NUMERICAL SOLUTIONS OF A DIFFUSIVE INTERFACE MODEL WITH PENG-ROBINSON EQUATION OF STATE

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Certificate of Originality

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PENG Qiujin

Dedicated to my family.

Abstract

This work is concerned with mathematical modeling and numerical simulations of the steady state and the movements of complex fluids involved in oil exploitation practice. Capillary pressure caused by surface tension at the interface between every two adjacent different phases of the mixture is viewed as the leading force in oil recovery from fractured oil reservoirs. Therefore, the interface between contiguous phases has become a critical mathematical modeling aspect.

The diffuse interface theory, or the phase field model, or the gradient theory, has been widely applied to model or understand the interface between different phases of oil mixture. Based on the assumption that the density of every substance is continuous over the whole fluid region, the total Helmholtz free energy often contains the homogeneous part $F_0(\mathbf{n})$ and the gradient contribution part $F_\nabla(\mathbf{n})$. The derivative of the total homogeneous free energy, $f_0(\mathbf{n})$, or of the gradient part of free energy, $f_\nabla(n)$, varies from substance to substance. Based on the original total free energy, the equilibrium state and the kinetic processes could be determined according to thermodynamic principles.

As for the fluid system related to the oil recovery process, we apply the homogeneous free energy density and the parameters of the gradient part of the free energy density provided by the widely used Peng-Robinson equation of state (EOS).

The fourth-order parabolic equation is derived and solved numerically by a convex-splitting scheme, the Crank-Nicolson scheme and a second order linearization scheme to describe the evolution processes of one-component, two-phase substances. The theoretical analyses of these numerical schemes have been obtained to demonstrate their mass conservation, energy stability, unique solvability and convergence.

The Euler-Lagrange (E-L) equation derived from this expression of total Helmholtz free energy to determine the equilibrium state of the fluid systems has also been studied. In this study, it is solved numerically by the original Newton iteration and a convex-splitting based Newton iterative method. Its theoretical analysis remains a part of our future work.

Numerical experiments have been carried out for both the fourth-order equation approach and the Euler-Lagrange equation approach. Our computational results match well with laboratory experimental data and are in good agreement with the well-known Young-Laplace equation.

Key Words: Diffuse interface theory, Peng-Robinson Equation of State, convex-splitting, energy stable schemes, convergence analysis

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Contents

List of Figures

List of Tables

Chapter 1

Introduction

1.1 Background

Mathematical modeling and numerical simulation of the multi-phase systems in the subsurface oil and gas reservoirs not only play a crucial role in reservoir engineering practice [36, 53, 94, 100], but also are crucial in solving or relieving many environmental problems, such as realizing the idea of injecting and storing the carbon dioxide into the subsurface depleted reservoirs and saline aquifers [1, 70, 79], which is an attractive and practical method to alleviate the greenhouse effect. There exist at least four major mechanisms to trap the injected carbon dioxide into subsurface for long term storage. They are structural stratigraphic trapping, residual fluid trapping, solubility trapping and mineral trapping. To understand these mechanisms deeply and explore new trapping methods, it is necessary to provide accurate modeling and simulation of the flow of these underground materials.

Capillary pressure caused by surface tension between two fluids can be the leading force in oil recovery from fractured oil reservoirs [14, 50]. There is a surface or an interface between any immiscible fluids or partially miscible fluids and between a fluid and a solid [67, 72]. From the molecular level, it could be found that the interior molecules are exposed to balanced forces. However, as for the molecules on the interface, the attractive pull and repulsive push, coming from their surrounding molecules are not balanced since the molecules around them are different. This anisotropic attractive force is the fundamental cause of the interfacial tension.

There are at least three methodologies that have been used to understand and model the interface between phases (see [85] and the references therein). The first approach is based on molecular scale. The molecular dynamics simulation or the molecular Monte Carlo simulation [31, 37, 119] is used with a given intermolecular potential function (e.g. Lennard-Johns potential). The molecular dynamics simulation has been applied to predict CO2-water interfacial tension under certain pressure and temperature conditions of geologic carbon dioxide storage [79]. Although it can describe the interface in detail, the central processing unit (CPU) intensive property limits its application to only a small part of simple substances. The second approach is sharp interface modeling. By using this method, the interface is simulated by a zero-thickness two-dimensional entity, and the molar or mass density undergoes a jump across the interface [51, 89]. This method can be applied to predict the shape and the dynamics of the interface with a given interface tension. Unfortunately, it cannot provide the details within the interface itself and predict the surface tension, which is a major interest in engineering. The third methodology is known as gradient theory [16, 59, 72], or diffuse interface theory [4, 19, 21, 116], or phase field theory [8, 32, 39, 54, 56, 80, 83]. By using this method, the interface is described as a continuous substance separating fluid regions. In this case, mass or molar density is constant in the regions occupied by either single phase, but varies continuously within the interface. This approach is more efficient than the methods from the molecular scale and can also provide the quantity of the surface tension [16, 71, 72]. In addition, methodologies combining different scales have also been applied. For example, diffusive interface model and molecular simulation have been combined to investigate the formation of carbon dioxide [98].

The diffusive interface theory becomes our first choice to model the complex oil fluids considering its advantages on both clear phenomenological descriptions on an appropriate scale and efficient numerical implementations. This theory was originally found by van der Waals [91] to study the interface based on thermodynamic principles [4], and was then extended by Cahn and Hilliard [16, 17, 18, 19, 20, 21]. According to this theory, the total Helmholtz free energy contains two parts, the homogeneous free energy $\mathbf{F}_0$, and the contribution from the gradient of the mass concentration, $\mathbf{F}_\nabla$. So far, the phase field method has been applied to investigate various materials, such as polymorphism, crystal nucleation and growth [7, 84, 101], thin film epitaxy [25, 54, 105], vesicle membranes [32], surfactants on two-phase fluid flow [34, 99], polycrystalline growth [41], Taylor flow in mini/microchannels [39], tumor growth [69], deformation of plasticity [95], electrohydrodynamic multiphase flows [114, 115], etc. The two parts of the total free energy for these substances have distinct forms according to the different features of the studied objects. One of the classical examples of the total free energy is the popular double-well Ginzburg-Landau free energy functional

$$\mathcal{E}(\varphi) = \int_\Omega \left[\frac{1}{4}(\varphi^2 - 1)^2 + \frac{1}{2}|\nabla\varphi|^2\right] d\mathbf{x} \tag{1.1}$$

for the order parameter φ. This typical energy has already been used to qualitatively model segregation, precipitation and phase-transition behaviors of alloys and liquid mixtures in geology, physics, materials science and biology fields, etc [13]. However, this typical double-well energy functional could not be applied to tell the differences of all kinds of oil-gas systems by just setting various quantitative parameters [85]. As for the petroleum fluids studied in reservoir engineering and oil industries, a realistic cubic equation of state (EOS) is required. The homogeneous free energy density and the coefficients of the gradient part given by the well known Peng-Robinson EOS are the preferred choice. The detailed description of the free energy provided by the Peng-Robinson EOS will be presented in next section.

