} + bRT. \quad (2.8)$$

In addition, as for the function  $f_2(u)$ , if  $u \in [0, \frac{1}{b}]$ , we get

$$F_2''(u) = -\frac{a(T)}{1+bu+bu(1-bu)} - \frac{a(T)(1-b^3u^2)}{(1+bu+bu(1-bu))^2}. \quad (2.9)$$

It is evident that  $F_2''(u)$  is a continuous function at the closed interval  $[0, \frac{1}{b}]$ . So, there exists  $\bar{C}_3, \bar{C}_4$  such that

$$-\bar{C}_3 \leq F_2''(u) \leq \bar{C}_4. \quad (2.10)$$

Combining (2.6)-(2.10), we can complete the proof of the Lemma 2.1.  $\square$

From (2.1) and (2.4), by using the variational derivative, we can obtain the SAV Peng-Robinson equation of state with dynamic boundary conditions

$$\left\{ \begin{array}{ll} u_t = -\mu & \text{in } \Omega \times (0, T], \\ u_{t,\Gamma} = -\mu_\Gamma & \text{on } \Gamma \times (0, T], \\ \mu + \kappa\mu_\Gamma = -c\Delta u - \kappa c\Delta_\Gamma u_\Gamma + \frac{r_1}{\sqrt{E_1[u]}}f(u) \\ \quad + \frac{\kappa r_2}{\sqrt{E_2[u_\Gamma]}}g(u_\Gamma) & \text{in } \bar{\Omega} \times (0, T], \\ r_{t,1} = \frac{1}{2\sqrt{E_1[u]}}(f(u), u_t) & \text{in } (0, T], \\ r_{t,2} = \frac{1}{2\sqrt{E_2[u_\Gamma]}}\langle g(u_\Gamma), u_{t,\Gamma} \rangle & \text{in } (0, T], \end{array} \right. \quad (2.11)$$

where  $f(u) := F'(u)$  and we can force  $g(u_\Gamma) = f(u_\Gamma) := F'(u_\Gamma)$ . Then  $\Delta_\Gamma$  means Laplace-Beltrami operator. Also,  $r_1(t) = \sqrt{E_1[u]}$  and  $r_2(t) = \sqrt{E_2[u_\Gamma]}$  are scalar auxiliary variables, respectively. In addition, the SAV Peng-Robinson equation of state has the initial value conditions

$$u(x, 0) = u_0(x), \quad r_1(0) = \sqrt{E_1[u(0)]}, \quad r_2(0) = \sqrt{E_2[u_\Gamma(0)]}. \quad (2.12)$$

And,  $u_\Gamma, \mu_\Gamma$  are the limits of  $u, \mu$  on the surface, which are

$$u|_\Gamma(x,t) = u_\Gamma(x,t), \quad \mu|_\Gamma(x,t) = \mu_\Gamma(x,t) \quad \text{on } \Gamma \times (0,T]. \quad (2.13)$$

There exist the unique solutions  $u, u_\Gamma$  in (2.11) such that

$$u \in C(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega)), \quad u_\Gamma \in C(0,T;H^1(\Gamma)) \cap L^2(0,T;H^2(\Gamma)). \quad (2.14)$$

The proof is similar to the way in [23] and we omit the process.

Then we reword the Peng-Robison equation of state in a weak formula: for any  $t \in (0,T]$ , finding  $(u, u_\Gamma, \mu, \mu_\Gamma, r_1, r_2) \in H^1(\Omega) \times H^1(\Gamma) \times L^2(\Omega) \times L^2(\Omega) \times C^1(0,T] \times C^1(0,T]$  such that

$$(u_t, \theta_1) = -(\mu, \theta_1), \quad \forall \theta_1 \in L^2(\Omega), \quad (2.15a)$$

$$\langle u_{t,\Gamma}, \theta_2 \rangle = -\langle \mu_\Gamma, \theta_2 \rangle, \quad \forall \theta_2 \in L^2(\Gamma), \quad (2.15b)$$

$$\begin{aligned} (\mu, v) + \kappa \langle \mu_\Gamma, v \rangle &= c(\nabla u, \nabla v) + \kappa c \langle \nabla_\Gamma u_\Gamma, \nabla_\Gamma v \rangle \\ &\quad + \frac{r_1}{\sqrt{E_1[u]}} (f(u), v) + \frac{\kappa r_2}{\sqrt{E_2[u_\Gamma]}} \langle g(u), v \rangle, \quad \forall v \in H^1(\bar{\Omega}), \end{aligned} \quad (2.15c)$$

$$r_{t,1} = \frac{1}{2\sqrt{E_1[u]}} (f(u), u_t), \quad (2.15d)$$

$$r_{t,2} = \frac{1}{2\sqrt{E_2[u_\Gamma]}} \langle g(u_\Gamma), u_{t,\Gamma} \rangle. \quad (2.15e)$$

### 3 Discrete SAV FEM scheme and its energy dissipation

In order to approximating the solution of the weak formula (2.15a)-(2.15e), we apply the finite element method in spatial. Assuming that  $V_h$  is a finite element space included in  $H^1(\bar{\Omega})$ . Then, there is a discrete finite element scheme as follows: finding a solution  $(u_h^{n+1}, u_{h,\Gamma}^{n+1}, \mu_h^{n+1}, \mu_{h,\Gamma}^{n+1}, r_{h,1}^{n+1}, r_{h,2}^{n+1}) \in [V_h]^4 \times \mathbb{R}^2$  satisfying that

$$(u_h^{n+1} - u_h^n, \theta_1) = -\Delta t (\mu_h^{n+1}, \theta_1), \quad \forall \theta_1 \in V_h, \quad (3.1a)$$

$$\langle u_{h,\Gamma}^{n+1} - u_{h,\Gamma}^n, \theta_2 \rangle = -\Delta t \langle \mu_{h,\Gamma}^{n+1}, \theta_2 \rangle, \quad \forall \theta_2 \in V_h, \quad (3.1b)$$

$$\begin{aligned} (\mu_h^{n+1}, v) + \kappa \langle \mu_{h,\Gamma}^{n+1}, v \rangle &= c(\nabla u_h^{n+1}, \nabla v) + \kappa c \langle \nabla_\Gamma u_{h,\Gamma}^{n+1}, \nabla_\Gamma v \rangle \\ &\quad + \frac{r_{h,1}^{n+1}}{\sqrt{E_1[u_h^n]}} (f(u_h^n), v) + \frac{\kappa r_{h,2}^{n+1}}{\sqrt{E_2[u_{h,\Gamma}^n]}} \langle g(u_h^n), v \rangle, \quad \forall v \in V_h, \end{aligned} \quad (3.1c)$$

$$r_{h,1}^{n+1} - r_{h,1}^n = \frac{1}{2\sqrt{E_1[u_h^n]}} (f(u_h^n), u_h^{n+1} - u_h^n), \quad (3.1d)$$

$$r_{h,2}^{n+1} - r_{h,2}^n = \frac{1}{2\sqrt{E_2[u_{h,\Gamma}^n]}} \langle g(u_{h,\Gamma}^n), u_{h,\Gamma}^{n+1} - u_{h,\Gamma}^n \rangle, \quad (3.1e)$$

with

$$u_h^0 = P_h u(x, 0), \quad r_{1,h}^0 = \sqrt{E_1[u_h^0]}, \quad r_{2,h}^0 = \sqrt{E_2[u_h^0]}, \quad (3.2)$$

where  $P_h : L^2 \rightarrow V_h$  is the  $L^2$  projection, and  $u_{h,\Gamma}$ ,  $\mu_{h,\Gamma}$  are the limit of  $u_h$ ,  $\mu_h$  on the surface  $\Gamma$ ,

$$u_h|_{\Gamma}(x, t) = u_{h,\Gamma}(x, t), \quad \mu_h|_{\Gamma}(x, t) = \mu_{h,\Gamma}(x, t). \quad (3.3)$$

Firstly, we present that the SAV FEM scheme satisfies the energy dissipation.

