STABILITY AND CONVERGENCE ANALYSIS OF SECOND-ORDER SCHEMES FOR A DIFFUSE INTERFACE MODEL WITH PENG-ROBINSON EQUATION OF STATE[*]

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Abstract

In this paper, we present two second-order numerical schemes to solve the fourth order parabolic equation derived from a diffuse interface model with Peng-Robinson Equation of state (EOS) for pure substance. The mass conservation, energy decay property, unique solvability and L^∞ convergence of these two schemes are proved. Numerical results demonstrate the good approximation of the fourth order equation and confirm reliability of these two schemes.

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1. Introduction

Multi-phase fluid mixture and its behaviors play important roles in many natural and engineering systems, especially in subsurface petroleum reservoirs [5,6,30–33]. It remains a challenge to understand and to model the complex interaction between phases, namely the physically distinct, separable portions of substance. In the classical theory known as the sharp interface model [9, 27, 39], an interface between two fluids is modeled as an infinitely thin, or sharp two-dimensional entity, and it is endowed with interface properties such as surface tension. In a more detailed continuum model called as the diffuse interface model, the sharp fluid-fluid interface is replaced by a small but finite-thickness layer in which the fluids may mix. Even though the concept of a diffuse interface was originally proposed a long time ago by van der Waals [36], its numerical simulation with realistic fluids has been investigated only in recent years [20, 22]. The diffuse interface theory is also known as the gradient theory [4, 10] in the chemical society, or phase field theory [3] in the fluid dynamics society. Unlike sharp interface models where surface tension must be provided as an input parameter, diffuse interface models have been used to predict surface tension [4, 10, 18, 19]. In particular, the surface tensions of petroleum fluids have been well predicted by diffuse interface models in one spatial dimension

together with Peng-Robinson Equation of State (EOS) [21], which is one of the most popular equations of state for hydrocarbon systems. However, little work has been carried out to investigate the numerical simulation of Peng-Robinson-EOS-equipped diffuse interface models in multiple spatial dimensions [22].

Inspired by the favorable properties of the Cahn-Hilliard equation and its derivation, we provide the fourth-order parabolic equation to describe the equilibrium state and the flow of the components in the crude oil in this article. Numerical experiments are our indispensable tools to investigate the solution to this equation. Previously proposed schemes for the Cahn-Hilliard equation [7,8,10–14,17,29,34,35,38] and other kinetics equations contain fourth order term [23,25,26,28,37] could be used as valuable references. The main contribution of this work is to develop two second-order energy stable numeircal schemes for the two-dimensional diffuse interface model with Peng-Robinson EOS of single component substance. The mass conservation and unique solvability are proved. The energy stability of these two schemes are achieved following the approach in [24]. However, it is not that smooth as we expected to obtain the L^∞ convergence of these two schemes attributed to the unboundedness of the free energy density of any given substance and its first and second order derivatives respect to the molar density. Taking the work of Li et al. [15] as reference, we overcome this difficulty with a nontrivial arguments.

The rest of this paper is organized as follows. In the second section, we present the mathematical model of the diffuse interface equation derived from the Peng-Robinson EOS and the scaled fourth order equation for multi-component substances and demonstrate its energy decreasing and mass conservation characters. In the third section, we present notations on the discrete space and some auxiliary lemmas. After that, the L^∞ convergence of the Crank-Nicolson scheme and the second order linearized scheme will be demonstrated in the fourth and fifth sections, respectively. And then, we provide the numerical results of these two schemes and compare them with previously published ones. The conclusion of this article will be provided in the end.

2. Mathematical Model of Fluid Systems with Diffuse Interface

We consider a fluid system consisting of fixed species amount on a fixed domain with spatially uniform-distributed given temperature.

2.1. Helmholtz free energy from Peng-Robinson EOS

Let M denote the number of components in the fluid mixture, n_i represent the molar concentration of the component i, and

$$\mathbf{n} = (n_1, n_2, \cdots, n_M)^T$$

be the molar concentrations of all components and $n = n_1 + n_2 + \cdots + n_M$ the molar density of the fluid. According to the diffuse interface model, the total Holmholtz free energy has the following form,

$$F(\mathbf{n}) = \int_\Omega f(\mathbf{n}) d\mathbf{x} = \int_\Omega f_0(\mathbf{n}) d\mathbf{x} + \int_\Omega f_\nabla(\mathbf{n}) d\mathbf{x}. \tag{2.1}$$

From Peng-Robinson EOS, the Helmholtz free energy $f_0(\mathbf{n})$ of a homogeneous fluid is given by

$$f_0(\mathbf{n}) = f_0^{\text{ideal}}(\mathbf{n}) + f_0^{\text{excess}}(\mathbf{n}),$$

$$f_0^{\text{ideal}}(\mathbf{n}) = RT \sum_{i=1}^{M} n_i \left(\ln n_i - 1 \right),$$

$$f_0^{\text{excess}}(\mathbf{n}) = -nRT \ln \left(1 - bn \right) + \frac{a(T)n}{2\sqrt{2}b} \ln \left(\frac{1 + (1 - \sqrt{2})bn}{1 + (1 + \sqrt{2})bn} \right).$$

Here T reprents the temperature of the mixture and R represents the universal gas constant (approximately $8.31432 \text{JK}^{-1}\text{mol}^{-1}$). The energy parameter $a = a(T)$ and the covolume parameter b are given by the following mixing rules,

$$a(T) = \sum_{i=1}^{M} \sum_{j=1}^{M} y_i y_j (a_i a_j)^{1/2} (1 - k_{ij}), \quad b = \sum_{i=1}^{M} y_i b_i,$$

where $y_i = n_i/n$ is the mole fraction of component i. The Peng-Robinson parameters a_i and b_i for pure-substance component i can be computed from the critical properties of the species as follows,

$$a_i = a_i(T) = 0.45724 \frac{R^2 T_{c_i}^2}{P_{c_i}} \left(1 + m_i \left(1 - \sqrt{\frac{T}{T_{c_i}}} \right) \right)^2, \quad b_i = 0.07780 \frac{RT_{c_i}}{P_{c_i}}. \quad (2.2)$$

The binary interaction coefficient k_{ij} of Peng-Robinson EOS is usually computed from experimental correlation. The critical temperature T_{c_i} and critical pressure P_{c_i} of a pure substance are intrinsic properties of the species, and they are available for most species encountered in application. The parameter m_i contained in the formula for a_i is experimentally correlated to the accentric parameter ω_i of the species by the following equations:

$$m_i = \begin{cases} 0.37464 + 1.54226\omega_i - 0.26992\omega_i^2, & \omega_i \leq 0.49, \\ 0.379642 + 1.485030\omega_i - 0.164423\omega_i^2 + 0.016666\omega_i^3, & \omega_i > 0.49. \end{cases}$$

The gradient part of the free energy density $f_\nabla(\mathbf{n})$ is in the following form,

$$f_\nabla(\mathbf{n}) = \frac{1}{2} \sum_{i,j=1}^{M} c_{ij} \nabla n_i \cdot \nabla n_j,$$

where the influence parameter c_{ij} is a function of temperature and molar concentrations which can also be provided by Peng-Robinson EOS in the mixing rule given by modified geometric mean as

$$c_{ij} = (1 - \beta_{ij})\sqrt{c_i c_j},$$

where the parameter β_{ij} is the binary interaction coefficient for the influence parameter. Stability of the interface requires β_{ij} to be included in the interval $[0, 1]$ and $\beta_{ij} = \beta_{ji}$. For most systems, β_{ij} is assumed to be zero. When $\beta_{ij} = 0$, the mixing rule is reduced to the simple geometric mean. The influence parameter of pure substance c_i is related to the Peng-Robinson parameters a_i and b_i by

$$c_i = a_i b_i^{2/3} \left(m_{1,i}^c \left(1 - \frac{T}{T_{c_i}} \right) + m_{2,i}^c \right), \quad (2.3)$$

where $m_{1,i}^c$ and $m_{2,i}^c$ are the coefficients correlated merely with the accentric factor ω_i of the component i by the following relations,

$$m_{1,i}^c = -\frac{10^{-16}}{1.2326 + 1.3757\omega_i}, \quad m_{2,i}^c = \frac{10^{-16}}{0.9051 + 1.5410\omega_i}.$$

2.2. A single component two-phase system

In this work, we would like to consider a single component two-phase system (i.e., the fluid being pure substance). In this case, the total Helmholtz free energy F is reduced to

$$F(n) = \int_\Omega f(n)d\mathbf{x} = \int_\Omega \left(f_0(n) + \frac{c}{2}|\nabla n|^2 \right) d\mathbf{x}. \tag{2.4}$$

The evolution of the molar concentration n can be written under mass conservation form

$$\frac{\partial n}{\partial t} = -\nabla \cdot J,$$

where J is the mass flux which has the form

$$J = -\nabla \frac{\delta f(n)}{\delta n}.$$

Therefore, giving periodic boundary condition, we have the following governing equation for a single component two-phase system:

$$\frac{\partial n(\mathbf{x}, t)}{\partial t} = -c\Delta^2 n(\mathbf{x}, t) + \Delta \mu_0(n(\mathbf{x}, t)), \tag{2.5a}$$

subjecting to the initial condition

$$n(\mathbf{x}, 0) = n_0(\mathbf{x}). \tag{2.5b}$$

For the energy density $f_0(n(\mathbf{x}, t))$, we have [24]

$$\frac{\partial f_0(n(\mathbf{x}, t))}{\partial t} = \frac{\partial f_0}{\partial n} \frac{\partial n}{\partial t} = \mu_0(n(\mathbf{x}, t)) \frac{\partial n(\mathbf{x}, t)}{\partial t}, \tag{2.6a}$$

where the first order derivative of $f_0(n)$ with respect to the molar density $n(\mathbf{x}, t)$ means the homogeneous chemical potential of the substance, the detailed form of which is as follows,

$$\mu_0(n) = RT \ln \left(\frac{n}{1 - bn} \right) + \frac{RTbn}{1 - bn} + \frac{a(T)}{2\sqrt{2}b} \ln \left(\frac{1 + (1 - \sqrt{2})bn}{1 + (1 + \sqrt{2})bn} \right) - \frac{a(T)n}{1 + 2bn - b^2n^2}. \tag{2.6b}$$

Lemma 2.1. *(Mass conservation.) If $n(\mathbf{x}, t)$ is a solution of the fourth order equation (2.5a)-(2.5b) under periodic boundary condition, then we can get the following mass conservation identity*

$$\frac{d}{dt} \int_\Omega n(\mathbf{x}, t)dx = 0. \tag{2.7}$$

The proof of this lemma is trivial. It can be obtained by integrating both sides of the equation (2.5a) over the domain Ω, using Green's theorem with the periodic boundary condition. Moreover, taking the inner product of (2.5a) with the term $c\Delta n(\mathbf{x}, t) - \mu_0(n(\mathbf{x}, t))$ under the periodic boundary condition, we can also obtain the following energy identity.

Lemma 2.2. *(Energy identity.) If $n(\mathbf{x}, t)$ is a solution of the fourth-order equation (2.5a)-(2.5b) under periodic boundary condition, the following energy identity can be guaranteed*

$$\frac{dF(n(\mathbf{x}, t))}{dt} = - \left\| \nabla \left(c\Delta n(\mathbf{x}, t) - \mu_0(n(\mathbf{x}, t)) \right) \right\|^2. \tag{2.8}$$

From this natural energy decay property of the fourth order equation (2.5a), it is reasonable for us to use it to approach the minimum of the total free energy, and the equilibrium state of the two-phase, single-component fluid system can be approximated by the steady solution of this equation.

3. Notations and Some Auxiliary Lemmas

We investigate the numerical solution of the fourth order equation (2.5a)-(2.5b) at the time interval $[0, T_m]$ on the domain $\Omega = [0, L]^2$. Here, T_m denotes the final time. Let $h_1 = L/M_1$, $h_2 = L/M_2$, $\triangle t = T_m/K$, $x_i = ih_1$, $y_j = jh_2$, $t_k = k\triangle t$. Denote

$$\Omega_h = \{(x_i,\ y_j) \mid 0 \le i \le M_1,\ 0 \le j \le M_2\}, \quad \Omega_\tau = \{t_k \mid 0 \le k \le K\},$$
$$\mathcal{V}_h = \{n \mid n = \{n_{ij}\},\ n_{i+M_1,j} = n_{ij},\ n_{i,j+M_2} = n_{ij}\}.$$

For $n \in \mathcal{V}_h$, denote

$$\delta_x n_{i+\frac{1}{2},j} = \frac{1}{h_1}\left(n_{i+1,j} - n_{i,j}\right), \qquad\qquad \delta_y n_{i,j+\frac{1}{2}} = \frac{1}{h_2}\left(n_{i,j+1} - n_{i,j}\right), \qquad (3.1a)$$

$$\delta_x^2 n_{ij} = \frac{1}{h_1^2}\left(n_{i+1,j} - 2n_{ij} + n_{i-1,j}\right), \qquad \delta_y^2 n_{ij} = \frac{1}{h_2^2}\left(n_{i,j+1} - 2n_{ij} + n_{i,j-1}\right), \qquad (3.1b)$$

$$\nabla_h n_{i+\frac{1}{2},j+\frac{1}{2}} = \left(\delta_x n_{i+\frac{1}{2},j}, \delta_y n_{i,j+\frac{1}{2}}\right)^T, \qquad \triangle_h n_{ij} = \left(\delta_x^2 + \delta_y^2\right) n_{ij}. \qquad (3.1c)$$

For a grid function $w = \left(w^0, w^1, \cdots, w^{K-1}, w^K\right)$ on Ω_τ, define

$$w^{n+\frac{1}{2}} = \frac{1}{2}\left(w^n + w^{n+1}\right), \quad \delta_t w^{n+\frac{1}{2}} = \frac{1}{\Delta t}\left(w^{n+1} - w^n\right), \quad 0 \le k \le K-1, \qquad (3.2a)$$

$$\hat{w}^{k+\frac{1}{2}} = 2w^{k-\frac{1}{2}} - w^{k-\frac{3}{2}} = w^k + \frac{1}{2}w^{k-1} - \frac{1}{2}w^{k-2}, \qquad\qquad 2 \le k \le K-1, \qquad (3.2b)$$

$$\hat{w}^{\frac{1}{2}} = w^0 + \frac{1}{2}w_t^0 \triangle t, \qquad\qquad \hat{w}^{\frac{3}{2}} = w^0 + \frac{3}{2}\triangle t w_t^0. \qquad (3.2c)$$

For $u, v \in \mathcal{V}_h$, their inner product is defined as $\langle u, v \rangle = h_1 h_2 \sum\limits_{i=1}^{M_1} \sum\limits_{j=1}^{M_2} u_{ij} v_{ij}$, and their Sobolev norms as

$$\|u\|_\infty = \max_{1 \le i \le M_1, 1 \le j \le M_2} |u_{ij}|, \qquad\qquad \|u\| = \sqrt{\langle u, u \rangle},$$

$$\|\delta_x u\| = \sqrt{h_1 h_2 \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} \left|\delta_x u_{i-\frac{1}{2},j}\right|^2}, \qquad\qquad \|\delta_y u\| = \sqrt{h_1 h_2 \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} \left|\delta_y u_{i,j-\frac{1}{2}}\right|^2},$$

$$\|\nabla_h u\| = \sqrt{h_1 h_2 \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} \left|\nabla_h u_{i+\frac{1}{2},j+\frac{1}{2}}\right|^2}, \qquad \|\triangle_h u\| = \sqrt{h_1 h_2 \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} |\triangle_h u_{ij}|^2}.$$

To demonstrate the solvability and the convergence of special numerical schemes, we will frequently use the following lemmas.