1.2 Formulation of the total Helmholtz free energy provided by the Peng-Robinson EOS

This section introduces the free energy provided by the Peng-Robinson equation of state (EOS) [82]. We consider a fluid system consisting of fixed species amount on a fixed domain with spatially uniform-distributed given temperature. Let M denote the number of components in the studied fluid mixture, n_i represents the molar concentration of the component i, and

$$\mathbf{n} = (n_1, n_2, \cdots, n_M)^T = \frac{(N_1, N_2, \cdots, N_M)^T}{V}$$

be the molar concentrations of all components and $n = n_1 + n_2 + \cdots + n_M$ be the molar density of the fluid. Based on the diffusive interface model, the total Holmholtz free energy is summation of homogeneous Helmholtz free energy density contribution, $F_0(\mathbf{n})$, and the concentration gradient $F_\nabla(\mathbf{n})$ in the following form,

$$\begin{aligned} F(\mathbf{n}) = F(\mathbf{n}; T, \Omega) &= \int_\Omega f(\mathbf{n}; T) d\mathbf{x} \\ &= F_0(\mathbf{n}; T, \Omega) + F_\nabla(\mathbf{n}; T, \Omega) \\ &= \int_\Omega f_0(\mathbf{n}; T) d\mathbf{x} + \int_\Omega f_\nabla(\mathbf{n}; T) d\mathbf{x}. \end{aligned} \tag{1.2}$$

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

$$f_0(\mathbf{n}) = f_0^{\text{ideal}}(\mathbf{n}) + f_0^{\text{excess}}(\mathbf{n}), \tag{1.3}$$

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

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

Here T denotes the temperature of the mixture and R represents the universal gas constant (approximately $8.31432 \mathrm{JK}^{-1}\mathrm{mol}^{-1}$). From this EOS model, for a mixture, the energy parameter $a = a(T)$ and the covolume parameter b are related to parameters of pure fluids by the following mixing rules:

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

where $y_i = n_i/n$ is the mole fraction of component i. The binary interaction coefficient k_{ij} of Peng-Robinson EOS, which is viewed as a constant for fixed species pair, is usually computed from experimental correlation. a_i and b_i are the Peng-Robinson parameters for pure-substance component i, which can be computed from the critical properties of the species:

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

$$b_i = 0.07780 \frac{R T_{c_i}}{P_{c_i}}.$$

Here, the critical pressure P_{c_i} and critical temperature T_{c_i} of a pure substance are intrinsic properties of the species, and they are available for most species encountered in application. The critical properties of selected species are provided in Table 1.1. The parameter m_i contained in the above formula of a_i is experimentally related to the accentric parameter ω_i of the species by the following equations:

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

The accentric parameter ω_i could in turn be obtained from its relationship with critical temperature T_{c_i}, critical pressure P_{c_i} and the normal boiling point T_{b_i} as

Table 1.1: Critical properties (Data from the Table 3.1 on Page 141 of the book by Firoozabadi [36]), ω and m (our computed results) of selected species.

symbol	T_c (K)	P_c	ω	m
C_1	190.58	4.604 MPa	0.0110	0.3916
C_2	305.42	4.880 MPa	0.0990	0.5247
nC_4	425.18	3.797 MPa	0.1990	0.6709
nC_{10}	617.7	2.099 MPa	0.489	1.0643
CO_2	304.14	73.75 bar	0.2390	0.7278
C6	507.40	30.12 bar	0.2960	0.8075
C7+	647.59	22.24 bar	0.7006	1.3451
N2	126.21	33.90 bar	0.0390	0.4344
C3	369.83	42.28 bar	0.1530	0.6043
iC4	407.80	36.04 bar	0.1830	0.6478
iC5	460.40	33.80 bar	0.2270	0.7108
nC5	469.70	33.70 bar	0.2510	0.7447

follows,

$$\begin{aligned}\omega_i &= \frac{3}{7}\left(\frac{\log_{10}\left(\frac{P_{c_i}}{14.695 \text{ PSI}}\right)}{\frac{T_{c_i}}{T_{b_i}} - 1}\right) - 1 \\ &= \frac{3}{7}\left(\frac{\log_{10}\left(\frac{P_{c_i}}{1 \text{ atm}}\right)}{\frac{T_{c_i}}{T_{b_i}} - 1}\right) - 1.\end{aligned}$$

Here, both PSI and atm are measure units of pressure. PSI is the abbreviation of "pounds per square inch", and atm refers to the standard atmosphere, which equals 101325 Pa. The units PSI and atm satisfy the relation 1atm = 14.695PSI.

The inhomogeneous term or the gradient contribution $f_\nabla(\mathbf{n})$ in (1.2) can be computed by the following relation

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

where the influence parameter c_{ij} is a function of temperature and molar concentrations, and can be also related to the parameter of pure substance by a mixing rule of modified geometric mean as follows

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

where the parameter β_{ij} is the binary interaction coefficient for the influence parameter. To maintain the stability of the interface, β_{ij} is required to be included in the interval $[0, 1]$ and $\beta_{ij} = \beta_{ji}$. For most systems, β_{ij} is viewed as zero. When $\beta_{ij} = 0$, this mixing rule is simplified to the geometric mean. The influence parameter of pure substance c_i is related by the parameters a_i and b_i by [16, 71, 72, 85]

$$c_i = a_i b_i^{2/3} \left(m_{1,i}^c \left(1 - \frac{T}{T_{c_i}} \right) + m_{2,i}^c \right), \tag{1.4}$$

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

$$m_{1,i}^c = -\frac{10^{-16}}{1.2326 + 1.3757\omega_i},$$

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

1.3 Literature review of numerical approaches for diffusive interface model

With the assistance of thermodynamical theory, both the equilibrium state and the kinetics of fluid system can be derived from the given free energy functional. Generally, the Euler-Lagrange equation derived from the variation of the free energy functional F with respect to n is applied to determine the equilibrium state of a fluid system. Moreover, the kinetics equation with the form $\partial\varphi/\partial t = N[\varphi]$ is obtained from the following two commonly used approaches [61]. The first equation is proposed based on the hypothesis that the free energy decreases along solution paths leaded by the second law of thermodynamics in the form

$$\frac{\partial \varphi(\mathbf{x},t)}{\partial t} = -K\frac{\delta F[\varphi_t(\cdot)]}{\delta \varphi(\mathbf{x},t)}, \tag{1.5}$$

where $\varphi_t(\cdot)$ denotes the order parameter field at time t, and K is a positive coefficient, which may depend on temperature T and on φ. A mass conserved constraint

$$\frac{d}{dt}\int_\Omega \varphi(\mathbf{x},t)d\mathbf{x} = 0 \tag{1.6}$$

is often imposed on this kind of kinetics equation by introducing a Lagrange multiplier. Another usually used kinetics equation is of the form

$$\frac{\partial \varphi(\mathbf{x},t)}{\partial t} = \nabla \cdot \left(\nabla\frac{\delta F[\varphi_t(\cdot)]}{\delta \varphi(\mathbf{x},t)}\right). \tag{1.7}$$