**Lemma 3.1.** *For the Peng-Robinson equation of state (3.1a)-(3.1e) and any  $n \leq \frac{T}{\Delta t}$ , we have*

$$\begin{aligned} & \frac{c}{2} \|\nabla u_h^{n+1}\|^2 + \frac{\kappa c}{2} \|\nabla_{\Gamma} u_{h,\Gamma}^{n+1}\|^2 + (r_{h,1}^{n+1})^2 + \kappa (r_{h,2}^{n+1})^2 \\ & \leq \frac{c}{2} \|\nabla u_h^n\|^2 + \frac{\kappa c}{2} \|\nabla_{\Gamma} u_{h,\Gamma}^n\|^2 + (r_{h,1}^n)^2 + \kappa (r_{h,2}^n)^2. \end{aligned} \quad (3.4)$$

*Proof.* Let  $\theta_1 = \mu_h^{n+1}$ ,  $\theta_2 = \mu_{h,\Gamma}^{n+1}$ ,  $v = u_h^{n+1} - u_h^n$  in (3.1a)-(3.1c), respectively, and multiplying (3.1d) and (3.1e) by  $2r_{h,1}^{n+1}$ ,  $\kappa \cdot 2r_{h,2}^{n+1}$ , respectively. We can derive

$$\begin{aligned} & \frac{c}{2} \|\nabla u_h^{n+1}\|^2 + \frac{\kappa c}{2} \|\nabla_{\Gamma} u_{h,\Gamma}^{n+1}\|^2 + (r_{h,1}^{n+1})^2 + \kappa (r_{h,2}^{n+1})^2 - \frac{c}{2} \|\nabla u_h^n\|^2 \\ & - \frac{\kappa c}{2} \|\nabla_{\Gamma} u_{h,\Gamma}^n\|^2 - (r_{h,1}^n)^2 - \kappa (r_{h,2}^n)^2 + \frac{c}{2} \|\nabla(u_h^{n+1} - u_h^n)\|^2 \\ & + \frac{\kappa c}{2} \|\nabla_{\Gamma}(u_{h,\Gamma}^{n+1} - u_{h,\Gamma}^n)\|^2 + (r_{h,1}^{n+1} - r_{h,1}^n)^2 + \kappa (r_{h,2}^{n+1} - r_{h,2}^n)^2 \\ & \leq -\Delta t \|\nabla \mu_h^{n+1}\|^2 - \kappa \Delta t \|\nabla_{\Gamma} \mu_{h,\Gamma}^{n+1}\|^2 \leq 0. \end{aligned} \quad (3.5)$$

Rewrite (3.5) and then Lemma 3.1 can be proved, immediately.  $\square$

Thus, the scheme is unconditionally energy stable by (3.5). Next, the following is used to describe how the SAV FEM scheme is implemented.  $b_{h,1}^n$ ,  $b_{h,2}^n$  are given as

$$b_{h,1}^n := \frac{P_h f(u_h^n)}{\sqrt{E_1[u_h^n]}}, \quad b_{h,2}^n := \frac{P_h g(u_{h,\Gamma}^n)}{\sqrt{E_2[u_{h,\Gamma}^n]}}. \quad (3.6)$$

Combining (3.1a)-(3.1e) to eliminate  $\mu_h^{n+1}$ ,  $\mu_{h,\Gamma}^{n+1}$ ,  $r_{h,1}^{n+1}$  and  $r_{h,2}^{n+1}$ , we derive

$$\begin{aligned} & (u_h^{n+1} - u_h^n, v) + \kappa \langle u_{h,\Gamma}^{n+1} - u_{h,\Gamma}^n, v \rangle \\ & = -\Delta t (c \langle \nabla u_h^{n+1}, \nabla v \rangle + \kappa c \langle \nabla u_{h,\Gamma}^{n+1}, \nabla v \rangle) \\ & - \Delta t \left( r_{h,1}^n + \frac{1}{2} (b_{h,1}^n, u_h^{n+1} - u_h^n) (b_{h,1}^n, v) + \kappa r_{h,2}^n \right. \\ & \left. + \frac{1}{2} \langle b_{h,2}^n, u_{h,\Gamma}^{n+1} - u_{h,\Gamma}^n \rangle \langle b_{h,2}^n, v \rangle \right). \end{aligned} \quad (3.7)$$

After defining  $d_{h,1}^n, d_{h,2}^n \in V_h$  as

$$d_{h,1}^n = \left(1 + \frac{\Delta t}{2} (b_{h,1}^n, b_{h,1}^n)\right) (u_h^n, v) - \Delta t r_{h,1}^n (b_{h,1}^n, v), \quad (3.8a)$$

$$d_{h,2}^n = \left(1 + \frac{\Delta t}{2} \langle b_{h,2}^n, b_{h,2}^n \rangle\right) \langle u_{h,\Gamma}^n, v \rangle - \Delta t r_{h,2}^n \langle b_{h,2}^n, v \rangle, \quad (3.8b)$$

Eq. (3.7) can be rewritten as

$$\begin{aligned} & \left(1 + \frac{\Delta t}{2} (b_{h,1}^n, b_{h,1}^n)\right) (u_h^{n+1}, v) + \left(1 + \frac{\Delta t}{2} \langle b_{h,2}^n, b_{h,2}^n \rangle\right) \langle u_{h,\Gamma}^{n+1}, v \rangle \\ & + c\Delta t (\nabla u_h^{n+1}, \nabla v) + \kappa c\Delta t \langle \nabla u_{h,\Gamma}^{n+1}, \nabla v \rangle \\ & = (d_{h,1}^n, v) + \langle d_{h,2}^n, v \rangle. \end{aligned} \quad (3.9)$$

In conclusion, we implement the SAV algorithm of the Peng-Robinson equation of state (3.1a)-(3.1e) as follows:

- i). Calculate  $b_{h,1}^n, b_{h,2}^n$  from (3.6).
- ii). Calculate  $d_{h,1}^n, d_{h,2}^n$  from (3.8a) and (3.8b).
- iii). Solve  $u_h^{n+1}, u_{h,\Gamma}^{n+1}$  from (3.9).
- iv). Update  $r_{h,1}^{n+1}, r_{h,2}^{n+1}$  from

$$\begin{aligned} r_{h,1}^{n+1} &= r_{h,1}^n + \frac{1}{2} (b_{h,1}^n, u_h^{n+1}) - \frac{1}{2} (b_{h,1}^n, u_h^n), \\ r_{h,2}^{n+1} &= r_{h,2}^n + \frac{1}{2} \langle b_{h,2}^n, u_{h,\Gamma}^{n+1} \rangle - \frac{1}{2} \langle b_{h,2}^n, u_{h,\Gamma}^n \rangle. \end{aligned}$$

- v). Go to the next time step.

Therefore, the discrete scheme of (3.1a)-(3.1e) is decoupled.

**Remark 3.1.** The unique solvability of the proposed SAV FEM scheme (3.1a)-(3.1e) is obvious since Eqs. (3.6)-(3.9) present the outline of solvability. In fact, it can be seen that the bilinear form

$$\begin{aligned} a(u_h^{n+1}, v) &= \left(1 + \frac{\Delta t}{2} (b_{h,1}^n, b_{h,1}^n)\right) (u_h^{n+1}, v) + \left(1 + \frac{\Delta t}{2} \langle b_{h,2}^n, b_{h,2}^n \rangle\right) \langle u_{h,\Gamma}^{n+1}, v \rangle \\ &+ c\Delta t (\nabla u_h^{n+1}, \nabla v) + \kappa c\Delta t \langle \nabla u_{h,\Gamma}^{n+1}, \nabla v \rangle \end{aligned}$$

is positive definite from the equation (3.9). We only need solve a linear system (3.9) and calculate three formulas (3.6)-(3.7) to obtain the numerical solution. That is to say, SAV method transform a nonlinear problem into a linear solver while keeping the unconditional stable. This is the glamorous advantage of SAV method!