Lemma 3.1. ([1,2]) *Let* $(H, (\cdot, \cdot))$ *be a finite dimensional inner product space,* $\|\cdot\|$ *the associated norm, and* $g : H \to H$ *be continuous. Assume moreover that*

$$\exists\ \alpha > 0, \quad \forall z \in H, \quad \|z\| = \alpha, \quad \langle g(z), z \rangle \ge 0.$$

Then there exists an element $z^* \in H$, *such that* $g(z^*) = 0$ *and* $\|z^*\| \le \alpha$.

Lemma 3.2. *For any grid function* $u, v \in \mathcal{V}_h$, *we have*

$$\langle \Delta_h u, v \rangle = \langle u, \Delta_h v \rangle = -\langle \nabla_h u \cdot \nabla_h v, 1 \rangle. \qquad (3.3)$$

Lemma 3.3. ([15]) *For any grid function $n \in \mathcal{V}_h$, we have*

$$\|n\|_\infty^2 \le k_0 \|n\| \left(\|\triangle_h n\| + \|n\| \right),$$

where k_0 is independent of the grid parameter h and the function n.

Referencing to the Lemma 4.2 given by [15], we can get the following similar result.

Lemma 3.4. *For any $u, v \in \mathcal{V}_h$ and $k \ge 1$, we have the following identity*

$$\sum_{l=0}^{k} u^{l+\frac{1}{2}} \delta_t v^{l+\frac{1}{2}} = \frac{1}{\Delta t} \left(u^{k+\frac{1}{2}} v^{k+1} - u^{\frac{1}{2}} v^0 \right) - \sum_{l=1}^{k} v^l \frac{u^{l+\frac{1}{2}} - u^{l-\frac{1}{2}}}{\Delta t}.$$

Proof. Observe that

$$\begin{aligned}
\sum_{l=0}^{k} u^{l+\frac{1}{2}} \delta_t v^{l+\frac{1}{2}} &= \sum_{l=0}^{k} u^{l+\frac{1}{2}} \frac{v^{l+1} - v^l}{\Delta t} \\
&= \frac{1}{\Delta t} \left[\sum_{l=1}^{k} \left(u^{l-\frac{1}{2}} - u^{l+\frac{1}{2}} \right) v^l + u^{k+\frac{1}{2}} v^{k+1} - u^{\frac{1}{2}} v^0 \right] \\
&= \frac{1}{\Delta t} \left(u^{k+\frac{1}{2}} v^{k+1} - u^{\frac{1}{2}} v^0 \right) - \sum_{l=1}^{k} v^l \frac{u^{l+\frac{1}{2}} - u^{l-\frac{1}{2}}}{\Delta t}.
\end{aligned}$$

This completes the proof. □

Similarly to the approach of Lemma 4.1 provided in [15], we can obtain the following helpful lemma.

Lemma 3.5. *Denote $e_{ij}^k = \bar{n}_{ij}^k - n_{ij}^k$, where $\bar{n}$ is the solution of (2.5a). For n, $\bar{n} \in \mathcal{V}_h$, there exists $\rho^l \in (0,1)$ and $\gamma_1 = \rho^l n^{l+\frac{1}{2}} + (1-\rho^l) n^{l-\frac{1}{2}}$, $\gamma_2 = \rho^l \bar{n}^{l+\frac{1}{2}} + (1-\rho^l) \bar{n}^{l-\frac{1}{2}}$, $\xi^l \in (\min\{\gamma_1, \gamma_2\}, \max\{\gamma_1, \gamma_2\})$, k, $l = 0, 1, 2, ..., K-1$, such that*

$$\frac{1}{\Delta t} \left[\mu_0(\bar{n}^{l+\frac{1}{2}}) - \mu_0(n^{l+\frac{1}{2}}) - \left(\mu_0(\bar{n}^{l-\frac{1}{2}}) - \mu_0(n^{l-\frac{1}{2}}) \right) \right]$$
$$= \mu_0' \left(\rho^l n^{l+\frac{1}{2}} + (1-\rho^l) n^{l-\frac{1}{2}} \right) \frac{e^{l+\frac{1}{2}} - e^{l-\frac{1}{2}}}{\Delta t} + \mu_0''(\xi^l) \left(\rho^l e^{l+\frac{1}{2}} + (1-\rho^l) e^{l-\frac{1}{2}} \right) \frac{\bar{n}^{l+\frac{1}{2}} - \bar{n}^{l-\frac{1}{2}}}{\Delta t}.$$

Proof. Note that

$$\frac{1}{\Delta t} \left[\mu_0(\bar{n}^{l+\frac{1}{2}}) - \mu_0(n^{l+\frac{1}{2}}) - \left(\mu_0(\bar{n}^{l-\frac{1}{2}}) - \mu_0(n^{l-\frac{1}{2}}) \right) \right]$$
$$= \mu_0' \left(\rho^l \bar{n}^{l+\frac{1}{2}} + (1-\rho^l) \bar{n}^{l-\frac{1}{2}} \right) \frac{\bar{n}^{l+\frac{1}{2}} - \bar{n}^{l-\frac{1}{2}}}{\Delta t} - \mu_0' \left(\rho^l n^{l+\frac{1}{2}} + (1-\rho^l) n^{l-\frac{1}{2}} \right) \frac{n^{l+\frac{1}{2}} - n^{l-\frac{1}{2}}}{\Delta t}$$
$$= \left[\mu_0' \left(\rho^l \bar{n}^{l+\frac{1}{2}} + (1-\rho^l) \bar{n}^{l-\frac{1}{2}} \right) - \mu_0' \left(\rho^l n^{l+\frac{1}{2}} + (1-\rho^l) n^{l-\frac{1}{2}} \right) \right] \frac{\bar{n}^{l+\frac{1}{2}} - \bar{n}^{l-\frac{1}{2}}}{\Delta t}$$
$$\qquad + \mu_0' \left(\rho^l n^{l+\frac{1}{2}} + (1-\rho^l) n^{l-\frac{1}{2}} \right) \left(\frac{\bar{n}^{l+\frac{1}{2}} - \bar{n}^{l-\frac{1}{2}}}{\Delta t} - \frac{n^{l+\frac{1}{2}} - n^{l-\frac{1}{2}}}{\Delta t} \right) \tag{3.4}$$
$$= \mu_0'(\rho^l n^{l+\frac{1}{2}} + (1-\rho^l) n^{l-\frac{1}{2}}) \frac{e^{l+\frac{1}{2}} - e^{l-\frac{1}{2}}}{\Delta t} + \mu_0''(\xi^l) \left(\rho^l e^{l+\frac{1}{2}} + (1-\rho^l) e^{l-\frac{1}{2}} \right) \frac{\bar{n}^{l+\frac{1}{2}} - \bar{n}^{l-\frac{1}{2}}}{\Delta t}. \tag{3.5}$$

In deriving (3.4), we treated $\mu_0 \left(\bar{u}^k + \Delta t \rho \delta_t \bar{u}^{k+\frac{1}{2}} \right) - \mu_0 \left(u^k + \Delta t \rho \delta_t u^{k+\frac{1}{2}} \right)$ as a function of $\rho \in [0, 1]$ and then use the mean-value theorem. To derive (3.5), we have also applied the differential mid-value theorem. $\qquad\square$

4. Crank-Nicolson Scheme

Define the grid function $\bar{n}^k, \bar{f}_0^k \in \mathcal{V}_h$ for $0 \le k \le K$ on Ω_h as follows,

$$\bar{n}_{ij}^k = n\left(x_i, y_j, t_k\right), \quad (\bar{f}_0)_{ij}^k = f_0^k\left(x_i, y_j\right), \quad 1 \le i \le M_1, \quad 1 \le j \le M_2.$$

Applying Taylor expansion to (2.5a) and (2.6a) for all $1 \le i \le M_1$, $1 \le j \le M_2$, we have

$$\frac{\bar{n}_{ij}^{k+1} - \bar{n}_{ij}^k}{\triangle t} + c \triangle_h^2 \bar{n}_{ij}^{k+\frac{1}{2}} - \triangle_h \mu_0 \left(\bar{n}_{ij}^{k+\frac{1}{2}} \right) = R_{ij}^{k+\frac{1}{2}}, \quad 0 \le k \le K - 1, \tag{4.1a}$$

$$\frac{(\bar{f}_0)_{ij}^{k+1} - (\bar{f}_0)_{ij}^k}{\triangle t} = \mu_0 \left(\bar{n}^{k+\frac{1}{2}} \right) \frac{\bar{n}_{ij}^{k+1} - \bar{n}_{ij}^k}{\triangle t} + S_{ij}^{k+\frac{1}{2}}, \quad 0 \le k \le K - 1, \tag{4.1b}$$

where there exists a constant m_1, such that for $0 \le k \le K - 1$

$$\left| R_{ij}^{k+\frac{1}{2}} \right| \le m_1 \left(h_1^2 + h_2^2 + \triangle t^2 \right), \qquad \left| S_{ij}^{k+\frac{1}{2}} \right| \le m_1 \left(h_1^2 + h_2^2 + \triangle t^2 \right), \tag{4.2}$$

with the initial conditions

$$\bar{n}_{ij}^0 = n_0\left(x_i, y_j\right), \qquad \bar{f}_{ij}^0 = f_0\left(\bar{n}_{ij}^0\right). \tag{4.3}$$

Omitting the local truncation error terms in (4.1a) and (4.1b), we can derive the Crank-Nicolson scheme of the fourth-order parabolic equation (2.5a) and (2.6a) for all $1 \le i \le M_1$, $1 \le j \le M_2$, $0 \le k \le K - 1$ as follows,

$$\frac{n_{ij}^{k+1} - n_{ij}^k}{\triangle t} + c \triangle_h^2 n_{ij}^{k+\frac{1}{2}} - \triangle_h \mu_0 \left(n_{ij}^{k+\frac{1}{2}} \right) = 0, \tag{4.4}$$

$$\frac{(f_0)_{ij}^{k+1} - (f_0)_{ij}^k}{\triangle t} = \mu_0 \left(n_{ij}^{k+\frac{1}{2}} \right) \frac{n_{ij}^{k+1} - n_{ij}^k}{\triangle t}. \tag{4.5}$$

Here, the total discrete free energy at $k\Delta t$, $k = 0, 1, 2, ..., K$, is defined as

$$F_h^k = \frac{c}{2} \left\| \nabla_h n^k \right\|^2 + \left\langle f_0^k, 1 \right\rangle, \tag{4.6}$$

and it is updated by the equation (4.5). We note that, there is a little inconsistence between the modified version of the discrete total energy as its original one due to the fact that $f_0^k \ne f_0(n^k)$. We apply the idea proposed in the work of Qiao. et al [24], to guarantee the energy decreasing property during the evolution process. The proof of the energy stability presented below will demonstrate how it plays the role. And the improvement of the consistence between the two energy expressions will be left as one aspect of our future work.

Lemma 4.1. *(Mass conservation.) The solution of the discrete equation (4.4) satisfies the mass conservation, that is, for any $0 \le k \le K - 1$,*

$$h_1 h_2 \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} n_{ij}^{k+1} = h_1 h_2 \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} n_{ij}^k.$$

Remark 4.1. The proof is classical. The mass conservation can be obtained spontaneously by multiplying $h_1 h_2 \triangle t$ to both sides of (4.4), summing for $i = 1, ..., M_1$, $j = 1, ..., M_2$, with supplement of the periodic boundary condition.

Lemma 4.2. *(Energy identity.) If the total discrete free energy at $k\triangle t$, $k = 0, 1, ...K$, is defined by (4.6), the discrete scheme provided by (4.4)-(4.5) can guarantee the following energy identity for any time step $\triangle t > 0$,*

$$\frac{F_h^{k+1} - F_h^k}{\triangle t} + \left\| \nabla_h w^{k+\frac{1}{2}} \right\|^2 = 0. \tag{4.7}$$

Proof. Define $w^{k+\frac{1}{2}}$, $k = 0, \ 1, \ 2, ..., K - 1$, as

$$w_{ij}^{k+\frac{1}{2}} = c \triangle_h n_{ij}^{k+\frac{1}{2}} - \mu_0 \left(n_{ij}^{k+\frac{1}{2}} \right).$$

Taking the inner product of (4.4) with $w^{k+\frac{1}{2}}$, we have

$$\frac{1}{\Delta t} \left\langle n^{k+1} - n^k, c\Delta_h \frac{n^{k+1} + n^k}{2} \right\rangle - \frac{1}{\Delta t} \left\langle n^{k+1} - n^k, \mu_0(n^{k+\frac{1}{2}}) \right\rangle + \left\langle \Delta_h w^{k+\frac{1}{2}}, w^{k+\frac{1}{2}} \right\rangle = 0.$$

By using integration by parts under periodic boundary condition and the equation (4.5), we have

$$\frac{c}{2\triangle t} \left(\left\| \nabla n^{k+1} \right\|^2 - \left\| \nabla n^k \right\|^2 \right) + \frac{1}{\triangle t} \left\langle f_0^{k+1} - f_0^k, 1 \right\rangle + \left\| -\nabla w^{k+\frac{1}{2}} \right\|^2 = 0.$$

Recombining the terms in the above formula, we can get

$$\frac{1}{\triangle t} \left(\frac{c}{2} \left\| \nabla n^{k+1} \right\|^2 + \left\langle f_0^{k+1}, 1 \right\rangle \right) - \frac{1}{\triangle t} \left(\frac{c}{2} \left\| \nabla n^k \right\|^2 + \left\langle f_0^k, 1 \right\rangle \right) + \left\| -\nabla w^{k+\frac{1}{2}} \right\|^2 = 0,$$

which is a detailed form of (4.7). This completes the proof. $\qquad \square$

Remark 4.2. We note that, this energy stability is respect to the modified energy expression (4.6), which is a little different with the discrete form of the original energy functional (2.4). In turn, one can not obtain the H^1 bound for the numerical solution, even if the numerical solution is required to be inside the domain $[\theta_0, 1/b - \theta_0]$, as in the following theorems.