Although (1.7) can not guarantee that the total free energy decreases along solution path, it satisfies the mass conservation (1.6) automatically. In addition, the fourth order term could be used to describe the surface diffusion [87]. These properties improve its application frequency greatly to simulate the flow process of multiphase systems by combining it with traditional momentum equations [8, 56]. The well-known Allen-Cahn equation and the Cahn-Hilliard equation derived from the Ginzburg-Landau free energy functional (1.1) are typical examples of the above two kinds of equation, respectively.

Due to the high nonlinearity and high order of the kinetics equations derived from the phase field model, it is unpractical to obtain the analytical solutions of these equations, not to mention to solve the equation systems derived from their combinations with moving process. Numerical methods become indispensable tools to approach the solutions for these equations and describe our desirable manifestation. To guarantee the reliability of the proposed numerical schemes, the stability is always the main consideration for constructing numerical schemes to solve equations with time-dependence. Up to now, there are at least two kinds of stable schemes for the phase field models, the traditional L^2 stable schemes and the energy stable schemes.

The classical L^2 stability often refers to the linearization difference schemes. The standard explicit Euler scheme is one of a basic L^2 stable schemes. Analysis has verified that the stability of this scheme can only be guaranteed when the time step is really small [117]. To lessen the limitation for the time step, some unconditional L^2 stable schemes, such as the backward Euler scheme with linearization for the nonlinear term [7], and a linear splitting scheme [28], have been proposed to solve the phase field crystal equation. In addition, similar strategy has been used to simulate an epitaxial growth model [86] and the Allen-Cahn and Cahn-Hilliard equations [104]. These schemes could be proved to be uniquely solvable and convergent with appropriate limitation for the discrete time step. However, the energy stability of these schemes could not be guaranteed, which is an important concern related to physical background.

Energy stability can be guaranteed by two main approaches, the stabilized schemes and the convex-splitting strategy. The stabilized schemes are obtained by adding stabilized terms on both sides of the partial differential equation [22, 68, 93, 113]. In this method, involved stabilization parameters are required to be large enough to ensure energy decreasing property and are dependent on unsettled solutions [87]. Convex splitting schemes are another significant energy stable ones. This method was first presented by Eyre [35], to give an unconditional energy stable scheme to solve the Cahn-Hilliard equation. In this case, the homogeneous part of the free energy density functional was decomposed into convex and concave parts, with the concave part treated explicitly and the convex part treated implicitly. This ingenious idea has been applied to various gradient flow systems and has achieved many successful results [9, 10, 23, 24, 92, 105, 107, 109, 110, 112]. Moreover, there are also other kinds of energy stable schemes for the equations derived from phase field models, such as linearization schemes [23, 45, 86], the Crank-Nicolson scheme [87], and so on [3, 6, 22, 28, 30, 38, 96].

With the unconditional stable property of these schemes, one can introduce adaptive strategies to adjust the time interval. Roughly speaking, one can use small time step when energy varies rapidly, while large time step can be used to save time, if energy evolves mildly. This strategy can resolve not only the steady state solution, but also the dynamical changes of solution accurately and efficiently [88, 117, 118]. Furthermore, one can also solve the elliptic partial differential equations without time-dependence by getting the steady state of these equations with a term of the partial derivative of unsolved variable with respect to time. In this case, all these stable schemes and adaptive strategies used to solve the time-dependent equation can be applied in this process.

Chapter 2

The fourth-order parabolic equation for a single-component two-phase system and its numerical approaches

The cubic Peng-Robinson EOS [82] is widely used to describe properties of the substances related to the underground oil and gas reservoirs. Kou et al. [59] derived Euler-Lagrange equations from this expression of free energy and provided adaptive finite element method for computing surface tension. Qiao et al. [85] converted the original elliptic equilibrium for the pure substance into a parabolic equation by introducing a derivative term of the molar density with respect to time since the final steady state of the time-dependent equation is equivalent to the equilibrium. A Lagrangian multiplier was used to guarantee the mass conservation. This second order parabolic equation was demonstrated to be energy stable and solved by a convex-splitting scheme. Numerical results provided in their work showed great consistence with the experimental results. This validates the reliability of the application of the diffusive interface theory and Peng-Robinson EOS on modeling the fluids related to the oil recovery process.

This work continues these previous achievements by investigating fourth-order parabolic equations to describe the equilibrium state and the flow of the components in the crude oil from the Peng-Robinson EOS due to the inspiration of the preferred properties and the derivation of the Cahn-Hilliard equation. Our work starts from the investigation of single-component, two-phase fluids. For this case, the homogeneous free energy density $f_0(n)$ is approximately a linear function. The nonconvexity of this function could not be visualized until a linear function was subtracted from $f_0(n)$, and the two minimizers of the obtained double-well function are of different orders, as shown in Qiao and Sun's paper [85]. As mentioned in their paper, evaluation of the contribution of this minute nonconvex perturbation to phase separation and capturing the different magnitude minimizers are challenging numerical tasks. Accurate and efficient numerical methods are our indispensable tools to meet this challenge. Here, we apply a convex-splitting scheme, the Crank-Nicolson scheme and a second order linearization scheme to solve the derived fourth-order parabolic equation for these fluids, sequentially. Moreover, their mass conservation, energy decay property and convergence are investigated.

This chapter is organized as follows. In the next section, it presents the derivation of the fourth-order parabolic equation for the multicomponent fluids in the subsurface oil reservoirs, which is also provided by Kou and Sun [58]; and demonstrate energy decrease and mass conservation characteristics of the equation for single-component, two-phase fluids. Notations on the discrete space and some auxiliary lemmata are presented in the second section. After that, a first order convex-splitting scheme, the Crank-Nicolson scheme and a second order linearization scheme and their unique solvability, convergence will be demonstrated successively. Then, it provides the numerical results obtained from using these schemes and compares them with experimental data. The conclusion of this chapter will be provided in the last part.