## 4 Error estimate

In this section, we present the error estimate in temporal and in spatial, respectively. In order to get the main result, we introduce the following lemmas.

**Lemma 4.1** ([25]). *Let us denote the Ritz projection operator by  $R_h: H^1 \rightarrow V_h$ , that is,*

$$(\nabla(u - R_h u), \nabla v) = 0, \quad \forall u \in H^1(\Omega), \quad v \in V_h, \quad (4.1)$$

with

$$\int_{\Omega} R_h u dx = \int_{\Omega} u dx.$$

If  $u \in H^{k+1}(\Omega)$ , it holds

$$\|u - R_h u\|_{L^2(\Omega)} \leq Ch^{k+1} \|u\|_{H^{k+1}(\Omega)}, \quad \|u - R_h u\|_{H^1(\Omega)} \leq Ch^k \|u\|_{H^{k+1}(\Omega)}. \quad (4.2)$$

Next, before discussing the error estimate in temporal, let us denote

$$D_t \phi^{n+1} := \frac{\phi^{n+1} - \phi^n}{\Delta t}$$

for any function value  $\{\phi^n\}_{n=0}^N$ , and the exact solution  $(u, u_{\Gamma}, \mu, \mu_{\Gamma}, r_1, r_2)$  satisfies

$$(u^{n+1} - u^n, \theta_1) = -\Delta t (\mu^{n+1}, \theta_1) + \Delta t (E_u^n, \theta_1), \quad \forall \theta_1 \in L^2(\Omega) \quad (4.3a)$$

$$\langle u_{\Gamma}^{n+1} - u_{\Gamma}^n, \theta_2 \rangle = -\Delta t \langle \mu_{\Gamma}^{n+1}, \theta_2 \rangle + \Delta t \langle E_{u_{\Gamma}}^n, \theta_2 \rangle, \quad \forall \theta_2 \in L^2(\Gamma), \quad (4.3b)$$

$$\begin{aligned} (\mu^{n+1}, v) + \kappa \langle \mu_{\Gamma}^{n+1}, v \rangle &= c(\nabla u^{n+1}, \nabla v) + \frac{r_1^{n+1}}{\sqrt{E_1[u^n]}} (f(u^n), v) + (E_{\mu}^n, v) \\ &\quad + \kappa c \langle \nabla_{\Gamma} u_{\Gamma}^{n+1}, \nabla_{\Gamma} v \rangle + \frac{\kappa r_2^{n+1}}{\sqrt{E_2[u_{\Gamma}^n]}} \langle g(u_{\Gamma}^n), v \rangle \\ &\quad + \kappa \langle E_{\mu, \Gamma}^n, v \rangle, \quad \forall v \in L^2(\Omega), \end{aligned} \quad (4.3c)$$

$$r_1^{n+1} - r_1^n = \frac{1}{2\sqrt{E_1[u^n]}} (f(u^n), u^{n+1} - u^n) + \Delta t E_{r,1}^n, \quad (4.3d)$$

$$r_2^{n+1} - r_2^n = \frac{1}{2\sqrt{E_2[u_{\Gamma}^n]}} \langle g(u_{\Gamma}^n), u_{\Gamma}^{n+1} - u_{\Gamma}^n \rangle + \Delta t E_{r,2}^n, \quad (4.3e)$$

where

$$|E_u^n| = |D_t u^{n+1} - \partial_t u^{n+1}| \leq \int_{t^n}^{t^{n+1}} |u_{tt}(\cdot, \tau)| d\tau, \quad (4.4a)$$

$$|E_{u, \Gamma}^n| = |D_t u_{\Gamma}^{n+1} - \partial_t u_{\Gamma}^{n+1}| \leq \int_{t^n}^{t^{n+1}} |u_{tt, \Gamma}(\cdot, s)| ds, \quad (4.4b)$$

$$|E_{r,1}^n| = \left| D_t r_1^{n+1} - \partial_t r_1^n - \frac{1}{2\sqrt{E_1[u^n]}} (f(u^n), D_t u^{n+1} - \partial_t u^n) \right|$$

$$\leq C \left( \int_{t^n}^{t^{n+1}} |r_{tt,1}(\tau)| d\tau + \int_{t^n}^{t^{n+1}} \int_{\Omega} |u_{tt,1}(x, \tau)| d\tau dx \right), \quad (4.4c)$$

$$|E_{r,2}^n| = \left| D_t r_2^{n+1} - \partial_t r_2^n - \frac{1}{2\sqrt{E_2[u_\Gamma^n]}} \langle g(u_\Gamma^n), D_t u_\Gamma^{n+1} - \partial_t u_\Gamma^n \rangle \right|$$

$$\leq C \left( \int_{t^n}^{t^{n+1}} |r_{tt,2}(\tau)| d\tau + \int_{t^n}^{t^{n+1}} \int_{\Gamma} |u_{tt,2}(x, \tau)| d\tau ds \right), \quad (4.4d)$$

$$E_\mu^n = r_1^{n+1} \left( \frac{f(u^{n+1})}{\sqrt{E_1(u^{n+1})}} - \frac{f(u^n)}{\sqrt{E_1(u^n)}} \right), \quad (4.4e)$$

$$E_{\mu,\Gamma}^n = r_2^{n+1} \left( \frac{g(u_\Gamma^{n+1})}{\sqrt{E_2(u_\Gamma^{n+1})}} - \frac{g(u_\Gamma^n)}{\sqrt{E_2(u_\Gamma^n)}} \right). \quad (4.4f)$$

**Lemma 4.2.** According to (2.14), assume that the following regularities hold

$$u \in L^\infty([0, T]; W_\infty^1(\Omega)), \quad u_t \in L^\infty([0, T]; H^1(\Omega)), \quad u_{tt} \in L^2((0, T); L^2(\Omega)), \quad (4.5a)$$

$$u_\Gamma \in L^\infty([0, T]; W_\infty^1(\Gamma)), \quad u_{t,\Gamma} \in L^\infty([0, T]; H^1(\Gamma)), \quad u_{tt,\Gamma} \in L^2((0, T); L^2(\Gamma)). \quad (4.5b)$$

Then, for any  $N \leq T/\Delta t$ , the error estimate in temporal satisfies

$$\max_{1 \leq n \leq N} (||E_u^n||_{L^2(\Omega)} + ||E_{u,\Gamma}^n||_{L^2(\Gamma)} + ||E_\mu^n||_{L^2(\Omega)} + ||E_{\mu,\Gamma}^n||_{L^2(\Gamma)} + |E_{r,1}^n| + |E_{r,2}^n|) \leq C\Delta t,$$

where  $C > 0$  is independent of  $\Delta t$ .