4.1. The unique solvability

4.1.1. Solvability

Theorem 4.1. *The discrete scheme (4.4)-(4.5) has at least one solution.*

Proof. The scheme (4.4) for all $1 \le i \le M_1$, $1 \le j \le M_2$, $0 \le k \le K - 1$, can be written as

$$w_{ij} - n_{ij}^k + \frac{c\triangle t}{2} \triangle_h^2 w_{ij} - \frac{\triangle t}{2} \triangle_h \mu_0 (w_{ij}) = 0, \tag{4.8}$$

where $w = n^{k+\frac{1}{2}}$. Define the map

$$g(w_{ij}) = w_{ij} - n_{ij}^k + \frac{c\triangle t}{2} \triangle_h^2 w_{ij} - \frac{\triangle t}{2} \triangle_h \mu_0 (w_{ij}).$$

Then

$$\langle g(w), w\rangle = \|w\|^2 - \langle n^k, w\rangle + \frac{c\triangle t}{2}\|\triangle_h w\|^2 - \frac{\triangle t}{2}\langle \triangle_h \mu_0(w), w\rangle$$

$$= \|w\|^2 - \langle n^k, w\rangle + \frac{c\triangle t}{2}\|\triangle_h w\|^2 + \frac{\triangle t}{2}\langle \mu_0'(w)\nabla_h w \cdot \nabla_h w, 1\rangle.$$

Therefore,

$$\langle g(w), w\rangle > \left[\|w\|^2 - \langle n^k, w\rangle\right] + \frac{c\triangle t}{2}\|\triangle_h w\|^2 - a(T)\triangle t\|\nabla_h w\|^2$$

$$\geq \left[\|w\|^2 - \|n^k\|\|w\|\right] + \frac{c\triangle t}{2}\|\triangle_h w\|^2 - \left(\frac{c\triangle t}{2}\|\triangle_h w\|^2 + \frac{a^2(T)\triangle t}{2c}\|w\|^2\right)$$

$$= \left(1 - \frac{a^2(T)\triangle t}{2c}\right)\|w\|^2 - \|n^k\|\|w\| \geq \left[\left(1 - \frac{a^2(T)\triangle t}{2c}\right)\|w\| - \|n^k\|\right]\|w\|.$$

When $\triangle t < \dfrac{c}{a^2(T)}$, it follows that $\dfrac{a^2(T)\triangle t}{2c} < \dfrac{1}{2}$, and

$$(g(w), w) \geq \left(\frac{1}{2}\|w\| - \|n^k\|\right)\|w\| = \frac{1}{2}\left(\|w\| - 2\|n^k\|\right)\|w\|.$$

If $\|w\| = 2\|n^k\|$, we have $\langle g(w), w\rangle \geq 0$. By Lemma 3.1, there is at least one solution w satisfying $\|w\| \leq 2\|n^k\|$. The solvability of the Crank-Nicolson scheme is proved. $\square$

Remark 4.3. It has to be noted that Theorem 4.1 can only guarantee the existence of the real value of the solution $\mathbf{n}^{k+1}$ for the equation (4.4). However, the reasonable value of each component of the vector $\mathbf{n}^{k+1}$ has to be in the open subset of the set of real numbers $(0, 1/b)$. This requirement for the solution from the physical background could not be guaranteed by this theorem. Numerically, this requirement could be guaranteed by selecting appropriate temporal steps since the program can only run ahead only if all the components of the vector $\mathbf{n}^{k+1}$ are in the region $(0, 1/b)$. Furthermore, all the components of the obtained numerical solution $\mathbf{n}^{k+1}$ are in a close subset of the reasonable $(0, 1/b)$ due to the finiteness of their total number, which could be written as $[\theta_0, 1/b - \theta_0]$, where $\theta_0 \in (0, 1/(2b))$ is a really small value.

In addition, the uniqueness of the reasonable solution of the discrete equation (4.4) is provided as follows.

4.1.2. Uniqueness of the solution

Theorem 4.2. *The discrete scheme* (4.4)-(4.5) *has at most one solution in the region* $[\theta_0, 1/b - \theta_0]$ *for any* $\theta_0 \in (0, 1/(2b))$ *if* $\Delta t < 2c/M^2$. *Here* $M = \max\{|\mu'(n)| : n \in [\theta_0, 1/b - \theta_0]\}$.

Proof. Suppose (4.8) has another solution z, $w_{ij} \in [\theta_0, 1/b - \theta_0]$ and $z_{ij} \in [\theta_0, 1/b - \theta_0]$ for all $1 \leq i \leq M_1$, $1 \leq j \leq M_2$, then

$$(z_{ij} - n_{ij}^k) + \frac{c\triangle t}{2}\triangle_h^2 z_{ij} - \frac{\triangle t}{2}\triangle_h \mu_0(z_{ij}) = 0. \tag{4.9}$$

Let $\epsilon_{ij} = w_{ij} - z_{ij}$, subtracting (4.9) from (4.8), we have

$$\epsilon_{ij} + \frac{c\triangle t}{2}\triangle_h^2 \epsilon_{ij} - \frac{\triangle t}{2}\left[\triangle_h \mu_0(w_{ij}) - \triangle_h \mu_0(z_{ij})\right] = 0. \tag{4.10}$$

Taking the inner product of (4.10) with ϵ, we obtain

$$\|\epsilon\|^2 + \frac{c\triangle t}{2}\|\triangle_h\epsilon\|^2 - \frac{\triangle t}{2}\langle\triangle_h\mu_0(w) - \triangle_h\mu_0(z),\epsilon\rangle = 0.$$

According to the Lemma 3.2, we have

$$\frac{\triangle t}{2}\langle\triangle_h\mu_0(w) - \triangle_h\mu_0(z),\epsilon\rangle = \frac{\triangle t}{2}\langle\mu_0(w) - \mu_0(z),\triangle_h\epsilon\rangle.$$

Then

$$\|\epsilon\|^2 + \frac{c\triangle t}{2}\|\triangle_h\epsilon\|^2 = \frac{\triangle t}{2}\langle\mu_0(w) - \mu_0(z),\triangle_h\epsilon\rangle = \frac{\triangle t}{2}\left\langle\frac{\partial\mu_0}{\partial n}(\xi)\epsilon,\Delta_h\epsilon\right\rangle$$

$$\leq \frac{\triangle t}{2}M\|\epsilon\|\|\Delta\epsilon\| \leq \frac{\Delta t M^2}{8c}\|\epsilon\|^2 + \frac{c\triangle t}{2}\|\triangle_h\epsilon\|^2.$$

where $\xi = cw + (1-c)z$, $c \in [0,1]$, satisfies $|\mu'(\xi)| < M$ spontaneously. Therefore,

$$\|\epsilon\|^2 + \frac{c\triangle t}{2}\|\triangle_h\epsilon\|^2 \leq \frac{\Delta t M^2}{8c}\|\epsilon\|^2 + \frac{c\triangle t}{2}\|\triangle_h\epsilon\|^2.$$

Thus $\|\epsilon\|^2 \leq \frac{\Delta t M^2}{8c}\|\epsilon\|^2$. If $\Delta t < \frac{8c}{M^2}$, $\epsilon = 0$. This completes the proof. $\square$

4.2. Convergence

For the convenience of presentation, we first introduce the following notations.

$$\alpha_{11} = \max\{|\mu_0'(n)| : n \in [\epsilon_1, 1/b - \epsilon_1]\}, \qquad \alpha_{12} = \max\{|\mu_0''(n)| : n \in [\epsilon_1, 1/b - \epsilon_1]\},$$

$$\alpha_{13} = \frac{\alpha_{11}^2}{4c} + \frac{1}{2}, \quad \alpha_{14} = \max\left\{\left|\frac{\bar{n}^{k+1} - \bar{n}^k}{\Delta t}\right|, k = 1, 2, ...K - 1.\right\},$$

$$\alpha_{15} = \frac{4\alpha_{11}^2}{c^2} + \frac{2\alpha_{12}\alpha_{14} + 2c + 2}{c}$$

$$\alpha_{16} = 2 + \frac{\alpha_{11}^2}{c} + \frac{4\alpha_{11}^2}{c^2} + \frac{4\alpha_{12}\alpha_{14}}{c} + \frac{\alpha_{11}^2}{c}\left(\frac{2\alpha_{11}^2}{c^2} + \frac{\alpha_{12}\alpha_{14}}{c}\right) + \max\left\{\frac{\alpha_{12}\alpha_{14}}{c}, \frac{2\alpha_{11}^2}{c^2}\right\},$$

$$C_{11} = \sqrt{\frac{|\Omega|}{4\alpha_{13}}}\exp(2\alpha_{13}(k+1)\Delta t)m_1,$$

$$C_{12} = \sqrt[4]{\frac{\alpha_{15}}{2\alpha_{13}\alpha_{16}}k_0^2|\Omega|^2}\exp\left(\left(\alpha_{13} + \frac{\alpha_{16}}{4}\right)(k+1)\Delta t\right)m_1.$$

Theorem 4.3. *Suppose the solution of the original fourth order equation (2.5a)-(2.5b) is sufficiently smooth, and there exists ϵ_1 such that for any $k = 0, 1, ..., K$, the solution of the Crank-Nicolson scheme (4.4), n^k and the solution of (4.1a) $\bar{n}^k \in [\epsilon_1, 1/b - \epsilon_1]$. If $\alpha_{13}\Delta t < 1/2$, then*

$$\|e^{k+1}\| \leq C_{11}\left(h_1^2 + h_2^2 + \Delta t^2\right);$$

if $\alpha_{15}\Delta t < \frac{1}{2}$, we can obtain

$$\|e^{k+1}\|_\infty \leq C_{12}\left(h_1^2 + h_2^2 + \Delta t^2\right).$$

Proof. We know $\bar{n}_{ij}^{k+1} = \bar{n}(x_i, y_j, t_k)$ is the solution of (4.1a), and n_{ij}^{k+1} is the solution of (4.4). Let $e_{ij}^k = \bar{n}_{ij}^k - n_{ij}^k$. Subtracting (4.4) from (4.1a), we have: for all $1 \le i \le M_1$, $1 \le j \le M_2$, $e_{ij}^0 = 0$, and

$$\frac{e_{ij}^{k+1} - e_{ij}^k}{\triangle t} + c\triangle_h^2 e_{ij}^{k+\frac{1}{2}} - \triangle_h \mu_0 \left(\bar{n}_{ij}^{k+\frac{1}{2}} \right) + \triangle_h \mu_0 \left(n_{ij}^{k+\frac{1}{2}} \right) = R_{ij}^{k+\frac{1}{2}}, \quad 0 \le k \le K-1. \quad (4.11)$$

Taking inner product of (4.11) with $e^{k+\frac{1}{2}} = \dfrac{e^{k+1} + e^k}{2}$, then

$$\frac{\left\| e^{k+1} \right\|^2 - \left\| e^k \right\|^2}{2\triangle t} + c \left\| \triangle_h e^{k+\frac{1}{2}} \right\|^2$$
$$= \left\langle \triangle_h \mu_0 \left(\bar{n}^{k+\frac{1}{2}} \right) - \triangle_h \mu_0 \left(n^{k+\frac{1}{2}} \right), e^{k+\frac{1}{2}} \right\rangle + \left\langle R^{k+\frac{1}{2}}, e^{k+\frac{1}{2}} \right\rangle.$$

According to Lemma 3.2, we have

$$\left\langle \triangle_h \mu_0 \left(\bar{n}^{k+\frac{1}{2}} \right) - \triangle_h \mu_0 \left(n^{k+\frac{1}{2}} \right), e^{k+\frac{1}{2}} \right\rangle$$
$$= \left\langle \mu_0 \left(\bar{n}^{k+\frac{1}{2}} \right) - \mu_0 \left(n^{k+\frac{1}{2}} \right), \triangle_h e^{k+\frac{1}{2}} \right\rangle = \left\langle \mu_0'(\xi^{k+\frac{1}{2}}) e^{k+\frac{1}{2}}, \Delta_h e^{k+\frac{1}{2}} \right\rangle$$
$$\le \alpha_{11} \left\| e^{k+\frac{1}{2}} \right\| \left\| \Delta_h e^{k+\frac{1}{2}} \right\| \le \frac{\alpha_{11}^2}{4c} \left\| e^{k+\frac{1}{2}} \right\|^2 + c \left\| \triangle_h e^{k+\frac{1}{2}} \right\|^2.$$

Using (4.2), we have

$$\left\langle R^{k+\frac{1}{2}}, e^{k+\frac{1}{2}} \right\rangle \le \left\| R^{k+\frac{1}{2}} \right\| \left\| \frac{e^{k+1} + e^k}{2} \right\|$$
$$\le \frac{|\Omega|}{2} m_1^2 \left(h_1^2 + h_2^2 + \Delta t^2 \right)^2 + \frac{\left\| e^{k+1} \right\|^2 + \left\| e^k \right\|^2}{4}.$$

Combining all the above results, we obtain

$$\left\| e^{k+1} \right\|^2 - \left\| e^k \right\|^2$$
$$\le \left(\frac{\alpha_{11}^2}{4c} + \frac{1}{2} \right) \left(\left\| e^{k+1} \right\|^2 + \left\| e^k \right\|^2 \right) \Delta t + |\Omega| \, m_1^2 \left(h_1^2 + h_2^2 + \Delta t^2 \right)^2 \Delta t. \quad (4.12)$$

Replacing the superscript k by l in (4.12) and summing up for l from 0 to k leads to

$$\left\| e^{k+1} \right\|^2 = \sum_{l=0}^k \left(\left\| e^{l+1} \right\|^2 - \left\| e^l \right\|^2 \right)$$
$$\le \sum_{l=0}^k \left(\frac{\alpha_{11}^2}{4c} + \frac{1}{2} \right) \left(\left\| e^{l+1} \right\|^2 + \left\| e^l \right\|^2 \right) \Delta t + (k+1) \, |\Omega| \, m_1^2 \left(h_1^2 + h_2^2 + \Delta t^2 \right)^2 \Delta t.$$

Thus,

$$\left\| e^{k+1} \right\|^2 \le \frac{\left(\frac{\alpha_{11}^2}{2c} + 1 \right) \Delta t}{1 - \left(\frac{\alpha_{11}^2}{4c} + \frac{1}{2} \right) \Delta t} \sum_{l=0}^k \left\| e^l \right\|^2 + \frac{(k+1) \, |\Omega| \, m_1^2}{1 - \left(\frac{\alpha_{11}^2}{4c} + \frac{1}{2} \right) \Delta t} \left(h_1^2 + h_2^2 + \Delta t^2 \right)^2 \Delta t.$$

If $\Delta t \le 1/ \left(\dfrac{\alpha_{11}^2}{2c} + 1 \right)$, then $\left(\dfrac{\alpha_{11}^2}{4c} + \dfrac{1}{2} \right) \Delta t \le \dfrac{1}{2}$, and

$$\left\| e^{k+1} \right\|^2 \le \left(\frac{\alpha_{11}^2}{c} + 2 \right) \Delta t \sum_{l=0}^k \left\| e^l \right\|^2 + 2(k+1) m_1^2 \left(h_1^2 + h_2^2 + \Delta t^2 \right)^2 \Delta t. \quad (4.13)$$