2.1 Derivation of the fourth-order parabolic equation

The fourth-order parabolic equation is established based on the reference of [58, 75]. We now consider a multicomponent fluid composed of M species with molar density n_i, $i = 1, ..., M$. The derivation of the fourth order equation comes from the following mass balance

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

where $\mathbf{n} = (n_1, n_2, \cdots, n_M)$ is the molar density vector, $n = n_1 + n_2 + \cdots + n_M$ and $\mathbf{h} = (h_1, h_2, \cdots, h_M)$ is the mass flux which relates to the chemical potential μ_1, $\cdots$, μ_M by the following constitutive equations,

$$h_i = -\sum_{j=1}^{M} \nabla \mu_i(\mathbf{n}), \quad i = 1, \cdots, M.$$

The chemical potential of i-th component μ_i in the above equation is the first order variational derivative of the total free energy (1.2) with respect to the molar density of i-th component n_i as follows,

$$\mu_i = \mu_i^0 - \sum_{j=i}^{M} \nabla \cdot c_{ij} \nabla n_j, \quad i = 1, 2, ..., M,$$

where the variable μ_i^0 is the first order derivative of the homogeneous free energy density (1.3) with respect to the i-th component molar density n_i. Therefore,

$$\frac{\partial n_i}{\partial t} = \Delta \mu = \Delta(\mu_i^0 - \sum_{j=i}^{M} \nabla \cdot c_{ij} \nabla n_j).$$

We note that, these equations for multi-component carbonization fluids involve cross-product terms of parameters and molar density for different substances. It is not an easy task to numerically decouple the molar density of one special component from equations for other substances while keeping appropriate consistence with their original continuous counterparts. To reduce the difficulties, our work starts from modeling single component substances. For this case, the total free energy is given by

$$F(n) = \int_{\Omega} \left[\frac{c}{2} |\nabla n|^2 + f_0(n) \right] d\mathbf{x}. \tag{2.1.1}$$

where the homogeneous energy density $f_0(n(\mathbf{x}, t))$ is in the following detailed form,

$$\begin{aligned} f_0(n) &= f_0^{\text{ideal}}(n) + f_0^{\text{excess}}(n) \\ &= f_0^{\text{ideal}}(n) + f_{01}^{\text{excess}}(n) + f_{02}^{\text{excess}}(n), \\ f_0^{\text{ideal}}(n) &= RTn \left(\ln n - 1 \right), \\ f_{01}^{\text{excess}}(n) &= -nRT \ln \left(1 - bn \right), \\ f_{02}^{\text{excess}}(n) &= \frac{a(T)n}{2\sqrt{2}b} \ln \left(\frac{1 + (1 - \sqrt{2})bn}{1 + (1 + \sqrt{2})bn} \right). \end{aligned} \tag{2.1.2}$$

Here $0 < n < \frac{1}{b}$. The homogeneous chemical potential is

$$\begin{aligned} \mu_0(n) =& RT \ln \left(\frac{n}{1 - bn} \right) + \frac{RTbn}{1 - bn} \\ &+ \frac{a(T)}{2\sqrt{2}b} \ln \left(\frac{1 + (1 - \sqrt{2})bn}{1 + (1 + \sqrt{2})bn} \right) - \frac{a(T)n}{1 + 2bn - b^2 n^2}. \end{aligned} \tag{2.1.3}$$

Given periodic boundary condition, the fourth-order parabolic equation for a single-component two-phase system with Peng-Robinson EOS is given as follows

$$\frac{\partial n(\mathbf{x}, t)}{\partial t} = -c\Delta^2 n(\mathbf{x}, t) + \Delta \mu_0(n(\mathbf{x}, t)), \tag{2.1.4a}$$

subjected to the initial condition

$$n(\mathbf{x}, 0) = n_0(\mathbf{x}). \tag{2.1.4b}$$

The evolution of the homogeneous free energy density satisfies

$$\frac{\partial f_0(n(\mathbf{x},t))}{\partial t} = \frac{\partial f_0}{\partial n}\frac{\partial n}{\partial t} = \mu_0(n(\mathbf{x},t))\frac{\partial n(\mathbf{x},t)}{\partial t}. \tag{2.1.5}$$

Lemma 2.1. *(Mass conservation). If $n(\mathbf{x},t)$ is a solution of the fourth order equation (2.1.4a) under periodic boundary condition, then we can get the following mass conservation identity*

$$\frac{d}{dt}\int_\Omega n(\mathbf{x},t)dx = 0. \tag{2.1.6}$$

Proof. Using the equation (2.1.4a), we can get

$$\begin{aligned}\frac{d}{dt}\int_\Omega n(\mathbf{x},t)dx &= \int_\Omega \left[-c\Delta^2 n(\mathbf{x},t) + \Delta\mu_0(n(\mathbf{x},t))\right] dx \\ &= \oint_\Gamma \frac{\partial\left[c\Delta n(\mathbf{x},t) - \mu_0(n(\mathbf{x},t))\right]}{\partial\nu} ds = 0,\end{aligned}$$

where Γ is the boundary Ω, and ν is the unit normal vector on Γ. □

Moreover, taking the inner product of (2.1.4a) with the term $c\Delta n(\mathbf{x},t)-\mu_0(n(\mathbf{x},t))$, we can obtain the following energy identity.

Lemma 2.2. *(Energy identity). If $n(\mathbf{x},t)$ is a solution of the fourth order equation (2.1.4a) under periodic boundary condition, the following energy identity can be guaranteed*

$$\frac{dF(n(\mathbf{x},t))}{dt} = -\left\|-\nabla\left(c\Delta n(\mathbf{x},t) - \mu_0(n(\mathbf{x},t))\right)\right\|^2. \tag{2.1.7}$$

From this natural energy decay property of the fourth order equation (2.1.4a), it is reasonable for us to use it to approach minimums of the total free energy, and steady states of the single-component, two-phase fluid system. In the following sections of this chapter, we will propose three numerical schemes under periodic boundary condition to solve (2.1.4a)-(2.1.4b) and study their stability and convergence properties.