*Proof.* Taking the temporal derivative of (2.15d) and (2.15e), respectively, we derive

$$r_{tt,1} = -\frac{1}{4\sqrt{E_1[u]^3}} ((f(u), u_t))^2 + \frac{1}{2\sqrt{E_1[u]}} ((f'(u), u_t^2) + (f(u), u_{tt})),$$

$$r_{tt,2} = -\frac{1}{4\sqrt{E_2[u_\Gamma]^3}} (\langle g(u_\Gamma), u_{t,\Gamma} \rangle)^2 + \frac{1}{2\sqrt{E_2[u_\Gamma]}} (\langle g'(u_\Gamma), u_{t,\Gamma}^2 \rangle + \langle g(u_\Gamma), u_{tt,\Gamma} \rangle).$$

From (2.14), we notice that  $u \in C(0, T; H^1(\Omega)) \cap L^2(0, T; H^2(\Omega))$  and  $u_\Gamma \in C(0, T; H^1(\Gamma)) \cap L^2(0, T; H^2(\Gamma))$ , so  $u \in L^\infty([0, T]; L^\infty(\Omega))$  and  $u_\Gamma \in L^\infty([0, T]; L^\infty(\Gamma))$ . Then, combining (2.5) and (4.5), using Young's inequality and imbedding theorems, we have

$$\int_0^T |r_{tt,1}|^2 dt \leq C \int_0^T (||u_t||_{L^4(\Omega)}^4 + ||u_{tt}||_{L^2(\Omega)}^2) dt$$

$$\leq C \int_0^T (||u_t||_{H^1(\Omega)}^4 + ||u_{tt}||_{L^2(\Omega)}^2) dt \leq C, \quad (4.6a)$$

$$\int_0^T |r_{tt,2}|^2 dt \leq C \int_0^T (||u_{t,\Gamma}||_{L^4(\Gamma)}^4 + ||u_{tt,\Gamma}||_{L^2(\Gamma)}^2) dt$$

$$\leq C \int_0^T (||u_{t,\Gamma}||_{H^1(\Gamma)}^4 + ||u_{tt,\Gamma}||_{L^2(\Gamma)}^2) dt \leq C. \quad (4.6b)$$

For (4.4e)-(4.4f), from (2.5), (4.6a), (4.6b) and using the mean value theorem, we deduce

$$\begin{aligned} \|E_\mu^n\|_{H^s(\Omega)} &= |r_1^{n+1}| \left\| \frac{f(u^{n+1})}{\sqrt{E_1(u^{n+1})}} - \frac{f(u^n)}{\sqrt{E_1(u^n)}} \right\|_{H^s(\Omega)} \\ &\leq \sup_{t \in [0, T]} |r_1(t)| \left( \|f(u^n)\|_{H^s(\Omega)} \frac{|E_1(u^n) - E_1(u^{n+1})|}{\sqrt{E_1(u^{n+1})E_1(u^n)(E_1(u^n) + E_1(u^{n+1}))}} \right. \\ &\quad \left. + \frac{\|f(u^{n+1}) - f(u^n)\|_{H^s(\Omega)}}{\sqrt{E_1(u^{n+1})}} \right) \leq C\Delta t, \end{aligned} \quad (4.7a)$$

$$\begin{aligned} \|E_{\mu, \Gamma}^n\|_{H^s(\Gamma)} &= |r_2^{n+1}| \left\| \frac{g(u_\Gamma^{n+1})}{\sqrt{E_2(u_\Gamma^{n+1})}} - \frac{g(u_\Gamma^n)}{\sqrt{E_2(u_\Gamma^n)}} \right\|_{H^s(\Gamma)} \\ &\leq \sup_{t \in [0, T]} |r_2(t)| \left( \|g(u_\Gamma^n)\|_{H^s(\Gamma)} \frac{|E_2(u_\Gamma^n) - E_2(u_\Gamma^{n+1})|}{\sqrt{E_2(u_\Gamma^{n+1})E_2(u_\Gamma^n)(E_2(u_\Gamma^n) + E_2(u_\Gamma^{n+1}))}} \right. \\ &\quad \left. + \frac{\|g(u_\Gamma^{n+1}) - g(u_\Gamma^n)\|_{H^s(\Gamma)}}{\sqrt{E_2(u_\Gamma^{n+1})}} \right) \leq C\Delta t. \end{aligned} \quad (4.7b)$$

Associating with (4.4a)-(4.4f), (4.7a)-(4.7b) and the assumption (4.5), we complete the proof.  $\square$

Now, we present the main result of this paper as follows.

**Theorem 4.1.** *Let  $(u, u_\Gamma, \mu, \mu_\Gamma, r_1, r_2)$  and  $(u_h, u_{h, \Gamma}, \mu_h, \mu_{h, \Gamma}, r_{h, 1}, r_{h, 2})$  be the solutions of (2.11) and (3.1a)-(3.1e), respectively, then for any  $N \leq T/\Delta t$ , we have the following error estimate*

$$\begin{aligned} &\max_{0 \leq l \leq N} (\|u^{l+1} - u_h^{l+1}\|_{H^1(\Omega)}^2 + \|u_\Gamma^{l+1} - u_{h, \Gamma}^{l+1}\|_{H^1(\Gamma)}^2 + (r_{h, 1}^{l+1} - r_1^{l+1})^2 + (r_{h, 2}^{l+1} - r_2^{l+1})^2) \\ &\leq Ch^{2k} + C\Delta t^2, \end{aligned} \quad (4.8)$$

where  $C > 0$  is independent of  $h$  and  $\Delta t$  and dependent of the regularized parameter  $\delta$  in (2.3).

*Proof.* Now we define

$$\begin{aligned} u_h^{n+1} - u^{n+1} &= (u_h^{n+1} - R_h u^{n+1}) - (u^{n+1} - R_h u^{n+1}) = \alpha_u^{n+1} - \beta_u^{n+1}, \\ u_{h, \Gamma}^{n+1} - u_\Gamma^{n+1} &= (u_{h, \Gamma}^{n+1} - R_h u_\Gamma^{n+1}) - (u_\Gamma^{n+1} - R_h u_\Gamma^{n+1}) = \alpha_{u, \Gamma}^{n+1} - \beta_{u, \Gamma}^{n+1}, \\ \mu_h^{n+1} - \mu^{n+1} &= (\mu_h^{n+1} - R_h \mu^{n+1}) - (\mu^{n+1} - R_h \mu^{n+1}) = \alpha_\mu^{n+1} - \beta_\mu^{n+1}, \\ \mu_{h, \Gamma}^{n+1} - \mu_\Gamma^{n+1} &= (\mu_{h, \Gamma}^{n+1} - R_h \mu_\Gamma^{n+1}) - (\mu_\Gamma^{n+1} - R_h \mu_\Gamma^{n+1}) = \alpha_{\mu, \Gamma}^{n+1} - \beta_{\mu, \Gamma}^{n+1}, \\ e_1^{n+1} &= r_{h, 1}^{n+1} - r_1^{n+1}, \quad e_2^{n+1} = r_{h, 2}^{n+1} - r_2^{n+1}. \end{aligned}$$