Gronwall's inequality leads to

$$\|e^{k+1}\| \leq \sqrt{\frac{|\Omega|}{4\alpha_{13}}} \exp\left(2\alpha_{13}(k+1)\Delta t\right) m_1 \left(h_1^2 + h_2^2 + \Delta t^2\right)$$

$$= C_{11} \left(h_1^2 + h_2^2 + \Delta t^2\right). \tag{4.14}$$

For estimating $\|\triangle_h e^{k+1}\|$, we take the inner product of (4.11) with $\delta_t e^{k+\frac{1}{2}} = \dfrac{e^{k+1} - e^k}{\Delta t}$. With the help of Lemma 3.2, we have

$$\left\|\frac{e^{k+1} - e^k}{\triangle t}\right\|^2 + \frac{c}{2\Delta t}\left(\|\triangle_h e^{k+1}\|^2 - \|\triangle_h e^k\|^2\right)$$

$$= \left\langle \mu_0\left(\bar{n}^{k+\frac{1}{2}}\right) - \mu_0\left(n^{k+\frac{1}{2}}\right), \delta_t \triangle_h e^{k+\frac{1}{2}}\right\rangle + \left\langle R^{k+\frac{1}{2}}, \frac{e^{k+1} - e^k}{\Delta t}\right\rangle.$$

The last term of above formula satisfies

$$\left\langle R^{k+\frac{1}{2}}, \frac{e^{k+1} - e^k}{\Delta t}\right\rangle \leq \left\|R^{k+\frac{1}{2}}\right\| \left\|\frac{e^{k+1} - e^k}{\Delta t}\right\| \leq \frac{|\Omega|}{2}m_1^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2 + \frac{1}{2}\left\|\frac{e^{k+1} - e^k}{\Delta t}\right\|^2.$$

Therefore,

$$\frac{1}{2}\left\|\frac{e^{k+1} - e^k}{\Delta t}\right\|^2 + \frac{c}{2\Delta t}\left(\|\triangle_h e^{k+1}\|^2 - \|\triangle_h e^k\|^2\right)$$

$$\leq \left\langle \mu_0\left(\bar{n}^{k+\frac{1}{2}}\right) - \mu_0\left(n^{k+\frac{1}{2}}\right), \delta_t \triangle_h e^{k+\frac{1}{2}}\right\rangle + \frac{|\Omega|}{2}m_1^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2. \tag{4.15}$$

Replacing the superscript k by l in (4.15), summing up for l from 0 to k and using Lemmas 3.4 and 3.5, we obtain

$$\frac{1}{2}\sum_{l=0}^{k}\left\|\frac{e^{l+1} - e^l}{\Delta t}\right\|^2 + \frac{c}{2\Delta t}\sum_{l=0}^{k}\left(\|\triangle_h e^{l+1}\|^2 - \|\triangle_h e^l\|^2\right)$$

$$\leq \sum_{l=0}^{k}\left\langle \mu_0\left(\bar{n}^{l+\frac{1}{2}}\right) - \mu_0\left(n^{l+\frac{1}{2}}\right), \delta_t \triangle_h e^{l+\frac{1}{2}}\right\rangle + \frac{|\Omega|}{2}(k+1)m_1^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2$$

$$= \frac{1}{\Delta t}\left\langle \mu_0'\left(\xi_1^{k+\frac{1}{2}}\right)e^{k+\frac{1}{2}}, \triangle_h e^{k+1}\right\rangle + \frac{|\Omega|}{2}(k+1)m_1^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2$$

$$- \sum_{l=1}^{k}\left\langle \mu_0''\left(\xi_2^l\right)\left(\rho^l e^{l+\frac{1}{2}} + (1-\rho^l)e^{l-\frac{1}{2}}\right)\frac{\bar{n}^{l+\frac{1}{2}} - \bar{n}^{l-\frac{1}{2}}}{\Delta t}, \triangle_h e^l\right\rangle$$

$$+ \sum_{l=1}^{k}\left\langle \mu_0'\left(\rho^l n^{l+\frac{1}{2}} + (1-\rho^l)n^{l-\frac{1}{2}}\right)\frac{e^{l+\frac{1}{2}} - e^{l-\frac{1}{2}}}{\Delta t}, \triangle_h e^l\right\rangle + \frac{\alpha_{12}\alpha_{14}}{2}\sum_{l=1}^{k}\left(\|e^{l+1}\| + \|e^l\|\right.$$

$$\left. + \|e^{l-1}\|\right)\|\triangle_h e^l\| + \alpha_{11}\sum_{l=1}^{k}\left[\left\|\frac{e^{l+1} - e^l}{2\Delta t}\right\| + \left\|\frac{e^l - e^{l-1}}{2\Delta t}\right\|\right]\|\triangle_h e^l\|$$

$$\leq \frac{c}{4\Delta t}\|\triangle_h e^{k+1}\|^2 + \frac{\alpha_{11}^2}{2c\Delta t}\left(\|e^{k+1}\|^2 + \|e^k\|^2\right) + \frac{|\Omega|}{2}(k+1)m_1^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2$$

$$+ \sum_{l=1}^{k}\left(\frac{\alpha_{12}\alpha_{14}}{4}\|e^{l+1}\|^2 + \frac{\alpha_{12}\alpha_{14}}{4}\|e^l\|^2 + \frac{\alpha_{12}\alpha_{14}}{4}\|e^{l-1}\|^2 + \frac{3\alpha_{12}\alpha_{14}}{4}\|\triangle_h e^l\|^2\right)$$

$$+ \sum_{l=1}^{k} \left(\frac{1}{4} \left\| \frac{e^{l+1} - e^l}{\Delta t} \right\|^2 + \frac{1}{4} \left\| \frac{e^l - e^{l-1}}{\Delta t} \right\|^2 + \frac{\alpha_{11}^2}{2} \left\| \Delta_h e^l \right\| \right).$$

Immediately,

$$\frac{c}{4\Delta t} \left\| \Delta_h e^{k+1} \right\|^2$$
$$\leq \frac{\alpha_{11}^2}{2c\Delta t} \left(\left\| e^{k+1} \right\|^2 + \left\| e^k \right\|^2 \right) + \frac{|\Omega|}{2} (k+1) m_1^2 \left(h_1^2 + h_2^2 + \Delta t^2 \right)^2 + \frac{\alpha_{11}^2}{2} \sum_{l=1}^{k} \left\| \Delta_h e^l \right\|^2$$
$$+ \sum_{l=1}^{k} \left(\frac{\alpha_{12}\alpha_{14}}{4} \left\| e^{l+1} \right\|^2 + \frac{\alpha_{12}\alpha_{14}}{4} \left\| e^l \right\|^2 + \frac{\alpha_{12}\alpha_{14}}{4} \left\| e^{l-1} \right\|^2 + \frac{3\alpha_{12}\alpha_{14}}{4} \left\| \Delta_h e^l \right\|^2 \right).$$

It naturally gives

$$\left\| \Delta_h e^{k+1} \right\|^2 \tag{4.16}$$
$$\leq \frac{2\alpha_{11}^2}{c^2} \left(\left\| e^{k+1} \right\|^2 + \left\| e^k \right\|^2 \right) + \frac{2|\Omega|}{c} (k+1) m_1^2 \left(h_1^2 + h_2^2 + \Delta t^2 \right)^2 \Delta t$$
$$+ \sum_{l=1}^{k} \left[\frac{\alpha_{12}\alpha_{14}}{c} \left(\left\| e^{l+1} \right\|^2 + \left\| e^l \right\|^2 + \left\| e^{l-1} \right\|^2 \right) + \left(\frac{3\alpha_{12}\alpha_{14}}{c} + \frac{2\alpha_{11}^2}{c} \right) \left\| \Delta_h e^l \right\|^2 \right] \Delta t. \tag{4.17}$$

Combining (4.13) and (4.17), we obtain

$$\left\| \Delta_h e^{k+1} \right\|^2 + \left\| e^{k+1} \right\|^2$$
$$\leq \left(1 + \frac{2\alpha_{11}^2}{c^2} + \frac{\alpha_{12}\alpha_{14}}{c} \right) \left\| e^{k+1} \right\|^2 + \max \left\{ \frac{3\alpha_{12}\alpha_{14}}{c}, \frac{2\alpha_{12}\alpha_{14}}{c} + \frac{2\alpha_{11}^2}{c^2} \right\} \Delta t \sum_{l=1}^{k} \left\| e^l \right\|^2$$
$$+ \left(\frac{3\alpha_{12}\alpha_{14}}{c} + \frac{2\alpha_{11}^2}{c} \right) \sum_{l=1}^{k} \left\| \Delta_h e^l \right\|^2 \Delta t + \frac{2|\Omega|}{c} (k+1) m_1^2 \left(h_1^2 + h_2^2 + \Delta t^2 \right)^2 \Delta t$$
$$\leq \left[2 + \frac{\alpha_{11}^2}{c} + \frac{4\alpha_{11}^2}{c^2} + \frac{4\alpha_{12}\alpha_{14}}{c} + \frac{\alpha_{11}^2}{c} \left(\frac{2\alpha_{11}^2}{c^2} + \frac{\alpha_{12}\alpha_{14}}{c} \right) \right.$$
$$\left. + \max \left\{ \frac{\alpha_{12}\alpha_{14}}{c}, \frac{2\alpha_{11}^2}{c^2} \right\} \right] \Delta t \sum_{l=0}^{k} \left\| e^l \right\|^2 + \left(\frac{4\alpha_{11}^2}{c^2} + \frac{2\alpha_{12}\alpha_{14} + 2c + 2}{c} \right) (k$$
$$+1) |\Omega| m_1^2 \left(h_1^2 + h_2^2 + \Delta t^2 \right)^2 \Delta t + \frac{3\alpha_{12}\alpha_{14} + 2\alpha_{11}^2}{c} \sum_{l=1}^{k} \left\| \Delta_h e^l \right\|^2 \Delta t$$
$$\leq \alpha_{16} \Delta t \sum_{l=1}^{k} \left(\left\| e^l \right\|^2 + \left\| \Delta_h e^l \right\|^2 \right) + (k+1)\alpha_{15} |\Omega| m_1^2 (h_1^2 + h_2^2 + \Delta t^2)^2 \Delta t.$$

Note that, the derivation of the last step bases on the fact that $\alpha_{11}^2/c < \alpha_{11}^2/c^2$ due to the coefficient $c \in (0,1)$. Gronwall's inequality yields

$$\left\| e^{k+1} \right\|^2 + \left\| \Delta_h e^{k+1} \right\|^2 \leq \frac{\alpha_{15}}{\alpha_{16}} \exp \left(\alpha_{16}(k+1)\Delta t \right) \cdot |\Omega| \left[m_1 \left(h_1^2 + h_2^2 + \triangle t^2 \right) \right]^2,$$

where $k = 0, 1, ..., K-1$. Using Lemma 3.3 and (4.14), we can get

$$\left\| e^{k+1} \right\|_{\infty}^2 \leq k_0 \left\| e^{k+1} \right\| \left(\left\| \triangle_h e^{k+1} \right\| + \left\| e^{k+1} \right\| \right)$$

$$\leq k_0 \sqrt{2 \left\| e^{k+1} \right\|^2 \left(\left\| e^{k+1} \right\|^2 + \left\| \triangle_h e^{k+1} \right\|^2 \right)}$$

$$\leq k_0 \sqrt{\frac{\alpha_{15}}{2\alpha_{13}\alpha_{16}}} \exp \left(\left(2\alpha_{13} + \frac{\alpha_{16}}{2} \right) (k+1)\triangle t \right) m_1^2 |\Omega| \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2.$$

Therefore,

$$\left\| e^{k+1} \right\|_\infty \leq C_{12} \left(h_1^2 + h_2^2 + \triangle t^2 \right).$$

The completes the proof of the theorem. $\qquad\square$

5. A Second Order Linearized Scheme

Applying Taylor expansion to (2.5a), (2.6a) for all $1 \leq i \leq M_1$, $1 \leq j \leq M_2$, we have

$$\frac{\bar{n}_{ij}^{k+1} - \bar{n}_{ij}^k}{\triangle t} + c\triangle_h^2 \bar{n}_{ij}^{k+\frac{1}{2}} - \triangle_h \mu_0 \left(\hat{\bar{n}}_{ij}^{k+\frac{1}{2}} \right) = \hat{R}_{ij}^{k+\frac{1}{2}}, \qquad 0 \leq k \leq K-1, \qquad (5.1a)$$

$$\frac{(\bar{f}_0)_{ij}^{k+1} - (\bar{f}_0)_{ij}^k}{\triangle t} = \mu_0 \left(\hat{\bar{n}}_{ij}^{k+\frac{1}{2}} \right) \frac{\bar{n}_{ij}^{k+1} - \bar{n}_{ij}^k}{\triangle t} + \hat{S}_{ij}^{k+\frac{1}{2}}, \qquad 0 \leq k \leq K-1, \qquad (5.1b)$$

with the following initial conditions

$$\bar{n}(\mathbf{x}_{ij}, 0) = n_0(\mathbf{x}_{ij}), \quad \bar{f}_0(n(\mathbf{x}_{ij}, 0)) = f_0^0(n(\mathbf{x}_{ij})), \qquad (5.2)$$

where there exists a constant m_2 such that

$$\left| \hat{R}_{ij}^{k+\frac{1}{2}} \right| \leq m_2 \left(h_1^2 + h_2^2 + \triangle t^2 \right), \quad \left| \hat{S}_{ij}^{k+\frac{1}{2}} \right| \leq m_2 \left(h_1^2 + h_2^2 + \triangle t^2 \right), \quad 0 \leq k \leq K-1. \qquad (5.3)$$

The difference scheme is constructed by omitting the local truncation error terms in the above two equations as follows: for all $1 \leq i \leq M_1$, $1 \leq j \leq M_2$,

$$\frac{n_{ij}^{k+1} - n_{ij}^k}{\triangle t} + c\triangle_h^2 n_{ij}^{k+\frac{1}{2}} - \triangle_h \mu_0 \left(\hat{n}_{ij}^{k+\frac{1}{2}} \right) = 0, \quad 0 \leq k \leq K-1, \qquad (5.4a)$$

subject to the initial condition

$$n(\mathbf{x}_{ij}, 0) = n_0(\mathbf{x}_{ij}). \qquad (5.4b)$$

As for all $1 \leq i \leq M_1$, $1 \leq j \leq M_2$, the discrete energy density $(f_0)_{ij}^{k+1}$ is computed by [24]

$$\frac{(f_0)_{ij}^{k+1} - (f_0)_{ij}^k}{\triangle t} = \mu_0 \left(\hat{n}_{ij}^{k+\frac{1}{2}} \right) \frac{n_{ij}^{k+1} - n_{ij}^k}{\triangle t}, \quad 0 \leq k \leq K-1, \qquad (5.5a)$$

with initial value

$$f_0(n(\mathbf{x}_{ij}, 0)) = f_0(n_0(\mathbf{x}_{ij})). \qquad (5.5b)$$

Similarly to derivations of the mass conservation and the energy decay property of the Crank-Nicolson scheme, these properties of the second order linearized scheme could be given by the following two lemmas.