2.2 Notations and some anxiliary lemmas

We investigate the solution of the fourth order equation (2.1.4a)-(2.1.4b) at the time interval $[0, T_m]$ on the domain $\Omega = [0, L_x] \times [0, L_y]$. Here, T_m denotes the final time. Let $h_1 = L_x/M_1$, $h_2 = L_y/M_2$, $\triangle t = T_m/K$, $x_i = ih_1$, $y_j = jh_2$, $t_k = k\triangle t$. Denote the spaces for the discrete grid points on Ω and temporal interval $[0, T_m]$ as follows,

$$\begin{aligned}
\Omega_h =& \left\{(x_i,\ y_j) \mid 0 \le i \le M_1,\ 0 \le j \le M_2\right\}, \\
\Omega_\tau =& \left\{t_k \mid 0 \le k \le K\right\}.
\end{aligned}$$

The space for the discrete periodic functional on Ω_h is denoted by

$$\mathcal{V}_h = \left\{n | n = \left\{n_{ij}\right\},\ n_{i+M_1,j} = n_{ij},\ n_{i,j+M_2} = n_{ij}\right\}.$$

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

$$\begin{aligned}
&\delta_x n_{i+\frac{1}{2},j} = \frac{1}{h_1}\left(n_{i+1,j} - n_{i,j}\right), && \delta_y n_{i,j+\frac{1}{2}} = \frac{1}{h_2}\left(n_{i,j+1} - n_{i,j}\right), \\
&\delta_x^2 n_{ij} = \frac{1}{h_1^2}\left(n_{i+1,j} - 2n_{ij} + n_{i-1,j}\right), && \delta_y^2 n_{ij} = \frac{1}{h_2^2}\left(n_{i,j+1} - 2n_{ij} + n_{i,j-1}\right), \\
&\nabla_h n_{i+\frac{1}{2},j+\frac{1}{2}} = \left(\delta_x n_{i+\frac{1}{2},j}, \delta_y n_{i,j+\frac{1}{2}}\right)^T, && \triangle_h n_{ij} = \left(\delta_x^2 + \delta_y^2\right) n_{ij}.
\end{aligned} \tag{2.2.1}$$

Define the function space on Ω_τ as

$$\mathcal{W}_\tau = \left\{w | w = \left(w^0, w^1, \cdots, w^{K-1}, w^K\right)\right\}.$$

For a grid function $w \in \mathcal{W}_\tau$, define

$$\begin{aligned}
&w^{k+\frac{1}{2}} = \frac{1}{2}\left(w^k + w^{k+1}\right), \quad \delta_t w^{k+\frac{1}{2}} = \frac{1}{\Delta t}\left(w^{k+1} - w^k\right), \quad 0 \le k \le K-1, \\
&\hat{w}^{k+\frac{1}{2}} = 2w^{k-\frac{1}{2}} - w^{k-\frac{3}{2}} = w^k + \frac{1}{2}w^{k-1} - \frac{1}{2}w^{n-2}, \quad 2 \le k \le K-1, \\
&\hat{w}^{\frac{1}{2}} = w^0 + \frac{1}{2}w_t^0 \triangle t, \quad \hat{w}^{\frac{3}{2}} = w^0 + \frac{3}{2}\triangle t w_t^0.
\end{aligned} \tag{2.2.2}$$

For $u, v \in \mathcal{V}_h$, their inner product is defined as

$$\langle u, v\rangle = h_1 h_2 \sum_{i=1}^{M_1}\sum_{j=1}^{M_2} u_{ij} v_{ij}, \tag{2.2.3}$$

and Sobolev norms are defined as

$$\|u\| = \sqrt{\langle u, u\rangle}, \qquad \|u\|_\infty = \max_{0\le i\le M_1, 0\le j\le M_2} |u_{ij}|,$$

$$\|\delta_x u\| = \sqrt{h_1 h_2 \sum_{i=0}^{M_1}\sum_{j=0}^{M_2} \left|\delta_x u_{i-\frac{1}{2},j}\right|^2}, \qquad \|\delta_y u\| = \sqrt{h_1 h_2 \sum_{i=1}^{M_1}\sum_{j=1}^{M_2} \left|\delta_y u_{i,j-\frac{1}{2}}\right|^2},$$

$$\|\nabla_h u\| = \sqrt{h_1 h_2 \sum_{i=0}^{M_1}\sum_{j=0}^{M_2} \left|\nabla_h u_{i+\frac{1}{2},j+\frac{1}{2}}\right|^2}, \qquad \|\triangle_h u\| = \sqrt{h_1 h_2 \sum_{i=1}^{M_1}\sum_{j=1}^{M_2} |\triangle_h u_{ij}|^2}.$$

For demonstrating the solvability and the convergence of our proposed numerical schemes, we will frequently use the following lemmas.

Lemma 2.3. *For any grid function u, $v \in \mathcal{V}_h$, we have*

$$\langle \Delta_h u, v\rangle = \langle u, \Delta_h v\rangle = -\langle \nabla_h u \cdot \nabla_h v, 1\rangle. \tag{2.2.4}$$

Lemma 2.4. *[63, 66, 86] For any grid function $u \in \mathcal{V}_h$, we have*

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

where k_0 is independent of the grid size h and the function u.

Lemma 2.5. *[2, 3, 87, 97] Let $(H, (\cdot,\cdot))$ be a finite dimensional inner product space, $\|\cdot\|$ be 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 2.6. *(Gronwall lemma)[87, 96] Let ξ be positive, and ν, a_k, $(k = 0, 1, 2, 3, ...)$ be nonnegative and satisfy*

$$a_k \leq (1 + \xi\tau)a_{k-1} + \nu\tau, \quad k = 1, 2, 3, ...,$$

then

$$a_k \leq \exp(\xi k\tau)(a_0 + \nu/\xi), \quad k = 1, 2, 3, ...$$

Referencing to the Lemma 4.2 given by [63], we can obtain the following similar results.

Lemma 2.7. *For any $u, v \in \mathcal{W}_\tau$ and $k \geq 1$, we have the following identities*

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

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

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

Proof.

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

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

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

This completes the proof. □

Lemma 2.8. *Suppose the function $\Phi(u)$ has continuous second-order derivative on any connected subset of R. For $u = (u^0, u^1, ..., u^K), \bar{u} = (\bar{u}^0, \bar{u}^1, ..., \bar{u}^K) \in \mathcal{W}_\tau$ and $k \in \{1, 2, ..., K-1\}$, there exist $\rho \in (0,1)$, $\alpha_1 = \rho u^{k+1} + (1-\rho)u^k$, $\alpha_2 = \rho \bar{u}^{k+1} + (1-\rho)\bar{u}^k$, and $\xi \in (\min\{\alpha_1, \alpha_2\}, \max\{\alpha_1, \alpha_2\})$ dependent on k such that*

$$
\begin{aligned}
\delta_t\left[\Phi\left(\bar{u}^{k+\frac{1}{2}}\right) - \Phi\left(u^{k+\frac{1}{2}}\right)\right] =& \Phi'\left(\rho u^{k+1} + (1-\rho)u^k\right)\delta_t\left(\bar{u}^{k+\frac{1}{2}} - u^{k+\frac{1}{2}}\right) \\
&+ \Phi''(\xi)\left(\rho\left(\bar{u}^{k+1} - u^{k+1}\right) + (1-\rho)\left(\bar{u}^k - u^k\right)\right)\delta_t \bar{u}^{k+\frac{1}{2}}.
\end{aligned}
$$

Proof.