From (2.11), (3.1a)-(3.1e) and (4.1), we have

$$(D_t \alpha_u^{n+1}, \theta_1) + (\alpha_\mu^{n+1}, \theta_1) = (D_t \beta_u^{n+1}, \theta_1) + (\beta_\mu^{n+1}, \theta_1) - (E_u^n, \theta_1), \quad (4.9a)$$

$$\langle D_t \alpha_{u,\Gamma}^{n+1}, \theta_2 \rangle + \langle \alpha_{\mu,\Gamma}^{n+1}, \theta_2 \rangle = \langle D_t \beta_{u,\Gamma}^{n+1}, \theta_2 \rangle + \langle \beta_{\mu,\Gamma}^{n+1}, \theta_2 \rangle - \langle E_{u,\Gamma}^n, \theta_2 \rangle, \quad (4.9b)$$

$$\begin{aligned} & (\alpha_{\mu}^{n+1}, v) + \kappa \langle \alpha_{\mu,\Gamma}^{n+1}, v \rangle - c \langle \nabla \alpha_u^{n+1}, \nabla v \rangle - \kappa c \langle \nabla_{\Gamma} \alpha_{u,\Gamma}^{n+1}, \nabla_{\Gamma} v \rangle \\ &= (\beta_{\mu}^{n+1}, v) + \kappa \langle \beta_{\mu,\Gamma}^{n+1}, v \rangle + \frac{e_1^{n+1}}{\sqrt{E_1(u^n)}} (f(u^n), v) \\ &+ \kappa \frac{e_2^{n+1}}{\sqrt{E_2(u_{h,\Gamma}^n)}} \langle g(u_{h,\Gamma}^n), v \rangle + r_{h,1}^{n+1} \left( \frac{f(u_h^n)}{\sqrt{E_1(u_h^n)}} - \frac{f(u^n)}{\sqrt{E_1(u^n)}}, v \right) \\ &+ \kappa r_{h,2}^{n+1} \left\langle \frac{g(u_{h,\Gamma}^n)}{\sqrt{E_2(u_{h,\Gamma}^n)}} - \frac{g(u_{\Gamma}^n)}{\sqrt{E_2(u_{\Gamma}^n)}}, v \right\rangle - (E_{\mu}^n, v) - \kappa \langle E_{\mu,\Gamma}^n, v \rangle, \end{aligned} \quad (4.9c)$$

$$D_t e_1^{n+1} - \frac{1}{2} \left( \frac{f(u_h^n)}{\sqrt{E_1(u_h^n)}}, D_t \alpha_u^{n+1} \right) = \frac{1}{2} \left( \frac{f(u_h^n)}{\sqrt{E_1(u_h^n)}} - \frac{f(u^n)}{\sqrt{E_1(u^n)}}, D_t u^{n+1} \right) - E_{r,1}^n, \quad (4.9d)$$

$$D_t e_2^{n+1} - \frac{1}{2} \left\langle \frac{g(u_{h,\Gamma}^n)}{\sqrt{E_2(u_{h,\Gamma}^n)}}, D_t \alpha_{u,\Gamma}^{n+1} \right\rangle = \frac{1}{2} \left\langle \frac{g(u_{h,\Gamma}^n)}{\sqrt{E_2(u_{h,\Gamma}^n)}} - \frac{g(u_{\Gamma}^n)}{\sqrt{E_2(u_{\Gamma}^n)}}, D_t u_{\Gamma}^{n+1} \right\rangle - E_{r,2}^n. \quad (4.9e)$$

Then substituting  $\theta_1 = \alpha_u^{n+1}$ ,  $\theta_2 = \alpha_{u,\Gamma}^{n+1}$ ,  $v = \alpha_u^{n+1}$  into (4.9a)-(4.9c), respectively, and multiplying (4.9d) and (4.9e) with  $2e_1^{n+1}$ ,  $2e_2^{n+1}$ , separately, we deduce

$$\begin{aligned} & \frac{c}{2} (\|\alpha_u^{n+1}\|_{H^1(\Omega)}^2 - \|\alpha_u^n\|_{H^1(\Omega)}^2) + \frac{\kappa c}{2} (\|\alpha_{u,\Gamma}^{n+1}\|_{H^1(\Gamma)}^2 - \|\alpha_{u,\Gamma}^n\|_{H^1(\Gamma)}^2) \\ &+ (e_1^{n+1})^2 - (e_1^n)^2 + (e_2^{n+1})^2 - (e_2^n)^2 \leq \sum_{i=1}^4 A_i \end{aligned} \quad (4.10)$$

with

$$\begin{aligned} A_1 &= \Delta t (D_t \beta_u^{n+1}, \alpha_u^{n+1}) - \Delta t (E_u^n, \alpha_u^{n+1}) + \kappa \Delta t \langle D_t \beta_{u,\Gamma}^{n+1}, \alpha_{u,\Gamma}^{n+1} \rangle \\ &- \kappa \Delta t \langle E_{u,\Gamma}^n, \alpha_{u,\Gamma}^{n+1} \rangle + \Delta t (E_{\mu}^n, \alpha_u^{n+1}) + \kappa \Delta t \langle E_{\mu,\Gamma}^n, \alpha_{u,\Gamma}^{n+1} \rangle, \\ A_2 &= -r_1^{n+1} \Delta t \left( \frac{f(u_h^n)}{\sqrt{E_1(u_h^n)}} - \frac{f(u^n)}{\sqrt{E_1(u^n)}}, \alpha_u^{n+1} \right) - \kappa r_2^{n+1} \Delta t \left\langle \frac{g(u_{h,\Gamma}^n)}{\sqrt{E_2(u_{h,\Gamma}^n)}} - \frac{g(u_{\Gamma}^n)}{\sqrt{E_2(u_{\Gamma}^n)}}, \alpha_{u,\Gamma}^{n+1} \right\rangle \\ &+ e_1^{n+1} \Delta t \left( \frac{f(u_h^n)}{\sqrt{E_1(u_h^n)}} - \frac{f(u^n)}{\sqrt{E_1(u^n)}}, D_t u^{n+1} \right) + \kappa e_2^{n+1} \Delta t \left\langle \frac{g(u_{h,\Gamma}^n)}{\sqrt{E_2(u_{h,\Gamma}^n)}} - \frac{g(u_{\Gamma}^n)}{\sqrt{E_2(u_{\Gamma}^n)}}, D_t u_{\Gamma}^{n+1} \right\rangle, \\ A_3 &= -e_1^{n+1} \Delta t \left( \frac{f(u_h^n)}{\sqrt{E_1(u_h^n)}}, D_t \beta_u^{n+1} \right) - \kappa e_2^{n+1} \Delta t \left\langle \frac{g(u_{h,\Gamma}^n)}{\sqrt{E_2(u_{h,\Gamma}^n)}}, D_t \beta_{u,\Gamma}^{n+1} \right\rangle - 2 \Delta t e_1^{n+1} E_{r,1}^n \\ &- 2 \kappa \Delta t e_2^{n+1} E_{r,2}^n - \frac{e_1^{n+1} \Delta t}{\sqrt{E_1(u^n)}} (f(u^n), \alpha_u^{n+1}) - \kappa \frac{e_2^{n+1} \Delta t}{\sqrt{E_2(u_{\Gamma}^n)}} \langle g(u_{\Gamma}^n), \alpha_{u,\Gamma}^{n+1} \rangle, \\ A_4 &= \frac{e_1^{n+1} \Delta t}{\sqrt{E_1(u_h^n)}} (f(u_h^n), D_t \alpha_u^{n+1}) + \kappa \frac{e_2^{n+1} \Delta t}{\sqrt{E_2(u_{h,\Gamma}^n)}} \langle g(u_{h,\Gamma}^n), D_t \alpha_{u,\Gamma}^{n+1} \rangle. \end{aligned}$$

Now, we estimate each term on the right hand side of (4.10). For  $A_1$ , by (4.2) and Lemma 4.2, we have

$$\begin{aligned}
 A_1 &\leq C\Delta t(\|D_t\beta_u^{n+1}\|_{L^2(\Omega)}^2 + \kappa\|D_t\beta_{u,\Gamma}^{n+1}\|_{L^2(\Gamma)}^2) + C\Delta t(\|\alpha_u^{n+1}\|_{L^2(\Omega)}^2 + \kappa\|\alpha_{u,\Gamma}^{n+1}\|_{L^2(\Gamma)}^2) \\
 &\quad + C\Delta t(\|E_u^n\|_{L^2(\Omega)}^2 + \kappa\|E_{u,\Gamma}^n\|_{L^2(\Gamma)}^2 + \|E_\mu^n\|_{L^2(\Omega)}^2 + \kappa\|E_{\mu,\Gamma}^n\|_{L^2(\Gamma)}^2) \\
 &\leq C\Delta t\|D_t\beta_u^{n+1}\|_{H^1(\Omega)}^2 + C\Delta t(\|\alpha_u^{n+1}\|_{L^2(\Omega)}^2 + \kappa\|\alpha_u^{n+1}\|_{L^2(\Gamma)}^2) \\
 &\quad + C\Delta t(\|E_u^n\|_{H^1(\Omega)}^2 + \|E_\mu^n\|_{H^1(\Omega)}^2) \\
 &\leq Ch^{2k} \int_{t^n}^{t^{n+1}} \|u_t\|_{H^{k+1}(\Omega)}^2 dt + C\Delta t(\|\alpha_u^{n+1}\|_{L^2(\Omega)}^2 + \|\alpha_u^{n+1}\|_{L^2(\Gamma)}^2) \\
 &\quad + C\Delta t^2 \int_{t^n}^{t^{n+1}} \|u_{tt}\|_{H^1(\Omega)}^2 dt + C\Delta t^3.
 \end{aligned}$$