Lemma 5.1. *(Mass conservation.)* *The solution of the discrete equation (5.4a)-(5.4b) also satisfies the mass conservation if periodic boundary condition is given, which means that for any $0 \leq k \leq K - 1$,*

$$h_1 h_2 \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} n_{ij}^{k+1} = h_1 h_2 \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} n_{ij}^k.$$

Lemma 5.2. *(Energy identity.)* *If the discrete total energy at $k\Delta t$, $k = 0, 1, ...K$, is defined by (4.6), then the discrete scheme provided by (5.4a)-(5.5a) also can guarantee the energy identity for any time step $\Delta t > 0$ as follows,*

$$\frac{F_h^{k+1} - F_h^k}{\triangle t} + \left\| -\nabla_h \hat{w}^{k+\frac{1}{2}} \right\|^2 = 0, \tag{5.6}$$

where $\hat{w}^{k+\frac{1}{2}} = c\triangle_h n^{k+\frac{1}{2}} - \mu_0(\hat{n}^{k+\frac{1}{2}})$.

5.1. The unique solvability and the convergence of the linearized scheme

Theorem 5.1. *The linearized scheme (5.4a)-(5.4b) is uniquely solvable.*

Proof. The scheme (5.4a) for all $1 \leq i \leq M_1$, $1 \leq j \leq M_2$, $0 \leq k \leq K - 1$ can be written as

$$n_{ij}^{k+1} + \frac{c\triangle t}{2} \triangle_h^2 n_{ij}^{k+1} = n_{ij}^k - \frac{c\triangle t}{2} \triangle_h^2 n_{ij}^k + \Delta t \triangle_h \mu_0 \left(\hat{n}_{ij}^{k+\frac{1}{2}} \right). \tag{5.7}$$

Suppose n^k, $\hat{n}^{k+\frac{1}{2}}$ have been determined. Then (5.7) is a linear equation about n^{k+1}. Consider its homogenous system as follows,

$$n_{ij}^{k+1} + \frac{c\triangle t}{2} \triangle_h^2 n_{ij}^{k+1} = 0, \quad 1 \leq i \leq M_1, \quad 1 \leq j \leq M_2. \tag{5.8}$$

Taking inner product of (5.8) with n^{k+1}, we have

$$\left\| n^{k+1} \right\|^2 + \frac{c\triangle t}{2} \left\| \triangle_h n^{k+1} \right\|^2 = 0. \tag{5.9}$$

It requires $n^{k+1} = 0$. Therefore (5.7) has a unique solution. □

Remark 5.1. Also, the above theorem can not guarantee that each component of the vector $\mathbf{n}^{k+1}$ is in the open subset of the set of real numbers $(0, 1/b)$. So far, we can only guarantee this from our numerical implementations. The exploration of theoretical analysis of this kind of discrete or continuous partial differential equations with high nonlinearity and singularity needs further future efforts.

For the convenience of presentation, the following notations are introduced.

$$\alpha_{21} = \max \left\{ |\mu_0'(n)| : \ n \in \left[\frac{\hat{\theta}}{2}, \frac{1}{b} - \frac{\hat{\theta}}{2} \right] \right\}, \quad \alpha_{22} = \max \left\{ |\mu_0''(n)| : \ n \in \left[\frac{\hat{\theta}}{2}, \frac{1}{b} - \frac{\hat{\theta}}{2} \right] \right\},$$

$$\alpha_{23} = \frac{2\alpha_{21}^2}{c} + 1, \quad \alpha_{24} = \max \left\{ \left| \frac{\bar{n}^{k+1} - \bar{n}^k}{\Delta t} \right|, k = 0, 1, ...K - 1. \right\},$$

$$\alpha_{25} = \frac{16\alpha_{21}^2 + 1}{c} + 1, \quad \alpha_{26} = \max\left\{\frac{13\alpha_{23}^2}{4}, 2\alpha_{21}^2 + 4\alpha_{22}\alpha_{24}\right\},$$

$$\alpha_{27} = \max\left\{2\alpha_{23} + \frac{16\alpha_{23}\alpha_{21}^2}{c^2} + \frac{5\alpha_{22}\alpha_{24}}{c}, \frac{2\alpha_{26}}{c}\right\},$$

$$C_{21} = \exp\left(\alpha_{23}t\right)\sqrt{\frac{|\Omega|}{\alpha_{23}}}m_2, \quad C_{22} = \sqrt[4]{\frac{2\alpha_{25}}{\alpha_{23}\alpha_{27}}k_0^2|\Omega|^2}\exp\left(\left(\frac{\alpha_{23} + \alpha_{27}}{2}\right)T_m\right)m_2.$$

Theorem 5.2. *Suppose the solution $\bar{n}(\mathbf{x}, t)$ to the fourth order equation (2.5a)-(2.5b) is sufficiently smooth, and there is a $\hat{\theta} \in (0, 1/(2b))$, such that $\bar{n}_{ij}^k \in \left[\hat{\theta}, 1/b - \hat{\theta}\right]$ for all $1 \leq i \leq M_1$, $1 \leq j \leq M_2$, $k = 0, 1, ..K$. If*

$$C_{22}(h_1^2 + h_2^2 + \Delta t^2) \leq \frac{1}{2}\hat{\theta}, \tag{5.10}$$

then the difference scheme (5.4a)-(5.4b) is convergent with second order in both time and space in the following detailed form

$$\left\|e^{k+1}\right\| \leq C_{21}\left(h_1^2 + h_2^2 + \triangle t^2\right), \quad \left\|e^{k+1}\right\|_\infty \leq C_{22}\left(h_1^2 + h_2^2 + \triangle t^2\right). \tag{5.11}$$

Proof. Since

$$\hat{\bar{n}}^{\frac{1}{2}} = \bar{n}^0 + \frac{\Delta t}{2}\bar{n}_t^0 = n^0 + \frac{\Delta t}{2}n_t^0 = \hat{n}^{\frac{1}{2}}, \qquad \hat{\bar{n}}^{\frac{3}{2}} = \bar{n}^0 + \frac{3\Delta t}{2}\bar{n}_t^0 = n^0 + \frac{3\Delta t}{2}n_t^0 = \hat{n}^{\frac{3}{2}},$$

we have

$$\mu_0\left(\hat{\bar{n}}^{\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{\frac{1}{2}}\right) = 0, \quad \mu_0\left(\hat{\bar{n}}^{\frac{3}{2}}\right) - \mu_0\left(\hat{n}^{\frac{3}{2}}\right) = 0.$$

Subtracting (5.4a) from (5.1a) for all $1 \leq i \leq M_1$, $1 \leq j \leq M_2$, we have $e_{ij}^0 = 0$ and

$$\frac{e_{ij}^{k+1} - e_{ij}^k}{\triangle t} + c\triangle_h^2 e_{ij}^{k+\frac{1}{2}} = \hat{R}_{ij}^{k+\frac{1}{2}}, \quad k = 0, 1, \tag{5.12}$$

$$\frac{e_{ij}^{k+1} - e_{ij}^k}{\triangle t} + c\triangle_h^2 e_{ij}^{k+\frac{1}{2}} - \triangle_h\mu_0\left(\hat{\bar{n}}_{ij}^{k+\frac{1}{2}}\right) + \triangle_h\mu_0\left(\hat{n}_{ij}^{k+\frac{1}{2}}\right) = \hat{R}_{ij}^{k+\frac{1}{2}}, \quad 2 \leq k \leq K - 1. \tag{5.13}$$

For the first step, taking inner product of (5.12) at $k = 0$ with $e^{\frac{1}{2}} = \frac{e^0 + e^1}{2}$ yields

$$\frac{\left\|e^1\right\|^2 - \left\|e^0\right\|^2}{2\triangle t} + c\left\|\triangle_h\left(\frac{e^0 + e^1}{2}\right)\right\|^2 = \left\langle\hat{R}^{\frac{1}{2}}, \frac{e^0 + e^1}{2}\right\rangle.$$

For the initial value, $\left\|e^0\right\| = 0$, so

$$\frac{\left\|e^1\right\|^2}{2\triangle t} + c\left\|\triangle_h\frac{e^1}{2}\right\|^2 = \left\langle\hat{R}^{\frac{1}{2}}, \frac{e^1}{2}\right\rangle. \tag{5.14}$$

Using (5.3), we get

$$\frac{\left\|e^1\right\|^2}{2\triangle t} + \frac{c}{4}\left\|\triangle_h e^1\right\|^2 \leq \frac{\left\|e^1\right\|^2}{4\triangle t} + \frac{\triangle t|\Omega|m_2^2\left(h_1^2 + h_2^2 + \triangle t^2\right)^2}{4}, \tag{5.15}$$

It yields

$$\left\|e^1\right\| \leq \sqrt{|\Omega|}m_2\triangle t\left(h_1^2 + h_2^2 + \triangle t^2\right), \tag{5.16}$$

$$\left\|\triangle_h e^1\right\| \leq \sqrt{\frac{|\Omega|\,\triangle t}{c}} m_2 \left(h_1^2 + h_2^2 + \triangle t^2\right). \tag{5.17}$$

According to Lemma 3.3,

$$\left\|e^1\right\|_\infty^2 \leq k_0 \left(\left\|\triangle_h e^1\right\| \left\|e^1\right\| + \left\|e^1\right\|^2\right)$$

$$\leq k_0 \left[\sqrt{\frac{\triangle t}{c}} m_2^2 |\Omega|\,\triangle t \left(h_1^2 + h_2^2 + \triangle t^2\right)^2 + |\Omega|\,m_2^2 \triangle t^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2\right].$$

If $\triangle t < 1/c$, then

$$\left\|e^1\right\|_\infty^2 \leq \frac{2\,|\Omega|\,k_0 \triangle t}{c} m_2^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2.$$

Besides, from (5.14) we also obtain

$$\frac{\left\|e^1\right\|^2}{2\triangle t} + \frac{c}{4} \left\|\triangle_h e^1\right\|^2 \leq \frac{\left\|e^1\right\|^2}{4} + \frac{|\Omega|\,m_2^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2}{4}.$$

Therefore,

$$\frac{\left\|e^1\right\|^2}{2\triangle t} \leq \frac{\left\|e^1\right\|^2}{4} + \frac{|\Omega|\,m_2^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2}{4}. \tag{5.18}$$

Secondly, to get the error at second time step $\left\|e^2\right\|_\infty$, we take the inner product of (5.12) with $k = 1$ and $e^{\frac{3}{2}} = \dfrac{e^1 + e^2}{2}$,

$$\frac{\left\|e^2\right\|^2 - \left\|e^1\right\|^2}{2\triangle t} + c \left\|\triangle_h \left(\frac{e^1 + e^2}{2}\right)\right\|^2 = \left\langle \hat{R}^{\frac{3}{2}}, \frac{e^1 + e^2}{2}\right\rangle.$$

Applying (5.3), we have

$$\frac{\left\|e^2\right\|^2 - \left\|e^1\right\|^2}{2\triangle t} \leq \frac{\left\|e^1\right\|^2 + \left\|e^2\right\|^2}{4\triangle t} + \frac{|\Omega|\,\triangle t}{2} m_2^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2. \tag{5.19}$$

From (5.19) and the estimation of $\left\|e^1\right\|^2$ by (5.16), we can get

$$\left\|e^2\right\| \leq \sqrt{5\,|\Omega|} m_2 \triangle t \left(h_1^2 + h_2^2 + \triangle t^2\right). \tag{5.20}$$

To get the estimation of $\left\|\Delta e^2\right\|$, taking the inner product of (5.12) when $k = 1$ with $\dfrac{e^2 - e^1}{\triangle t}$, we have

$$\left\|\frac{e^2 - e^1}{\triangle t}\right\|^2 + \frac{c}{2\triangle t} \left(\left\|\triangle_h e^2\right\|^2 - \left\|\triangle_h e^1\right\|^2\right)$$

$$= \left\langle \hat{R}^{\frac{3}{2}}, \frac{e^2 - e^1}{\triangle t}\right\rangle \leq \left\|\frac{e^2 - e^1}{\triangle t}\right\|^2 + \frac{|\Omega|}{4} m_2^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2,$$

from which, we obtain

$$\left\|\triangle_h e^2\right\|^2 \leq \left\|\triangle_h e^1\right\|^2 + \frac{|\Omega|\,\Delta t}{2c} m_2^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2.$$

Combining the above equation with (5.17), we get

$$\left\| \triangle_h e^2 \right\|^2 \leq \frac{3 \left| \Omega \right| \triangle t}{2c} m_2^2 \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2. \tag{5.21}$$

Similar to the first case, combining the equation (5.20) and (5.21) leads to

$$\left\| e^2 \right\|_\infty^2 \leq k_0 \left(\left\| \triangle_h e^2 \right\| \left\| e^2 \right\| + \left\| e^2 \right\|^2 \right)$$

$$\leq k_0 \left[\sqrt{\frac{15 \triangle t}{2c}} \left| \Omega \right| m_2^2 \triangle t \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2 + 5 \left| \Omega \right| m_2^2 \triangle t^2 \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2 \right]. \tag{5.22}$$

If $\Delta t < 1/c$, then

$$\left\| e^2 \right\|_\infty^2 \leq \frac{8 k_0 \left| \Omega \right| \triangle t}{c} m_2^2 \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2. \tag{5.23}$$

At the third step, we derive the estimation for $\left\| e^{k+1} \right\|$ and $\left\| e^{k+1} \right\|_\infty$ by mathematical induction. Suppose (5.11) is true for l from 0 to k ($0 \leq k \leq K - 1$). Then if (5.10) is satisfied, we have

$$\left\| e^k \right\|_\infty \leq C_{22} (h_1^2 + h_2^2 + \Delta t^2) \leq \frac{1}{2} \hat{\theta}, \quad 1 \leq l \leq k.$$

Then it follows that

$$n_{ij}^k \in \left[\hat{\theta}/2, 1/b - \hat{\theta}/2 \right], \quad 1 \leq i \leq M_1, \quad 1 \leq j \leq M_2, \quad 0 \leq l \leq k.$$

Taking inner product of (5.13) with $e^{k+\frac{1}{2}} = \dfrac{e^k + e^{k+1}}{2}$, we obtain

$$\frac{\left\| e^{k+1} \right\|^2 - \left\| e^k \right\|^2}{2 \triangle t} + c \left\| \triangle_h e^{k+\frac{1}{2}} \right\|^2$$

$$= \left\langle \triangle_h \mu_0 \left(\hat{\bar{n}}^{k+\frac{1}{2}} \right) - \triangle_h \mu_0 \left(\hat{n}^{k+\frac{1}{2}} \right), e^{k+\frac{1}{2}} \right\rangle + \left\langle \hat{R}^{k+\frac{1}{2}}, \frac{e^k + e^{k+1}}{2} \right\rangle.$$