$$
\begin{aligned}
&\delta_t\left[\Phi\left(\bar{u}^{k+\frac{1}{2}}\right) - \Phi\left(u^{k+\frac{1}{2}}\right)\right] \\
&\quad = \frac{1}{\Delta t}\left\{\left[\Phi\left(\bar{u}^{k+1}\right) - \Phi\left(\bar{u}^k\right)\right] - \left[\Phi\left(u^{k+1}\right) - \Phi\left(u^k\right)\right]\right\}
\end{aligned}
$$

$$= \frac{1}{\Delta t}\left\{\left[\Phi\left(\bar{u}^k + \Delta t \delta_t \bar{u}^{k+\frac{1}{2}}\right) - \Phi\left(\bar{u}^k\right)\right] - \left[\Phi\left(u^k + \Delta t \delta_t u^{k+\frac{1}{2}}\right) - \Phi\left(u^k\right)\right]\right\}$$

$$= \Phi'\left(\bar{u}^k + \rho\Delta t \delta_t \bar{u}^{k+\frac{1}{2}}\right)\delta_t \bar{u}^{k+\frac{1}{2}} - \Phi'\left(u^k + \rho\Delta t \delta_t u^{k+\frac{1}{2}}\right)\delta_t u^{k+\frac{1}{2}} \tag{2.2.5}$$

$$= \Phi'\left(\rho\bar{u}^{k+1} + (1-\rho)\bar{u}^k\right)\delta_t \bar{u}^{k+\frac{1}{2}} - \Phi'\left(\rho u^{k+1} + (1-\rho)u^k\right)\delta_t u^{k+\frac{1}{2}}$$

$$= \left[\Phi'\left(\rho\bar{u}^{k+1} + (1-\rho)\bar{u}^k\right) - \Phi'\left(\rho u^{k+1} + (1-\rho)u^k\right)\right]\delta_t \bar{u}^{k+\frac{1}{2}}$$

$$+ \Phi'\left(\rho u^{k+1} + (1-\rho)u^k\right)\delta_t\left(\bar{u}^{k+\frac{1}{2}} - u^{k+\frac{1}{2}}\right)$$

$$= \Phi''(\xi)\left(\rho\left(\bar{u}^{k+1} - u^{k+1}\right) + (1-\rho)\left(\bar{u}^k - u^k\right)\right)\delta_t \bar{u}^{k+\frac{1}{2}}$$

$$+ \Phi'\left(\rho u^{k+1} + (1-\rho)u^k\right)\delta_t\left(\bar{u}^{k+\frac{1}{2}} - u^{k+\frac{1}{2}}\right). \tag{2.2.6}$$

This completes the proof. □

In the derivation (2.2.5), we treat $\Phi\left(\bar{u}^k + \Delta t\rho\delta_t \bar{u}^{k+\frac{1}{2}}\right) - \Phi\left(u^k + \Delta t\rho\delta_t u^{k+\frac{1}{2}}\right)$ as a function of $\rho \in [0,1]$ and then use the differential mid-value theorem.

2.3 A convex-splitting scheme for the fourth-order parabolic equation

In this section, we will provide a first order convex-splitting scheme for the fourth-order parabolic equation of pure substance (2.1.4a) and investigate its unconditional stability, unique solvability and L^∞ cconvergence.

2.3.1 The first-order convex-splitting scheme

For the gradient part of the total free energy $F_\nabla = \int_\Omega \frac{c}{2}|\nabla n(\mathbf{x},t)|^2 d\mathbf{x}$, we have

$$\mu_\nabla = \frac{\delta F_\nabla}{\delta n} = -c\Delta n(\mathbf{x},t). \tag{2.3.1}$$

For the homogeneous part of the total free energy, selecting

$$f_{01}(n) = f_0^{\text{ideal}}(n) + f_{01}^{\text{excess}}(n) = RTn\left(\ln n - 1\right) - nRT\ln\left(1 - bn\right),$$

$$f_{02}(n) = -f_{02}^{\text{excess}}(n) = -\frac{a(T)n}{2\sqrt{2}b} \ln\left(\frac{1+(1-\sqrt{2})bn}{1+(1+\sqrt{2})bn}\right),$$

then we have $f_0 = f_{01} - f_{02}$, and

$$\mu_{01}(n) = \mu_0^{\text{ideal}}(n) + \mu_{01}^{\text{excess}}(n) = RT\ln n - RT\ln(1-bn) + RT\frac{bn}{1-bn},$$

$$\mu_{02}(n) = -\mu_{02}^{\text{excess}}(n) = -\frac{a(T)}{2\sqrt{2}b} \ln\left(\frac{1+(1-\sqrt{2})bn}{1+(1+\sqrt{2})bn}\right) + \frac{a(T)n}{1+bn+bn(1-bn)}.$$

Therefore,

$$\begin{aligned}
\frac{\partial^2 f_{01}(n)}{\partial n^2} &= \frac{\partial \mu_{01}(n)}{\partial n} = \frac{RT}{n} + \frac{bRT(2-bn)}{(1-bn)^2} \\
&= \frac{RT\,(1-bn)^2}{n\,(1-bn)^2} + \frac{bRTn(2-bn)}{n\,(1-bn)^2} \\
&= RT\frac{(1-bn)^2 + bn(2-bn)}{n\,(1-bn)^2} = \frac{RT}{n\,(1-bn)^2} > 0, \qquad (2.3.2)
\end{aligned}$$

$$\frac{\partial^2 f_{02}(n)}{\partial n^2} = \frac{\partial \mu_{02}(n)}{\partial n} = \frac{2a(T)\,(1+bn)}{(1+2bn-b^2n^2)^2} > 0. \qquad (2.3.3)$$

So $f_0(n)$ can be convexly split with $f_0(n) = f_{01}(n) - f_{02}(n)$. The convex splitting of total energy described in (2.1.1) is $F = F_c - F_e$, where

$$\begin{aligned}
F_c &= \int_\Omega \left[\frac{c}{2}|\nabla n(\mathbf{x},t)|^2 + f_{01}\right] d\mathbf{x} \\
&= \int_\Omega \left[\frac{c}{2}|\nabla n(\mathbf{x},t)|^2 + RTn\,(\ln n - 1) - nRT\ln(1-bn)\right] d\mathbf{x}, \qquad (2.3.4)
\end{aligned}$$

$$F_e = \int_\Omega f_{02} dx = -\int_\Omega \frac{a(T)n}{2\sqrt{2}b} \ln\left(\frac{1+(1-\sqrt{2})bn}{1+(1+\sqrt{2})bn}\right) d\mathbf{x}. \qquad (2.3.5)$$