In view of (4.5), we yield

$$\begin{aligned}
 A_2 &\leq C\Delta t(\|\alpha_u^{n+1}\|_{L^2(\Omega)}^2 + \kappa\|\alpha_{u,\Gamma}^{n+1}\|_{L^2(\Gamma)}^2) + C\Delta t((e_1^{n+1})^2 + (e_2^{n+1})^2) \\
 &\quad + C\Delta t\left(\left\|\frac{f(u_h^n)}{\sqrt{E_1(u_h^n)}} - \frac{f(u^n)}{\sqrt{E_1(u^n)}}\right\|_{L^2(\Omega)}^2 + \kappa\left\|\frac{g(u_{h,\Gamma}^n)}{\sqrt{E_2(u_{h,\Gamma}^n)}} - \frac{g(u_\Gamma^n)}{\sqrt{E_2(u_\Gamma^n)}}\right\|_{L^2(\Gamma)}^2\right). \quad (4.11)
 \end{aligned}$$

The last term on the right hand side of (4.11) can be treated as follows

$$\begin{aligned}
 &\frac{f(u_h^n)}{\sqrt{E_1(u_h^n)}} - \frac{f(u^n)}{\sqrt{E_1(u^n)}} \\
 &= \frac{f(u^n)(E_1(u^n) - E_1(u_h^n))}{\sqrt{E_1(u_h^n)E_1(u^n)(E_1(u^n) + E_1(u_h^n))}} + \frac{f(u_h^n) - f(u^n)}{\sqrt{E_1(u_h^n)}} \\
 &= J_1 + J_2, \quad (4.12a)
 \end{aligned}$$

$$\begin{aligned}
 &\frac{g(u_{h,\Gamma}^n)}{\sqrt{E_2(u_{h,\Gamma}^n)}} - \frac{g(u_\Gamma^n)}{\sqrt{E_2(u_\Gamma^n)}} \\
 &= \frac{g(u_\Gamma^n)(E_2(u_\Gamma^n) - E_2(u_{h,\Gamma}^n))}{\sqrt{E_2(u_{h,\Gamma}^n)E_2(u_\Gamma^n)(E_2(u_\Gamma^n) + E_2(u_{h,\Gamma}^n))}} + \frac{g(u_{h,\Gamma}^n) - g(u_\Gamma^n)}{\sqrt{E_2(u_{h,\Gamma}^n)}} \\
 &= J_3 + J_4. \quad (4.12b)
 \end{aligned}$$

Note that  $f(u_h)$ ,  $f'(u_h)$ ,  $g(u_{h,\Gamma})$ ,  $g'(u_{h,\Gamma})$  all have upper bounds by (2.5), then the terms  $J_1$ ,  $J_2$ ,  $J_3$ ,  $J_4$  are bounded by

$$\begin{aligned}
 \|J_1\|_{L^2(\Omega)} &\leq C\|f(u^n)\|_{L^2(\Omega)}\|u^n - u_h^n\|_{L^2(\Omega)} \\
 &\leq C\delta^{-1}(\|\alpha_u^n\|_{L^2(\Omega)} + \|\beta_u^n\|_{L^2(\Omega)}), \quad (4.13a)
 \end{aligned}$$

$$\begin{aligned}
\|J_3\|_{L^2(\Gamma)} &\leq C\|g(u_\Gamma^n)\|_{L^2(\Gamma)}\|u_\Gamma^n - u_{h,\Gamma}^n\|_{L^2(\Gamma)} \\
&\leq C\delta^{-1}(\|\alpha_{u,\Gamma}^n\|_{L^2(\Gamma)} + \|\beta_{u,\Gamma}^n\|_{L^2(\Gamma)}) \\
&\leq C\delta^{-1}(\|\alpha_u^n\|_{L^2(\Gamma)} + \|\beta_u^n\|_{H^1(\Omega)}),
\end{aligned} \tag{4.13b}$$

$$\begin{aligned}
\|J_2\|_{L^2(\Omega)} &\leq C\|f(u_h^n) - f(u^n)\| \\
&\leq C(\|f'(u^n)\|_{L^2(\Omega)}\|u^n - u_h^n\|_{L^2(\Omega)}) \\
&\leq C\delta^{-1}(\|\alpha_u^n\|_{L^2(\Omega)} + \|\beta_u^n\|_{L^2(\Omega)}),
\end{aligned} \tag{4.13c}$$

$$\begin{aligned}
\|J_4\|_{L^2(\Gamma)} &\leq C\|g(u_{h,\Gamma}^n) - g(u_\Gamma^n)\| \\
&\leq C(\|g'(u_\Gamma^n)\|_{L^2(\Gamma)}\|u_\Gamma^n - u_{h,\Gamma}^n\|_{L^2(\Gamma)}) \\
&\leq C\delta^{-1}(\|\alpha_{u,\Gamma}^n\|_{L^2(\Gamma)} + \|\beta_{u,\Gamma}^n\|_{L^2(\Gamma)}) \\
&\leq C\delta^{-1}(\|\alpha_u^n\|_{L^2(\Gamma)} + \|\beta_u^n\|_{H^1(\Omega)}).
\end{aligned} \tag{4.13d}$$

Combining (4.12a)-(4.13d), applying trace theorem and interpolation theory, we have

$$\begin{aligned}
&\left\| \frac{f(u_h^n)}{\sqrt{E_1(u_h^n)}} - \frac{f(u^n)}{\sqrt{E_1(u^n)}} \right\|_{L^2(\Omega)}^2 + \kappa \left\| \frac{g(u_{h,\Gamma}^n)}{\sqrt{E_2(u_{h,\Gamma}^n)}} - \frac{g(u_\Gamma^n)}{\sqrt{E_2(u_\Gamma^n)}} \right\|_{L^2(\Gamma)}^2 \\
&\leq C\delta^{-1}(\|\beta_u^n\|_{L^2(\Omega)}^2 + \|\alpha_u^n\|_{L^2(\Omega)}^2 + \|\alpha_u^n\|_{L^2(\Gamma)}^2 + \|\beta_u^n\|_{H^1(\Omega)}^2) \\
&\leq C\delta^{-1}h^{2k}\|u^n\|_{H^{k+1}(\Omega)}^2 + C\delta^{-1}(\|\alpha_u^n\|_{L^2(\Omega)}^2 + \|\alpha_{u,\Gamma}^n\|_{L^2(\Gamma)}^2).
\end{aligned} \tag{4.14}$$