Since

$$\hat{\bar{n}}^{k+\frac{1}{2}} - \hat{n}^{k+\frac{1}{2}}$$

$$= \bar{n}^k + \frac{1}{2} \bar{n}^{k-1} - \frac{1}{2} \bar{n}^{k-2} - \left(n^k + \frac{1}{2} n^{k-1} - \frac{1}{2} n^{k-2} \right) = e^k + \frac{1}{2} e^{k-1} - \frac{1}{2} e^{k-2},$$

we have

$$\mu_0 \left(\hat{\bar{n}}^{k+\frac{1}{2}} \right) - \mu_0 \left(\hat{n}^{k+\frac{1}{2}} \right) = \mu'(\hat{\xi}^{k+\frac{1}{2}}) \left(e^k + \frac{1}{2} e^{k-1} - \frac{1}{2} e^{k-2} \right),$$

where $\hat{\xi}^{k+\frac{1}{2}} = \hat{\lambda}^{k+\frac{1}{2}} \hat{\bar{n}}^{k+\frac{1}{2}} + (1 - \hat{\lambda}^{k+\frac{1}{2}}) \hat{n}^{k+\frac{1}{2}}$, $\hat{\lambda}^{k+\frac{1}{2}} \in [0,1]$. According to Lemma 3.2, we get

$$\left\langle \triangle_h \mu_0 \left(\hat{\bar{n}}^{k+\frac{1}{2}} \right) - \triangle_h \mu_0 \left(\hat{n}^{k+\frac{1}{2}} \right), e^{k+\frac{1}{2}} \right\rangle = \left\langle \mu_0 \left(\hat{\bar{n}}^{k+\frac{1}{2}} \right) - \mu_0 \left(\hat{n}^{k+\frac{1}{2}} \right), \triangle_h e^{k+\frac{1}{2}} \right\rangle$$

$$\leq \left\| \mu'(\hat{\xi}^{k+\frac{1}{2}}) \left(e^k + \frac{1}{2} e^{k-1} - \frac{1}{2} e^{k-2} \right) \right\| \left\| \triangle_h e^{k+\frac{1}{2}} \right\|$$

$$\leq \alpha_{21} \left[\left\| e^k \right\| + \frac{1}{2} \left\| e^{k-1} \right\| + \frac{1}{2} \left\| e^{k-2} \right\| \right] \left\| \triangle_h e^{k+\frac{1}{2}} \right\|$$

$$\leq \frac{\alpha_{21}^2}{2c} \left[\left\|e^k\right\|^2 + \frac{1}{2}\left\|e^{k-1}\right\|^2 + \frac{1}{2}\left\|e^{k-2}\right\|^2 \right] + c \left\|\Delta_h e^{k+\frac{1}{2}}\right\|^2. \tag{5.24}$$

Whereupon

$$\frac{\left\|e^{k+1}\right\|^2 - \left\|e^k\right\|^2}{2\triangle t} + c \left\|\triangle_h e^{k+\frac{1}{2}}\right\|^2$$

$$\leq \frac{\alpha_{21}^2}{2c} \left[\left\|e^k\right\|^2 + \frac{1}{2}\left\|e^{k-1}\right\|^2 + \frac{1}{2}\left\|e^{k-2}\right\|^2 \right] + c \left\|\Delta_h e^{k+\frac{1}{2}}\right\|^2 + \left\langle \hat{R}^{k+\frac{1}{2}}, \frac{e^k + e^{k+1}}{2} \right\rangle.$$

Accordingly,

$$\frac{\left\|e^{k+1}\right\|^2 - \left\|e^k\right\|^2}{2\triangle t} \tag{5.25}$$

$$\leq \frac{\alpha_{21}^2}{2c} \left[\left\|e^k\right\|^2 + \frac{1}{2}\left\|e^{k-1}\right\|^2 + \frac{1}{2}\left\|e^{k-2}\right\|^2 \right] + \frac{\left\|e^k\right\|^2 + \left\|e^{k+1}\right\|^2}{4} + \frac{|\Omega|}{2}m_2^2\left(h_1^2 + h_2^2 + \triangle t^2\right)^2.$$

Replacing the superscript k by l in (5.25) and summing up for l from 2 to k, we get

$$\sum_{l=2}^k \frac{\left\|e^{l+1}\right\|^2 - \left\|e^l\right\|^2}{2\triangle t} \leq \frac{\alpha_{21}^2}{2c} \left[\sum_{l=2}^k \left\|e^l\right\|^2 + \frac{1}{2}\sum_{l=1}^{k-1} \left\|e^l\right\|^2 + \frac{1}{2}\sum_{l=1}^{k-2} \left\|e^l\right\|^2 \right]$$

$$+ \sum_{l=2}^k \frac{\left\|e^l\right\|^2 + \left\|e^{l+1}\right\|^2}{4} + \frac{|\Omega|}{2}\sum_{l=2}^k m_2^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2. \tag{5.26}$$

Combining (5.18) with (5.26) and multiplying $2\Delta t$ to both side, we obtain

$$\left(1 - \frac{\Delta t}{2}\right) \left\|e^{k+1}\right\|^2$$

$$\leq \frac{\alpha_{21}^2}{c} \left[\sum_{l=2}^k \left\|e^l\right\|^2 + \frac{1}{2}\sum_{l=1}^{k-1} \left\|e^l\right\|^2 + \frac{1}{2}\sum_{l=1}^{k-2} \left\|e^l\right\|^2 \right] \Delta t + \frac{\Delta t}{2} \left[\sum_{l=2}^k \left\|e^l\right\|^2 + \sum_{l=3}^k \left\|e^l\right\|^2 \right]$$

$$+ |\Omega| \Delta t \sum_{l=2}^k m_2^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2 + \frac{\left\|e^2\right\|^2 + \left\|e^1\right\|^2}{2}\Delta t$$

$$+ |\Omega| \Delta t m_2^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2 + \frac{\left\|e^1\right\|^2 \Delta t}{2} + \frac{|\Omega| m_2^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2}{2}\Delta t$$

$$\leq \frac{2\alpha_{21}^2}{c}\Delta t \sum_{l=1}^k \left\|e^l\right\|^2 + \Delta t \sum_{l=1}^k \left\|e^l\right\|^2 + (k+1)|\Omega| \Delta t m_2^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2$$

$$= \alpha_{23}\Delta t \sum_{l=1}^k \left\|e^l\right\|^2 + (k+1)|\Omega| m_2^2 \triangle t \left(h_1^2 + h_2^2 + \triangle t^2\right)^2.$$

If $\Delta t < 1$, then

$$\left\|e^{k+1}\right\|^2 \leq 2\alpha_{23}\Delta t \sum_{l=1}^k \left\|e^l\right\|^2 + 2(k+1)|\Omega| m_2^2 \triangle t \left(h_1^2 + h_2^2 + \triangle t^2\right)^2. \tag{5.27}$$

The Gronwall's inequality yields

$$\left\|e^{k+1}\right\| \leq \exp\left(\alpha_{23}(k+1)\Delta t\right) \sqrt{\frac{|\Omega|}{\alpha_{23}}} m_2 \left(h_1^2 + h_2^2 + \triangle t^2\right) = C_{21}\left(h_1^2 + h_2^2 + \triangle t^2\right). \tag{5.28}$$

For estimating $\left\|\Delta_h e^{k+1}\right\|$, we take the inner product of (5.13) with $\delta_t e^{k+\frac{1}{2}} = \dfrac{e^{k+1} - e^k}{\Delta t}$, then

$$\left\|\frac{e^{k+1} - e^k}{\triangle t}\right\|^2 + \frac{c}{2\Delta t}\left(\left\|\triangle_h e^{k+1}\right\|^2 - \left\|\triangle_h e^k\right\|^2\right)$$

$$= \left\langle \triangle_h \mu_0\left(\hat{\hat{n}}^{k+\frac{1}{2}}\right) - \triangle_h \mu_0\left(\hat{n}^{k+\frac{1}{2}}\right), \delta_t e^{k+\frac{1}{2}} \right\rangle + \left\langle \hat{R}^{k+\frac{1}{2}}, \frac{e^{k+1} - e^k}{\Delta t} \right\rangle.$$

Similar to the derivation of (5.24), we have

$$\left\langle \triangle_h \mu_0\left(\hat{\hat{n}}^{k+\frac{1}{2}}\right) - \triangle_h \mu_0\left(\hat{n}^{k+\frac{1}{2}}\right), \delta_t e^{k+\frac{1}{2}} \right\rangle = \left\langle \mu_0\left(\hat{\hat{n}}^{k+\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{k+\frac{1}{2}}\right), \delta_t \triangle_h e^{k+\frac{1}{2}} \right\rangle.$$

Also, we obtain

$$\left\langle \hat{R}^{k+\frac{1}{2}}, \frac{e^{k+1} - e^k}{\Delta t} \right\rangle \leq \frac{|\Omega|\, m_2^2(h_1^2 + h_2^2 + \Delta t^2)^2}{2} + \frac{1}{2}\left\|\frac{e^{k+1} - e^k}{\triangle t}\right\|^2.$$

Therefore, we have

$$\frac{1}{2}\left\|\frac{e^{k+1} - e^k}{\triangle t}\right\|^2 + \frac{c}{2\Delta t}\left(\left\|\triangle_h e^{k+1}\right\|^2 - \left\|\triangle_h e^k\right\|^2\right)$$

$$\leq \left\langle \mu_0\left(\hat{\hat{n}}^{k+\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{k+\frac{1}{2}}\right), \delta_t \triangle_h e^{k+\frac{1}{2}} \right\rangle + \frac{|\Omega|\, m_2^2(h_1^2 + h_2^2 + \Delta t^2)^2}{2}. \qquad (5.29)$$

Replacing the superscript k by l in (5.29) and summing up for l from 0 to k, we get

$$\frac{1}{2}\sum_{l=0}^{k}\left\|\frac{e^{l+1} - e^l}{\triangle t}\right\|^2 + \frac{c}{2\Delta t}\left\|\triangle_h e^{k+1}\right\|^2$$

$$\leq \sum_{l=0}^{k}\left\langle \mu_0\left(\hat{\hat{n}}^{l+\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{l+\frac{1}{2}}\right), \delta_t \triangle_h e^{l+\frac{1}{2}} \right\rangle + \sum_{l=0}^{k}\frac{|\Omega|\, m_2^2(h_1^2 + h_2^2 + \Delta t^2)^2}{2}. \qquad (5.30)$$

According to Lemma 3.4, we have

$$\sum_{l=0}^{l=k}\left\langle \mu_0\left(\hat{\hat{n}}^{l+\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{l+\frac{1}{2}}\right), \delta_t \triangle_h e^{l+\frac{1}{2}} \right\rangle$$

$$- \sum_{l=1}^{k}\left\langle \frac{\mu_0\left(\hat{\hat{n}}^{l+\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{l+\frac{1}{2}}\right) - \left[\mu_0\left(\hat{\hat{n}}^{l-\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{l-\frac{1}{2}}\right)\right]}{\Delta t}, \Delta_h e^l \right\rangle$$

$$= \frac{1}{\Delta t}\left\langle \mu_0\left(\hat{\hat{n}}^{k+\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{k+\frac{1}{2}}\right), \Delta_h e^{k+1} \right\rangle - \left\langle \frac{\mu_0\left(\hat{\hat{n}}^{\frac{5}{2}}\right) - \mu_0\left(\hat{n}^{\frac{5}{2}}\right)}{\Delta t}, \Delta_h e^2 \right\rangle$$

$$- \sum_{l=3}^{k}\left\langle \frac{\mu_0\left(\hat{\hat{n}}^{l+\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{l+\frac{1}{2}}\right) - \left(\mu_0\left(\hat{\hat{n}}^{l-\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{l-\frac{1}{2}}\right)\right)}{\Delta t}, \Delta_h e^l \right\rangle.$$

Here,

$$\mu_0\left(\hat{\hat{n}}^{k+\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{k+\frac{1}{2}}\right) = \mu_0'(\hat{\rho}^{k+\frac{1}{2}}\hat{\hat{n}}^{k+\frac{1}{2}} + (1 - \hat{\rho}^{k+\frac{1}{2}})\hat{n}^{k+\frac{1}{2}})\left(\hat{\hat{n}}^{k+\frac{1}{2}} - \hat{n}^{k+\frac{1}{2}}\right)$$

$$= \mu_0'(\hat{\rho}^{k+\frac{1}{2}}\hat{\hat{n}}^{k+\frac{1}{2}} + (1 - \hat{\rho}^{k+\frac{1}{2}})\hat{n}^{k+\frac{1}{2}})\left(e^k + \frac{1}{2}e^{k-1} - \frac{1}{2}e^{k-2}\right),$$

$$\mu_0\left(\hat{\hat{u}}^{\frac{5}{2}}\right) - \mu_0\left(\hat{u}^{\frac{5}{2}}\right) = \mu_0'(\hat{\rho}^{\frac{5}{2}}\hat{\hat{n}}^{\frac{5}{2}} + (1-\hat{\rho}^{\frac{5}{2}})\hat{n}^{\frac{5}{2}})\left(e^2 - e^1 + \frac{3}{2}e^1 - \frac{3}{2}e^0\right).$$

Therefore, we have

$$\frac{1}{\Delta t}\left\langle \mu_0\left(\hat{\hat{u}}^{k+\frac{1}{2}}\right) - \mu_0\left(\hat{u}^{k+\frac{1}{2}}\right), \Delta_h e^{k+1}\right\rangle$$
$$= \frac{1}{\Delta t}\left\langle \mu_0'(\hat{\rho}^{k+\frac{1}{2}}\hat{\hat{n}}^{k+\frac{1}{2}} + (1-\hat{\rho}^{k+\frac{1}{2}})\hat{n}^{k+\frac{1}{2}})\left(e^k + \frac{1}{2}e^{k-1} - \frac{1}{2}e^{k-2}\right), \Delta_h e^{k+1}\right\rangle$$
$$\leq \frac{c}{4\Delta t}\left\|\Delta_h e^{k+1}\right\|^2 + \frac{2\alpha_{21}^2}{c\Delta t}\left(\left\|e^k\right\|^2 + \frac{1}{2}\left\|e^{k-1}\right\|^2 + \frac{1}{2}\left\|e^{k-2}\right\|^2\right),$$

and

$$-\left\langle \frac{\mu_0\left(\hat{\hat{u}}^{\frac{5}{2}}\right) - \mu_0\left(\hat{u}^{\frac{5}{2}}\right)}{\Delta t}, \Delta_h e^2\right\rangle$$
$$= -\frac{1}{\Delta t}\left\langle \mu_0'(\hat{\rho}^{\frac{5}{2}}\hat{\hat{n}}^{\frac{5}{2}} + (1-\hat{\rho}^{\frac{5}{2}})\hat{n}^{\frac{5}{2}})\left(e^2 - e^1 + \frac{3}{2}e^1 - \frac{3}{2}e^0\right), \Delta_h e^2\right\rangle$$
$$\leq \alpha_{21}\left\|\frac{e^2 - e^1}{\Delta t} + \frac{3}{2}\frac{e^1 - e^0}{\Delta t}\right\|\left\|\Delta_h e^2\right\| \leq \frac{1}{4}\left[\left\|\frac{e^2 - e^1}{\Delta t}\right\|^2 + \left\|\frac{e^1 - e^0}{\Delta t}\right\|^2\right] + \frac{13\alpha_{21}^2}{4}\left\|\Delta_h e^2\right\|^2.$$