Denote $\mu(n) = \dfrac{\delta F}{\delta n}(n) = \mu_c - \mu_e$, then $\mu(n) = \mu_\nabla + \mu_0$, and

$$\mu_c = \frac{\delta F_c}{\delta n}(n) = \mu_\nabla + \mu_{01} = -c\Delta n(\mathbf{x},t) + RT\ln n - RT\ln(1-bn) + RT\frac{bn}{1-bn},$$

$$\mu_e = \frac{\delta F_e}{\delta n}(n) = \mu_{02} = -\frac{a(T)}{2\sqrt{2}b} \ln\left(\frac{1+(1-\sqrt{2})bn}{1+(1+\sqrt{2})bn}\right) + \frac{a(T)n}{1+bn+bn(1-bn)}. \quad (2.3.6)$$

Define the total discrete energy F_h to be

$$F_h(n) = \frac{c}{2}\left\|\nabla_h n\right\|^2 + \langle f_{01}(n), 1\rangle - \langle f_{02}(n), 1\rangle. \quad (2.3.7)$$

Lemma 2.9. *(Existence of a convex-splitting of the discrete total free energy.) Suppose both n and $\Delta_h n$ are periodic. Define the energies*

$$F_h^c(n) = \frac{c}{2}\left\|\nabla_h n\right\|^2 + \langle f_{01}(n), 1\rangle, \quad F_h^e(n) = \langle f_{02}(n), 1\rangle. \quad (2.3.8)$$

Then the gradients of the respective energies are $\frac{\delta F_h^c}{\delta n} = -c\Delta_h n + \mu_{01}(n)$ *and* $\frac{\delta F_h^e}{\delta n} = \mu_{02}(n)$*, and F_h^c and F_h^e are convex, admitting the convex splitting $F_h = F_h^c - F_h^e$.*

Proof. Calculating the (discrete) variation of F_h^c and using summation-by-parts give

$$\frac{dF_h^c}{d\varepsilon}(n+\varepsilon\tilde{n})|_{\varepsilon=0} = \langle -c\Delta_h n, \tilde{n}\rangle + \langle \mu_{01}(n), \tilde{n}\rangle.$$

A calculation of the second variation reveals

$$\frac{d^2F_h^c}{d\varepsilon^2}(n+\varepsilon\tilde{n})|_{\varepsilon=0} = c\left\|\nabla_h \tilde{n}\right\|^2 + \langle \mu_{01}'(n), \tilde{n}^2\rangle \geq 0.$$

For F_h^e, we have

$$\frac{dF_h^e}{d\varepsilon}(n+\varepsilon\tilde{n})|_{\varepsilon=0} = \langle \mu_{02}(n), \tilde{n}\rangle,$$

$$\frac{d^2F_h^e}{d\varepsilon^2}(n+\varepsilon\tilde{n})|_{\varepsilon=0} = \langle \mu_{02}'(n), \tilde{n}^2\rangle \geq 0.$$

These verify the convexity of the discrete functionals F_h^c and F_h^e. Since it is obvious that $F_h = F_h^c - F_h^e$, the proof is completed. $\square$

We now describe the fully discrete scheme in detail. Define the discrete chemical potential $\tilde{\mu}$ to be

$$\begin{aligned}\tilde{\mu}(n^{k+1}, n^k) &= \frac{\delta F_h^c}{\delta n}(n^{k+1}) - \frac{\delta F_h^e}{\delta n}(n^k) \\ &= -c\Delta_h n^{k+1} + \mu_{01}\left(n^{k+1}\right) - \mu_{02}\left(n^k\right). \end{aligned} \tag{2.3.9}$$

The total discrete scheme for the original fourth order equation is the following: given n_{ij}^k, find periodic n_{ij}^{k+1} such that

$$\frac{n_{ij}^{k+1} - n_{ij}^k}{\Delta t} = \Delta_h \tilde{\mu} = -c\Delta_h^2 n_{ij}^{k+1} + \Delta_h \mu_{01}\left(n_{ij}^{k+1}\right) - \Delta_h \mu_{02}\left(n_{ij}^k\right). \tag{2.3.10}$$

2.3.2 Mass conservation and unconditional energy stability

Lemma 2.10. *The solution of the discrete equation (2.3.10) satisfies the mass conservation, which means, for any* $0 \le k \le K-1$,

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

Proof. Denote $\tilde{\mu}_{ij}^{k+\frac{1}{2}} = \tilde{\mu}\left(n_{ij}^{k+1}, n_{ij}^k\right)$. Multiplying $h_1 h_2 \Delta t$ to both sides of (2.4.4a) and summing for $i = 1, ..., M_1,\ j = 1, ..., M_2$, with the periodic boundary condition, we obtain

$$\begin{aligned}&h_1 h_2 \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} \left(n_{ij}^{k+1} - n_{ij}^k\right) \\ &= -h_1 h_2 \triangle t \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} \Delta_h \tilde{\mu}\left(n_{ij}^{k+1}, n_{ij}^k\right) \\ &= -h_1 h_2 \triangle t \sum_{j=1}^{M_2} \frac{1}{h_1^2} \sum_{i=1}^{M_1} \left[\left(\tilde{\mu}_{i+1,j}^{k+\frac{1}{2}} - \tilde{\mu}_{ij}^{k+\frac{1}{2}}\right) - \left(\tilde{\mu}_{ij}^{k+\frac{1}{2}} - \tilde{\mu}_{i-1,j}^{k+\frac{1}{2}}\right)\right] \\ &\quad - h_1 h_2 \triangle t \sum_{i=1}^{M_1} \frac{1}{h_2^2} \sum_{j=1}^{M_2} \left[\left(\tilde{\mu}_{i,j+1}^{k+\frac{1}{2}} - \tilde{\mu}_{ij}^{k+\frac{1}{2}}\right) - \left(\tilde{\mu}_{ij}^{k+\frac{1}{2}} - \tilde{\mu}_{i,j-1}^{k+\frac{1}{2}}\right)\right]\end{aligned}$$

$$= 0.$$

This completes the proof. □

Theorem 2.1. *(Energy stability.) The scheme (2.3.10) for the fourth order equation (2.1.4a) is unconditional energy stable, which means that*

$$F_h(n^{k+1}) \leq F_h(n^k) \tag{2.3.11}$$

is satisfied for any time step $\Delta t > 0$.