Again, by using (2.5), (4.4c) and (4.4d), we have

$$\begin{aligned}
A_3 &\leq C\Delta t((e_1^{n+1})^2 + (e_2^{n+1})^2) + C\delta^{-1}\Delta t(\|D_t\beta_u^{n+1}\|_{L^2(\Omega)}^2 + \|D_t\beta_{u,\Gamma}^{n+1}\|_{L^2(\Gamma)}^2) \\
&\quad + C\Delta t(\|E_{r,1}^{n+1}\|_{L^2(\Omega)}^2 + \|E_{r,2}^{n+1}\|_{L^2(\Gamma)}^2) + C\delta^{-1}\Delta t(\|\alpha_u^{n+1}\|_{L^2(\Omega)}^2 + \|\alpha_{u,\Gamma}^{n+1}\|_{L^2(\Gamma)}^2) \\
&\leq C\Delta t((e_1^{n+1})^2 + (e_2^{n+1})^2) + C\delta^{-1}\Delta t(\|D_t\beta_u^{n+1}\|_{L^2(\Omega)}^2 + \|D_t\beta_{u,\Gamma}^{n+1}\|_{H^1(\Omega)}^2) \\
&\quad + C\Delta t(\|E_{r,1}^{n+1}\|_{L^2(\Omega)}^2 + \|E_{r,2}^{n+1}\|_{L^2(\Gamma)}^2) + C\delta^{-1}\Delta t(\|\alpha_u^{n+1}\|_{L^2(\Omega)}^2 + \|\alpha_{u,\Gamma}^{n+1}\|_{L^2(\Gamma)}^2) \\
&\leq C\Delta t((e_1^{n+1})^2 + (e_2^{n+1})^2) + C\delta^{-1}h^{2k} \int_{t^n}^{t^{n+1}} \|u_t\|_{H^{k+1}(\Omega)}^2 dt + C\Delta t^3 \\
&\quad + C\delta^{-1}\Delta t(\|\alpha_u^{n+1}\|_{L^2(\Omega)}^2 + \|\alpha_{u,\Gamma}^{n+1}\|_{L^2(\Gamma)}^2).
\end{aligned}$$

Then, by Young's inequality and Taylor expansion,  $A_4$  satisfies

$$A_4 \leq C\varepsilon(e_1^{n+1})^2 + C\varepsilon(e_2^{n+1})^2 + C\Delta t^2.$$

We combine the estimates for each term  $A_i$ ,  $1 \leq i \leq 4$ , and (4.14) to get

$$\begin{aligned}
&\frac{1}{2}(\|\alpha_u^{n+1}\|_{H^1(\Omega)}^2 - \|\alpha_u^n\|_{H^1(\Omega)}^2 + \|\alpha_{u,\Gamma}^{n+1}\|_{H^1(\Gamma)}^2 - \|\alpha_{u,\Gamma}^n\|_{H^1(\Gamma)}^2) \\
&\quad + ((e_1^{n+1})^2 - (e_1^n)^2) + ((e_2^{n+1})^2 - (e_2^n)^2)
\end{aligned}$$

$$\begin{aligned}
&\leq C(1+\delta^{-1})\Delta t(\|\alpha_u^{n+1}\|_{L^2(\Omega)}^2 + \|\alpha_u^n\|_{L^2(\Omega)}^2 + \|\alpha_{u,\Gamma}^{n+1}\|_{L^2(\Gamma)}^2 + \|\alpha_{u,\Gamma}^n\|_{L^2(\Gamma)}^2) \\
&\quad + C\Delta t^2 \int_{t^n}^{t^{n+1}} \|u_{tt}(s)\|_{H^1(\Omega)}^2 ds + C\Delta t^3 + Ch^{2k} \int_{t^n}^{t^{n+1}} \|u_t\|_{H^{\max(1,k+1)}(\Omega)}^2 dt \\
&\quad + Ch^{2k}\Delta t(\|u^n\|_{H^{k+1}(\Omega)}^2 + \|\mu^{n+1}\|_{H^{k+1}(\Omega)}^2) + C\Delta t(e_1^{n+1})^2 + (e_2^{n+1})^2. \tag{4.15}
\end{aligned}$$

Note that

$$\|\alpha_u^0\|_{L^2(\Omega)} + h\|\nabla\alpha_u^0\|_{L^2(\Omega)} + \|\alpha_{u,\Gamma}^0\|_{L^2(\Gamma)} + h\|\nabla\alpha_{u,\Gamma}^0\|_{L^2(\Gamma)} + |e_1^0| + |e_2^0| \leq Ch^{k+1}.$$

When summing (4.15) from  $n=1, \dots, l$ , ( $1 \leq l \leq N$ ), by discrete Gronwall's inequality, there exists small positive constants  $h_1$  and  $\Delta t_1$ , such that when  $h < h_1$  and  $\Delta t < \Delta t_1$ ,

$$\|\alpha_u^{l+1}\|_{H^1(\Omega)}^2 + \|\alpha_{u,\Gamma}^{l+1}\|_{H^1(\Gamma)}^2 + (e_1^{l+1})^2 + (e_2^{l+1})^2 \leq C(h^{2k} + \Delta t^2), \tag{4.16}$$

which is the desired result of Theorem 4.8.  $\square$

## 5 Numerical example

In this section, we present a numerical example to show theoretical result and simulate the interactions between solid walls with dynamic boundary conditions. We choose domain  $\bar{\Omega} = [0, L]^2$ , where  $L = 2E - 8$  meters, and suppose the temperature  $T$  is 350K. In the subdomain of  $[\frac{3L}{8}, \frac{5L}{8}]^2$ , we assume it as the gas of isobutane, then the rest of the domain is filled with the liquid of isobutane. Such an assume is opposite to the experiments in [7, 8, 12].

We use SAV FEM scheme to calculate with four different time steps  $\Delta t = 1E - 2, 5E - 3, 7.5E - 4$ , respectively. The approximate solution obtained with time step  $\Delta t = 1E - 6$  is selected as the basic solution for calculating the error. From Table 1, we can observe that the SAV scheme has the first order convergence.

Next, we will numerically simulate the evolution of molar density over time at the gas-liquid interface in two-dimensional space. As can be seen from Fig. 1, the initial contact surface in the bulk is square. As time goes on, it gets rounder slowly. Finally, the shape of the bubble for the gas becomes a circle. At the same time, the phenomenon of gradient decline will also appear on the surface. Fig. 2 shows that the surface tension contribution of Helmholtz free energy density at the gas-liquid interface also decreases

Table 1: The  $L^2(\Omega)$  errors and the temporal convergence of the approximate solutions for the molar density at  $t=0.1$  on the uniform  $200 \times 200$  mesh.

Time step size	$L^2$ error	Rate of $L^2$ error
1E-2	5.836E-6	-
5E-3	3.024E-6	0.9481
7.5E-4	1.523E-6	0.9895

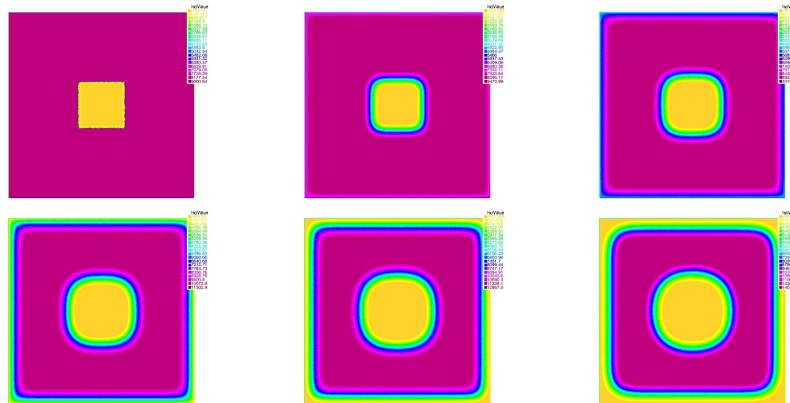


Figure 1: The simulated dynamical evolution of the molar density at time  $t=0,1,2,3,4,7$  with  $\delta=0.02$ ,  $\kappa=1$ ,  $\Delta t=1E-3$  and a  $200 \times 200$  grid, when the Peng-Robinson equation of state equipped with dynamic boundary conditions.