Its follows from Lemma 3.5 that

$$\frac{1}{\Delta t}\left[\mu_0(\hat{\hat{n}}^{l+\frac{1}{2}}) - \mu_0(\hat{n}^{l+\frac{1}{2}}) - \left(\mu_0(\hat{\hat{n}}^{l-\frac{1}{2}}) - \mu_0(\hat{n}^{l-\frac{1}{2}})\right)\right]$$
$$= \mu_0'(\hat{\rho}^l\hat{n}^{l+\frac{1}{2}} + (1-\hat{\rho}^l)\hat{n}^{l-\frac{1}{2}})\frac{e^l - e^{l-1} + \frac{1}{2}(e^{l-1} - e^{l-2}) - \frac{1}{2}(e^{l-2} - e^{l-3})}{\Delta t}$$
$$+ \mu_0''(\hat{\xi}^l)\left(\hat{\rho}^l\hat{e}^{l+\frac{1}{2}} + (1-\hat{\rho}^l)\hat{e}^{l-\frac{1}{2}}\right)\frac{\bar{n}^l - \bar{n}^{l-1} + \frac{1}{2}(\bar{n}^{l-1} - \bar{n}^{l-2}) - \frac{1}{2}(\bar{n}^{l-2} - \bar{n}^{l-3})}{\Delta t},$$

where $\hat{\rho}^l \in (0,1)$ and $\hat{\xi}^l \in \left(\min\{\gamma_1, \gamma_2\}, \max\{\gamma_1, \gamma_2\}\right)$. Consequently, we have

$$-\sum_{l=3}^{k}\left\langle \frac{\mu_0\left(\hat{\hat{n}}^{l+\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{l+\frac{1}{2}}\right) - \left(\mu_0\left(\hat{\hat{n}}^{l-\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{l-\frac{1}{2}}\right)\right)}{\Delta t}, \Delta_h e^l\right\rangle$$
$$= -\sum_{l=3}^{k}\left\langle \mu_0'(\hat{\rho}^l\hat{n}^{l+\frac{1}{2}} + (1-\hat{\rho}^l)\hat{n}^{l-\frac{1}{2}})\frac{e^l - e^{l-1} + \frac{1}{2}(e^{l-1} - e^{l-2}) - \frac{1}{2}(e^{l-2} - e^{l-3})}{\Delta t}, \Delta_h e^l\right\rangle$$
$$- \sum_{l=3}^{k}\left\langle \mu_0''(\xi^l)\left(\hat{\rho}^l\hat{e}^{l+\frac{1}{2}} + (1-\hat{\rho}^l)\hat{e}^{l-\frac{1}{2}}\right)\frac{\bar{n}^l - \bar{n}^{l-1} + \frac{\bar{n}^{l-1} - \bar{n}^{l-2}}{2} - \frac{\bar{n}^{l-2} - \bar{n}^{l-3}}{2}}{\Delta t}, \Delta_h e^l\right\rangle. \quad (5.31)$$

The first term of the right hand side of (5.31) satisfies

$$-\sum_{l=3}^{k}\left\langle \mu_0'(\hat{\rho}^l\hat{n}^{l+\frac{1}{2}} + (1-\hat{\rho}^l)\hat{n}^{l-\frac{1}{2}})\frac{e^l - e^{l-1} + \frac{1}{2}(e^{l-1} - e^{l-2}) - \frac{1}{2}(e^{l-2} - e^{l-3})}{\Delta t}, \Delta_h e^l\right\rangle$$
$$\leq \frac{1}{4}\sum_{l=3}^{k}\left\|\frac{e^l - e^{l-1}}{\Delta t}\right\|^2 + \alpha_{21}^2\sum_{l=3}^{k}\left\|\Delta_h e^l\right\|^2 + \frac{1}{8}\sum_{l=3}^{k}\left\|\frac{e^{l-1} - e^{l-2}}{\Delta t}\right\|^2$$
$$+ \frac{\alpha_{21}^2}{2}\sum_{l=3}^{k}\left\|\Delta_h e^l\right\|^2 + \frac{1}{8}\sum_{l=3}^{k}\left\|\frac{e^{l-2} - e^{l-3}}{\Delta t}\right\|^2 + \frac{\alpha_{21}^2}{2}\sum_{l=3}^{k}\left\|\Delta_h e^l\right\|^2. \quad (5.32)$$

As for the second term of (5.31), we have

$$
\left| \sum_{l=3}^{k} \left\langle \mu_0''(\xi^l) \left(\hat{\rho}^l \hat{e}^{l+\frac{1}{2}} + (1 - \hat{\rho}^l) \hat{e}^{l-\frac{1}{2}} \right) \frac{\bar{n}^l - \bar{n}^{l-1} + \frac{\bar{n}^{l-1} - \bar{n}^{l-2}}{2} - \frac{\bar{n}^{l-2} - \bar{n}^{l-3}}{2}}{\Delta t}, \Delta_h e^l \right\rangle \right|
$$

$$
\leq 2 \sum_{l=3}^{k} \alpha_{22} \alpha_{24} \left[\left\| \hat{\rho} e^l \right\| + \left\| \left(1 - \frac{\hat{\rho}}{2} \right) e^{l-1} \right\| + \left\| \left(\frac{1}{2} - \hat{\rho} \right) e^{l-2} \right\| + \left\| \frac{1 - \hat{\rho}}{2} e^{l-3} \right\| \right] \left\| \Delta_h e^l \right\|
$$

$$
= \sum_{l=3}^{k} \alpha_{22} \alpha_{24} \left\| e^l \right\|^2 + \sum_{l=2}^{k-1} \alpha_{22} \alpha_{24} \left\| e^l \right\|^2 + \sum_{l=1}^{k-2} \frac{\alpha_{22} \alpha_{24}}{4} \left\| e^l \right\|^2
$$

$$
+ \sum_{l=1}^{k-3} \frac{\alpha_{22} \alpha_{24}}{4} \left\| e^l \right\|^2 + 4 \alpha_{22} \alpha_{24} \sum_{l=3}^{k} \left\| \Delta_h e^l \right\|^2.
$$

Hence,

$$
\sum_{l=0}^{l=k} \left\langle \mu_0 \left(\hat{\bar{u}}^{l+\frac{1}{2}} \right) - \mu_0 \left(\hat{u}^{l+\frac{1}{2}} \right), \delta_t \Delta_h e^{l+\frac{1}{2}} \right\rangle \tag{5.33}
$$

$$
= \frac{1}{\Delta t} \left\langle \mu_0 \left(\hat{\bar{u}}^{k+\frac{1}{2}} \right) - \mu_0 \left(\hat{u}^{k+\frac{1}{2}} \right), \Delta_h e^{k+1} \right\rangle - \left\langle \frac{\mu_0 \left(\hat{\bar{u}}^{\frac{5}{2}} \right) - \mu_0 \left(\hat{u}^{\frac{5}{2}} \right)}{\Delta t}, \Delta_h e^2 \right\rangle
$$

$$
- \sum_{l=3}^{k} \left\langle \frac{\mu_0 \left(\hat{\bar{u}}^{l+\frac{1}{2}} \right) - \mu_0 \left(\hat{u}^{l+\frac{1}{2}} \right) - \left(\mu_0 \left(\hat{\bar{u}}^{l-\frac{1}{2}} \right) - \mu_0 \left(\hat{u}^{l-\frac{1}{2}} \right) \right)}{\Delta t}, \Delta_h e^l \right\rangle
$$

$$
\leq \frac{c}{4\Delta t} \left\| \Delta_h e^{k+1} \right\|^2 + \frac{2\alpha_{21}^2}{c\Delta t} \left(\left\| e^k \right\|^2 + \frac{1}{4} \left\| e^{k-1} \right\|^2 + \frac{1}{4} \left\| e^{k-2} \right\|^2 \right)
$$

$$
+ \frac{1}{2} \sum_{l=0}^{k-1} \left\| \frac{e^{l+1} - e^l}{\Delta t} \right\|^2 + \alpha_{26} \sum_{l=2}^{k} \left\| \Delta_h e^l \right\|^2
$$

$$
+ \sum_{l=3}^{k} \alpha_{22} \alpha_{24} \left\| e^l \right\|^2 + \sum_{l=2}^{k-1} \alpha_{22} \alpha_{24} \left\| e^l \right\|^2 + \sum_{l=1}^{k-2} \frac{\alpha_{22} \alpha_{24}}{4} \left\| e^l \right\|^2 + \sum_{l=1}^{k-3} \frac{\alpha_{22} \alpha_{24}}{4} \left\| e^l \right\|^2.
$$

Combining (5.33) with (5.30), we get

$$
\frac{1}{2} \sum_{l=0}^{k} \left\| \frac{e^{l+1} - e^l}{\Delta t} \right\|^2 + \frac{c}{2\Delta t} \left\| \Delta_h e^{k+1} \right\|^2
$$

$$
\leq \frac{c}{4\Delta t} \left\| \Delta_h e^{k+1} \right\|^2 + \frac{2\alpha_{21}^2}{c\Delta t} \left(\left\| e^k \right\|^2 + \frac{1}{2} \left\| e^{k-1} \right\|^2 + \frac{1}{2} \left\| e^{k-2} \right\|^2 \right)
$$

$$
+ \frac{1}{2} \sum_{l=0}^{k-1} \left\| \frac{e^{l+1} - e^l}{\Delta t} \right\|^2 + \alpha_{26} \sum_{l=2}^{k} \left\| \Delta_h e^l \right\|^2 + \sum_{l=3}^{k} \alpha_{22} \alpha_{24} \left\| e^l \right\|^2 + \sum_{l=2}^{k-1} \alpha_{22} \alpha_{24} \left\| e^l \right\|^2
$$

$$
+ \sum_{l=1}^{k-2} \frac{\alpha_{22} \alpha_{24}}{4} \left\| e^l \right\|^2 + \sum_{l=1}^{k-3} \frac{\alpha_{22} \alpha_{24}}{4} \left\| e^l \right\|^2 + \sum_{l=0}^{k} \frac{|\Omega| \, m_2^2 (h_1^2 + h_2^2 + \Delta t^2)^2}{2}. \tag{5.34}
$$

Therefore,

$$
\frac{c}{4\Delta t} \left\| \Delta_h e^{k+1} \right\|^2 \leq \frac{2\alpha_{21}^2}{c\Delta t} \left(\left\| e^k \right\|^2 + \frac{1}{4} \left\| e^{k-1} \right\|^2 + \frac{1}{4} \left\| e^{k-2} \right\|^2 \right) + \alpha_{26} \sum_{l=2}^{k} \left\| \Delta_h e^l \right\|^2
$$

$$
+ \sum_{l=3}^{k} \alpha_{22} \alpha_{24} \left\| e^l \right\|^2 + \sum_{l=2}^{k-1} \alpha_{22} \alpha_{24} \left\| e^l \right\|^2 + \sum_{l=1}^{k-2} \frac{\alpha_{22} \alpha_{24}}{4} \left\| e^l \right\|^2
$$

$$+ \sum_{l=1}^{k-3} \frac{\alpha_{22}\alpha_{24}}{4} \left\| e^l \right\|^2 + \sum_{l=0}^{k} \frac{|\Omega|\, m_2^2(h_1^2 + h_2^2 + \Delta t^2)^2}{2}. \qquad (5.35)$$

Accordingly,

$$\left\| \triangle_h e^{k+1} \right\|^2 \leq \frac{8\alpha_{21}^2}{c^2} \left(\left\| e^k \right\|^2 + \frac{1}{2} \left\| e^{k-1} \right\|^2 + \frac{1}{2} \left\| e^{k-2} \right\|^2 \right) + \frac{4\alpha_{26}}{c} \Delta t \sum_{l=2}^{k} \left\| \Delta_h e^l \right\|^2$$

$$+ \sum_{l=3}^{k} \frac{4\alpha_{22}\alpha_{24}}{c} \Delta t \left\| e^l \right\|^2 + \sum_{l=2}^{k-1} \frac{4\alpha_{22}\alpha_{24}}{c} \Delta t \left\| e^l \right\|^2 + \sum_{l=1}^{k-2} \frac{\alpha_{22}\alpha_{24}}{c} \Delta t \left\| e^l \right\|^2$$

$$+ \sum_{l=1}^{k-3} \frac{\alpha_{22}\alpha_{24}}{c} \Delta t \left\| e^l \right\|^2 + \sum_{l=0}^{k} \frac{2\,|\Omega|\, m_2^2(h_1^2 + h_2^2 + \Delta t^2)^2}{c} \Delta t. \qquad (5.36)$$

According to (5.27), if $\Delta t < 1$, we get

$$\left\| e^{k+1} \right\|^2 \leq 2\alpha_{23}\Delta t \sum_{l=1}^{k} \left\| e^l \right\|^2 + 2(k+1)\,|\Omega|\, m_2^2 \triangle t \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2.$$

Combining the above results, (5.27) with (5.36), we have

$$\left\| e^{k+1} \right\|^2 + \left\| \triangle_h e^{k+1} \right\|^2$$

$$\leq 2\alpha_{23}\Delta t \sum_{l=1}^{k} \left\| e^l \right\|^2 + 2(k+1)\,|\Omega|\, m_2^2 \triangle t \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2 + \frac{4\alpha_{26}}{c} \Delta t \sum_{l=2}^{k} \left\| \Delta_h e^l \right\|^2$$

$$+ \frac{8\alpha_{21}^2}{c^2} \left[2\alpha_{23}\Delta t \sum_{l=1}^{k-1} \left\| e^l \right\|^2 + 2k\,|\Omega|\, m_2^2 \triangle t \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2 \right]$$

$$+ \frac{4\alpha_{21}^2}{c^2} \left[2\alpha_{23}\Delta t \sum_{l=1}^{k-2} \left\| e^l \right\|^2 + 2(k-1)\,|\Omega|\, m_2^2 \triangle t \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2 \right]$$

$$+ \frac{4\alpha_{21}^2}{c^2} \left[2\alpha_{23}\Delta t \sum_{l=1}^{k-3} \left\| e^l \right\|^2 + 2(k-2)\,|\Omega|\, m_2^2 \triangle t \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2 \right]$$

$$+ \sum_{l=3}^{k} \frac{4\alpha_{22}\alpha_{24}}{c} \Delta t \left\| e^l \right\|^2 + \sum_{l=2}^{k-1} \frac{4\alpha_{22}\alpha_{24}}{c} \Delta t \left\| e^l \right\|^2 + \sum_{l=1}^{k-2} \frac{\alpha_{22}\alpha_{24}}{c} \Delta t \left\| e^l \right\|^2$$

$$+ \sum_{l=1}^{k-3} \frac{\alpha_{22}\alpha_{24}}{c} \Delta t \left\| e^l \right\|^2 + \sum_{l=0}^{k} \frac{2\,|\Omega|\, m_2^2(h_1^2 + h_2^2 + \Delta t^2)^2}{c} \Delta t$$

$$\leq \left(2\alpha_{23} + \frac{32\alpha_{23}\alpha_{21}^2}{c^2} + \frac{10\alpha_{22}\alpha_{24}}{c} \right) \Delta t \sum_{l=1}^{k} \left\| e^l \right\|^2 + \frac{4\alpha_{26}}{c} \Delta t \sum_{l=1}^{k} \left\| \Delta_h e^l \right\|^2$$

$$+ (k+1) \left(2 + \frac{32\alpha_{21}^2}{c^2} + \frac{2}{c} \right) |\Omega|\, \alpha_{22}^2(h_1^2 + h_2^2 + \Delta t^2)^2 \Delta t$$

$$\leq 2\alpha_{27}\Delta t \sum_{l=1}^{k} \left(\left\| e^l \right\|^2 + \left\| \Delta_h e^l \right\|^2 \right) + 2(k+1)\alpha_{25}\,|\Omega|\, m_2^2(h_1^2 + h_2^2 + \Delta t^2)^2 \Delta t.$$