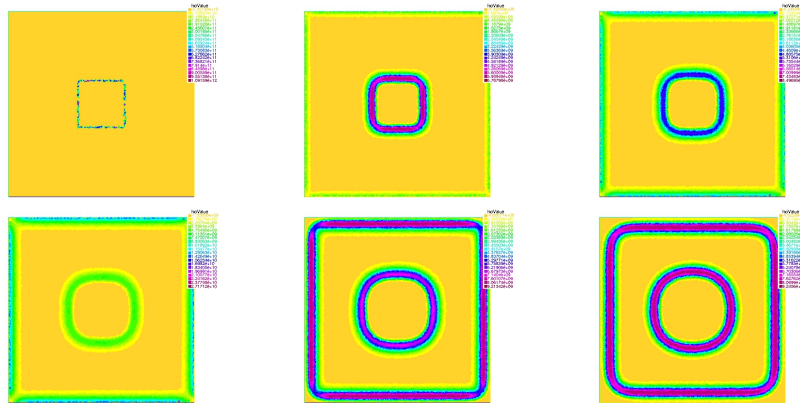


Figure 2: The simulated surface tension contribution of Helmholtz free energy density at time  $t=0,1,2,3,4,7$  with  $\delta=0.001$ ,  $\kappa=1$ ,  $\Delta t=1E-3$  and a  $200 \times 200$  grid, when the Peng-Robinson equation of state equipped with dynamic boundary conditions.

gradually in the bulk and on the surface, and becomes circular finally. These show the interactions of materials in the bulk and the interactions with solid walls. For comparison, we also consider the case with periodic boundary conditions on the surface under the same assumption. As shown in Figs. 3 and 4, the shapes of the bubble and the surface tension contribution become circular as well. Obviously, the density and the surface tension contribution do not evolve on the surface.

Fig. 5 shows that the mass of the whole system is conserved. In Fig. 6, we can clearly see that the energy decline rate is relatively fast at the beginning. As time goes on, the energy decline rate is significantly reduced, which indicates the energy is stable.



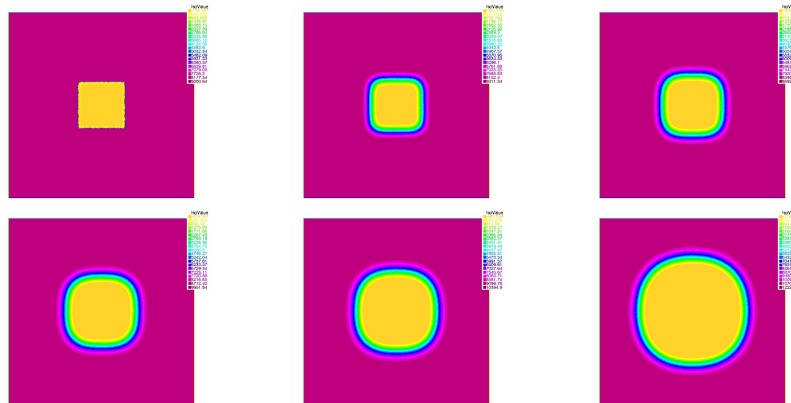


Figure 3: The simulated dynamical evolution of the molar density at time  $t=0,1,2,3,4,7$  with  $\delta=0.001$ ,  $\Delta t=1E-3$  and a  $200 \times 200$  grid, when the Peng-Robinson equation of state equipped with periodic boundary conditions.

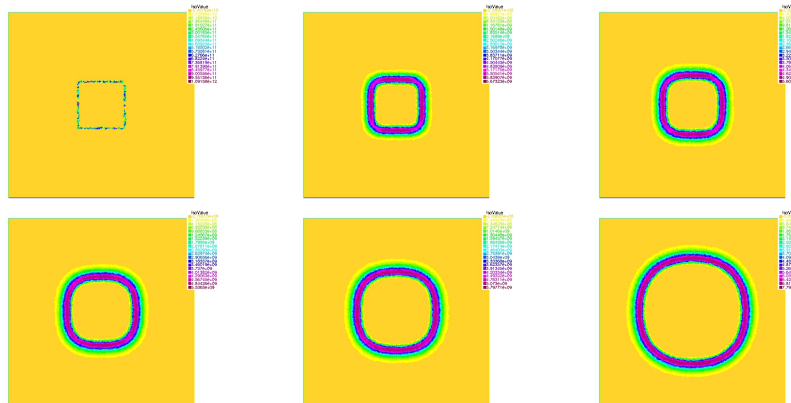


Figure 4: The simulated surface tension contribution of Helmholtz free energy density at time  $t=0,1,2,3,4,7$  with  $\delta=0.001$ ,  $\Delta t=1E-3$  and a  $200 \times 200$  grid, when the Peng-Robinson equation of state equipped with periodic boundary conditions.

## 6 Conclusions

In this paper, we focused on the Peng-Robinson equation of state with dynamic boundary conditions. Comparing with the classical boundary conditions, the system with the dynamic boundary conditions considered the interactions with solid walls, and it was better to simulate the two intersecting interfaces. Firstly, we introduced the the Peng-Robinson equation of state, and adopted the regularization method on the nonlinear term. For purpose of solving the Peng-Robinson equation of state, we used the SAV method in temporal and finite element method in spatial, and derived the energy dissipation law of the discrete SAV FEM scheme. Next, we proven that the scheme is convergent. At last, by a numerical example, we confirmed the theoretical result.

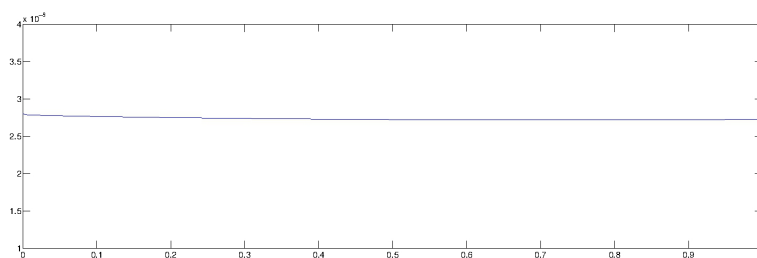


Figure 5: Conservation of mass.

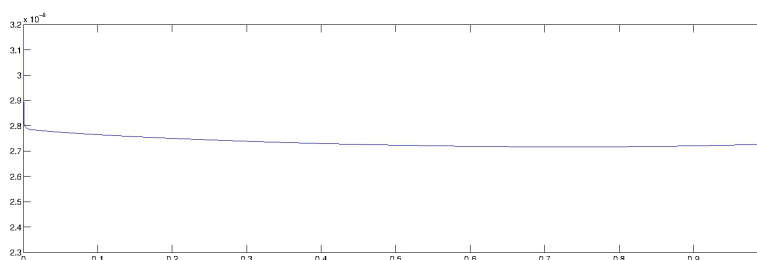


Figure 6: Decrease of energy.

In turn, in the resulting numerical scheme, the positivity preserving property for both  $1+u$  and  $1-u$  are not available, due to the explicit treatment of the nonlinear singular terms. Meanwhile, there have been many related works of positivity-preserving analysis for numerical schemes to various gradient flow models in recent years, such as the Cahn-Hilliard equation with Flory-Huggins or Flory-Huggins-Degennes energy, the Poisson-Nernst-Planck and Poisson-Nernst-Planck-Cahn-Hilliard system, liquid thin film coarsening model, reaction diffusion equations with detailed balance, etc. The point-wise positivity of the numerical solution has been theoretically established in these existing works [26–38].

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