Using the Gronwall's inequality yields

$$\left\| e^{k+1} \right\|^2 + \left\| \triangle_h e^{k+1} \right\|^2 \leq \frac{\alpha_{25}}{\alpha_{27}} \exp\left(\alpha_{27}(k+1)\Delta t \right) \cdot |\Omega| \left[m_2 \left(h_1^2 + h_2^2 + \triangle t^2 \right) \right]^2,$$

where $k = 0, 1, ..., K - 1$. Using Lemma 3.3 and (5.28), we can get

$$\left\| e^{k+1} \right\|_\infty^2 \leq k_0 \left\| e^{k+1} \right\| \left(\left\| \triangle_h e^{k+1} \right\| + \left\| e^{k+1} \right\| \right) \leq k_0 \sqrt{2 \left\| e^{k+1} \right\|^2 \left(\left\| e^{k+1} \right\|^2 + \left\| \triangle_h e^{k+1} \right\|^2 \right)}$$

$$\leq k_0 \sqrt{\frac{2\alpha_{25}}{\alpha_{23}\alpha_{27}}} \exp \left((\alpha_{23} + \alpha_{27}) (k+1)\Delta t \right) m_2^2 |\Omega| \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2 .$$

Therefore,

$$\left\| e^{k+1} \right\|_\infty \leq C_{22} \left(h_1^2 + h_2^2 + \triangle t^2 \right) .$$

6. A Numerical Example

In this section, we use the two second order numerical schemes to obtain the steady state of the fourth order parabolic equations (2.5a)-(2.5b). The substance isobutane (nC4) is selected for comparing with the results of second order parabolic equation provided in [22]. The critical properties and the normal boiling point of this substance are provided in Table 6.1. The parameters $a(T)$, b and $c(T)$ are calculated by the formulas (2.2) and (2.3). For comparison with the results in [22], all the following numerical results are implemented on the domain $\Omega = [0, L]^2$ with $L = 2 \times 10^{-8}$ meters. The initial condition is set as: the molar density equals the liquid isobutane under a saturated pressure in the region $[0.3L, 0.7L]$, the rest of the domain is filled with a saturated isobutane gas. The periodic boundary condition is imposed.

Table 6.1: Critical properties (Data from Table 3.1 of the book of Firoozabadi [6]), ω and m (our computed results) of the selected substance, isobutane (nC4).

symbol	T_c, K	P_c	ω	m
$n\mathrm{C}_4$	425.18	3.797 MPa	0.1990	0.6709

6.1. Numerical accuracy test

In this subsection, we check the convergence rate in time of the Crank-Nicolson scheme (4.4)-(4.5) and the second order linearized scheme (5.4a)-(5.4b). Here, the exact solution is defined by the molar density at $T_m = 10^{-7}$ obtained from $\Delta t = 10^{-11}$ on a 400×400 meshes on the domain Ω. The l^2 norm of errors at several time points and the convergence rate of these schemes are provided by Table 6.2.

Table 6.2: The temporal convergence of the two schemes at $T_m = 10^{-7}$. (a) The Crank-Nicolson Scheme; (b) The linearized scheme.

Δt	l^2 error	rate of convergence
1.0e-10	2.7107e-5	-
2.0e-10	1.0925e-4	2.0109
4.0e-10	4.3783e-4	2.0027
8.0e-10	0.0018	2.0396
1.0e-9	0.0027	2.0002

(a)

Δt	l^2 error	rate of convergence
1.0e-10	0.0022	-
2.0e-10	0.0047	1.0952
4.0e-10	0.0096	1.0304
8.0e-10	0.0194	1.0150
1.0e-9	0.0244	1.0253

(b)

It is clear that the Crank-Nicolson scheme has exactly second order temporal convergence rate and the linearized scheme has only first order temporal convergence rate. The loss of the
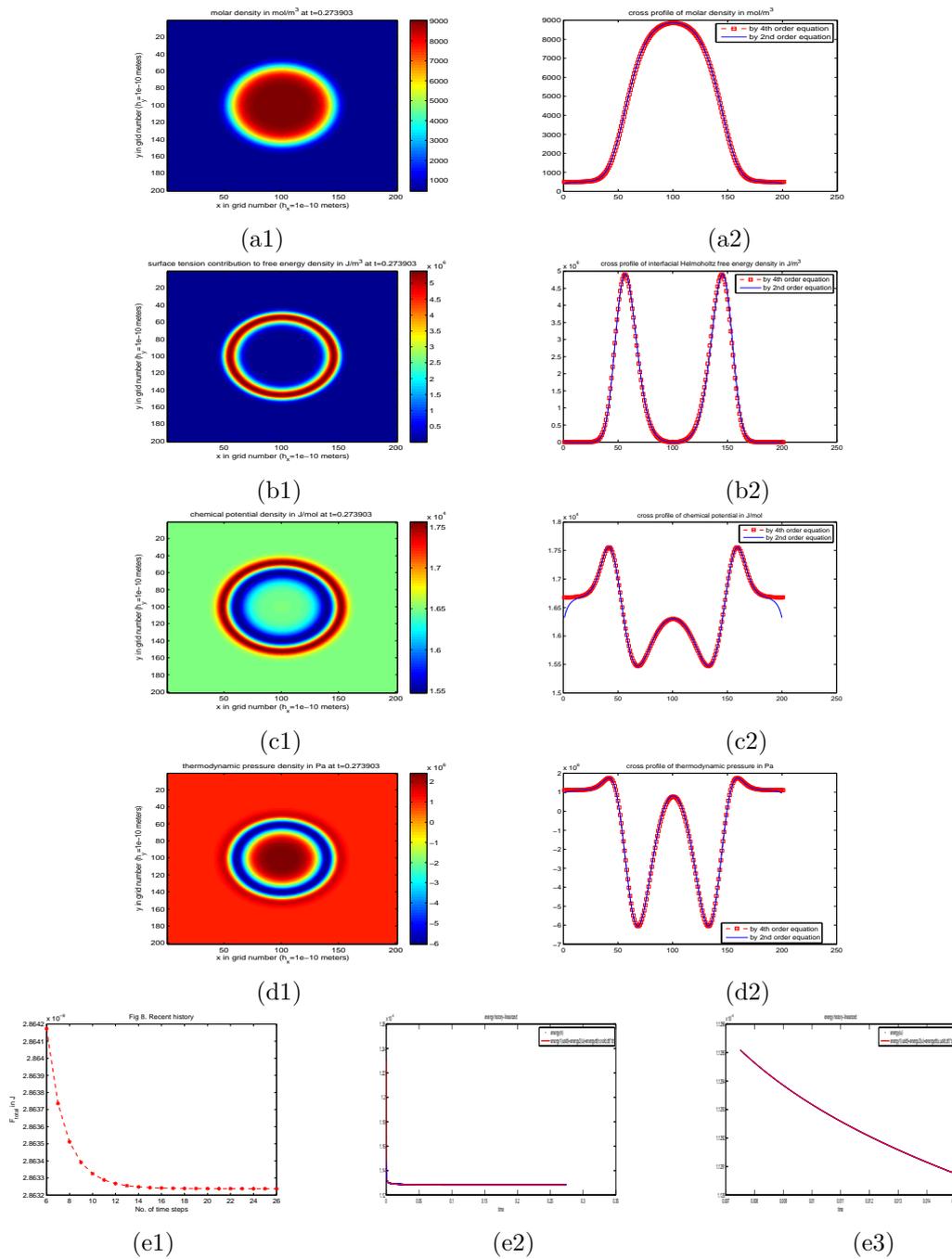
Fig. 6.1. Numerical results given by the fourth order equation at steady state: (a1) molar density, (b1) interfacial Helmholtz free energy density, (c1) chemical potential density, (d1) thermodynamic pressure density, cross profile of molar (a2), interfacial Helmholtz free energy (b2), chemical potential (c2), thermodynamic pressure (d2) density; total energy evolution history given by second order equation (e1), fourth order equation (e2), current energy evolution history given by fourth-order equation.

convergence rate of the linearized scheme may arise from its large truncation error. However, at every time step, the Crank-Nicolson scheme takes several steps of the Newton iteration due

to its nonlinear character, while the linearized scheme does not have this extra cost. So it is worthy of carrying out the long time simulation with the linearized scheme.

6.2. Spatial distribution of molar density and other chemical properties

Here, the homogeneous contribution of chemical potential μ_0 is defined as (2.6b). The surface tension contribution to the Helmholtz free energy density $f_{intfTens}$ is also defied as [22]

$$f_{intfTens} = 2f_{\nabla}(n) = c\nabla n \cdot \nabla n. \tag{6.1}$$

And the thermodynamic pressure p_0 is defined as [22]

$$p_0 = n\left(\frac{\partial f_0}{\partial n}\right) - f_0 = n\mu_0 - f_0$$
$$= \frac{nRT}{1 - bn} - \frac{n^2 a(T)}{1 + 2bn - b^2 n^2} = \frac{RT}{v - b} - \frac{a(T)}{v(v + b) + b(v - b)}. \tag{6.2}$$

Since the evolution history and the steady state obtained from the two schemes are very close, the results offered by either one can illustrate the same phenomenon. Hereafter, we use the solution obtained from the linearized scheme to calculate all the variables of interest. The whole domain Ω is discretized by 200×200 rectangular meshes. Figure 6.1 provides the molar density, interfacial Helmholtz free energy density, homogeneous chemical potential, the thermodynamic pressure and the total energy evolution history calculated from the solution of the four-order equation. The steady state is defined by the condition that the relative error between two neighboring time step is less than 10^{-8}. From Figure 6.1, we can see that the fourth-order parabolic equation can describe dramatically changing of n, $f_{intTens}$, μ_0, p_0 and guarantee the energy decreasing property.

6.3. Calculation of interface tension and verification against Young-Laplace eqn

The surface tension σ is defined as the net contractive force per unit length with a unit of N/m mechanically or the work for creating a unit area of interface with a unit of J/m^2. Here
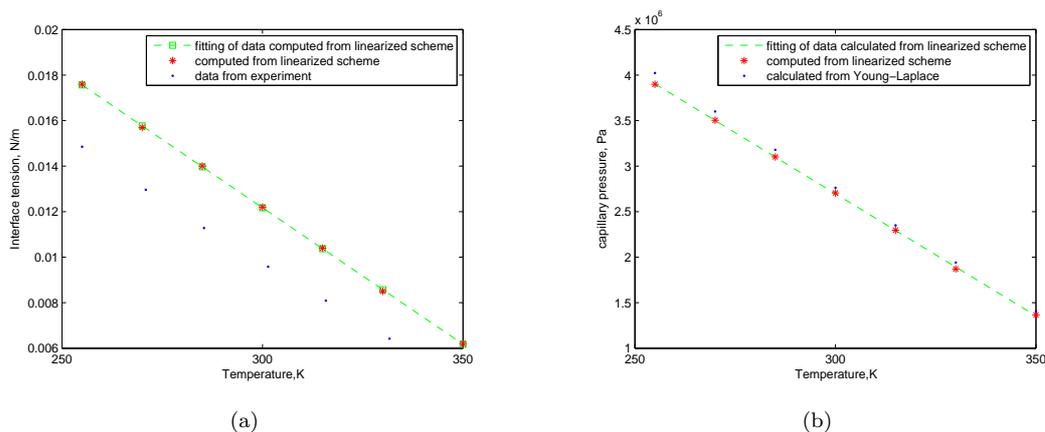

Fig. 6.2. Comparison between numerical predictions given by second order linearized scheme and laboratory data: (a) surface tension (N/m); (b) capillary pressure.

we use the formula [6, 22]

$$\sigma = \frac{\partial F}{\partial A} = \frac{F(n) - F_0(n_{bulk})}{A}. \tag{6.3}$$

with the assumption that σ is spatially constant within the interface for the given system. The numerator term of the equation (6.3) evaluates the contribution of the surface tension to the total free energy at equilibrium state. Here, the volume of the liquid droplet is assumed as a constant all the time and becomes a perfect circle at steady state. The radius of the droplet is also $r = 2 \times 10^{-8} \times (0.16/\pi)^{1/2} = 4.514 \times 10^{-9}$. The length of the circle $A = 2\pi \times 4,514 \times 10^{-9}$ meters. The surface tension ranging from $250K$ to $350K$ are plotted in Figure 6.2 (a) comparing with the laboratory results provided in Table 2 of [16]. We can see that, the difference between the surface tension trend calculated by the steady state of our fourth order equation and the experimental data is small from the engineering point of view.

The pressure is calculated by the well-known Young-Laplace equation as $P_c = P_{liquid} - P_{gas} = \sigma/r$ [6, 22]. The pressure of liquid drop P_{liquid} is picked from the central grid point $(101, 101)$ and the pressure of gas region P_{gas} is calculated at the point $(51, 51)$. The difference between the two is the capillary pressure $p_0 = P_{liquid} - P_{gas}$. On the other hand, the capillary pressure predicted by Young-Laplace equation is $p = \sigma/r$. The capillary pressure P_c from temperature $250K$ to $350K$ obtained from these two methods are plotted in Figure 6.2 (b). These two methods agree with errors around or smaller than 6%.

7. Conclusions

In this paper, we have derived the fourth-order parabolic equation on a two-dimensional rectangular domain Ω and provided two second order energy stable schemes to solve it. Here, we should point out that, our energy stability was obtained on an modified form of the original total discrete energy. There is still a minor gap between our modified energy stability and the direct discretization in terms of the original variable n. To make up this gap is left as one aspect of our future work. The mass conservation, energy decreasing property, and the convergence of these two schemes are provided. To overcome the difficulty in deriving the convergence of these two schemes, which contributes to the possible unboundness of the chemical potential μ_0 and its derivative, μ_0', on the definitional domain $(0, 1/b)$, we impose a reasonable hypothesis that the exact solution to the fourth-order equation and the numerical solution to these two schemes at every step are in a subset of $(0, 1/b)$, which is in the form of $[\theta, 1/b - \theta]$. The numerical results showed in the above section demonstrate the effectiveness of the fourth-order equation and these two schemes.

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