Proof. From the convexity of of the discrete energy $F_h^c(n)$ and $F_h^e(n)$, we can obtain

$$\begin{aligned}
F_h^c(n^{k+1}) - F_h^c(n^k) &\leq \left\langle \delta_n F_h^c(n^{k+1}), n^{k+1} - n^k \right\rangle, \\
F_h^e(n^k) - F_h^e(n^{k+1}) &\leq \left\langle \delta_n F_h^e(n^k), n^k - n^{k+1} \right\rangle.
\end{aligned}$$

Therefore,

$$\begin{aligned}
F_h(n^{k+1}) - F_h(n^k) = &\left(F_h^c(n^{k+1}) - F_h^e(n^{k+1})\right) - \left(F_h^c(n^k - F_h^e(n^k)\right) \\
= &F_h^c(n^{k+1}) - F_h^c(n^k) + F_h^e(n^k) - F_h^e(n^{k+1}) \\
\leq &\left\langle \delta_n F_h^c(n^{k+1}), n^{k+1} - n^k \right\rangle + \left\langle \delta_n F_h^e(n^k), n^k - n^{k+1} \right\rangle \\
\leq &\left\langle \delta_n F_h^c(n^{k+1}) - \delta_n F_h^e(n^k), n^{k+1} - n^k \right\rangle \\
= &\left\langle \tilde{\mu}(n^{k+1}, n^k), \Delta t \Delta_h \tilde{\mu}(n^{k+1}, n^k) \right\rangle \\
= &- \Delta t \left\| \nabla_h \tilde{\mu}(n^{k+1}, n^k) \right\|^2 \\
\leq &0.
\end{aligned}$$

This completes the proof. □

2.3.3 Unconditional unique solvability

Define $\mathcal{M}_0$ to be all the functions in $\mathcal{V}_h$ with zero average as follows,

$$\mathcal{M}_0 = \left\{ n \in \mathcal{V}_h \mid \frac{1}{M_1 M_2} \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} n_{i,j} = 0 \right\}.$$

The symmetry and positive definite property of the discrete operator under the periodic condition yields the following lemma.

Lemma 2.11. *[110] For any $n_0 \in \mathcal{M}_0$, there exists a unique periodic solution $\check{n}_0 \in \mathcal{M}_0$ such that $-\Delta_h \check{n}_0 = n_0$.*

Note that, the requirement of $\check{n}_0,\ n_0 \in \mathcal{M}_0$ attributes to the zero average of the functions in $\mathcal{V}_h$ manipulated by Δ_h. From this lemma, we define the inverse of operator L_0, L_0^{-1}, as $\check{n}_0 = L_0^{-1} n_0$. Naturally, L_0^{-1} is also symmetrical and positive definite.

Theorem 2.2. *(Unique solvability). The difference scheme (2.3.9)-(2.3.10) is uniquely solvable for any time step $\Delta t > 0$.*

Proof. Define $L = \Delta t L_0 = -\Delta t \Delta_h$. It is obvious that, both the operator L and its inverse L^{-1} are symmetrical and positive definite. For $n \in \mathcal{V}_h$, denote

$$\tilde{n}_{ij} = n_{ij} - \frac{1}{M_1 M_2} \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} n_{ij},$$

then we have $\tilde{n} \in \mathcal{M}_0$. As for $k = 0, 1, ..., K-1$, define a functional on $\mathcal{V}_h$ as follows,

$$G(n) = \frac{1}{2} \langle L^{-1}(\tilde{n}), \tilde{n} \rangle - \langle L^{-1}(\tilde{n}), \tilde{n}^k \rangle + F_h^c(n) - \langle n, \delta_n F_h^e(n^k) \rangle, \qquad (2.3.12)$$

For any $n_0 \in \mathcal{M}_0$,

$$\begin{aligned} G(n + \lambda n_0) =& \frac{1}{2} \langle L^{-1}(\tilde{n} + \lambda n_0), \tilde{n} + \lambda n_0 \rangle - \langle L^{-1}(\tilde{n} + \lambda n_0), \tilde{n}^k \rangle \\ &+ F_h^c(n + \lambda n_0) - \langle n + \lambda n_0, \delta_n F_h^e(n^k) \rangle. \end{aligned}$$

So we have

$$\frac{dG(n + \lambda n_0)}{d\lambda} |_{\lambda=0}$$

$$= \langle L^{-1}(\tilde{n} + \lambda n_0 - \tilde{n}^k), n_0\rangle + \langle \delta_n F_h^c(n + \lambda n_0), n_0\rangle - \langle \delta_n F_h^e(n^k), n_0\rangle \mid_{\lambda=0}$$

$$= \langle L^{-1}(\tilde{n} - \tilde{n}^k), n_0\rangle + \langle \delta_n F_h^c(n), n_0\rangle - \langle \delta_n F_h^e(n^k), n_0\rangle,$$

it follows that

$$\delta_n G(n) = L^{-1}(\tilde{n} - \tilde{n}^k) + \delta_n F_h^c(n) - \delta_n F_h^e(n^k),$$

and

$$\frac{d^2 G(n + \lambda n_0)}{d\lambda^2} \mid_{\lambda=0} = \langle L^{-1}(n_0), n_0\rangle + \langle \delta_n^2 F_h^c(n), n_0^2\rangle.$$

The convexity of F_h^c and the positive definiteness of L^{-1} guarantee the convexity of $G(n)$ on $\mathcal{V}_h$. Supposing n^{k+1} solves (2.3.9)-(2.3.10), we can obtain

$$n^{k+1} - n^k + L\left(\frac{\delta F_h^e}{\delta n}(n^{k+1}) - \frac{\delta F_h^e}{\delta n}(n^k)\right) = 0. \tag{2.3.13}$$

The mass conservation of the solution of discrete equations (2.3.9)-(2.3.10) yields

$$\begin{aligned}\delta_n G(n^{k+1}) =& L^{-1}(\tilde{n}^{k+1} - \tilde{n}^k) + \left(\frac{\delta F_h^e}{\delta n}(n^{k+1}) - \frac{\delta F_h^e}{\delta n}(n^k)\right)\\ =& L^{-1}(n^{k+1} - n^k) + \left(\frac{\delta F_h^e}{\delta n}(n^{k+1}) - \frac{\delta F_h^e}{\delta n}(n^k)\right)\\ =& 0.\end{aligned}$$

Therefore, n^{k+1} solves (2.3.9)-(2.3.10) if and only if $\delta_n G(n^{k+1}) = 0$. The convexity of the functional $G(n)$ implies that it is uniquely minimized by n^{k+1}. $\square$

2.3.4 Convergence

Denote

$$\alpha_{11} = \max\left\{|\mu_{01}'(n)| : \ n \in \left[\epsilon_1, \frac{1}{b} - \epsilon_1\right]\right\}, \quad \alpha_{12} = \max\left\{|\mu_{01}''(n)| : \ n \in \left[\epsilon_1, \frac{1}{b} - \epsilon_1\right]\right\},$$

$$\alpha_{21} = \max\left\{|\mu_{02}'(n)| : \ n \in \left[\epsilon_1, \frac{1}{b} - \epsilon_1\right]\right\} \le a(T), \quad \alpha_{13} = \frac{c + \alpha_{11}^2 + a(T)^2}{c},$$

$$\alpha_{22} = \max\left\{|\mu''_{02}(n)| : \ n \in \left[\epsilon_1, \frac{1}{b} - \epsilon_1\right]\right\}, \quad \alpha_{15} = \frac{\alpha_{11}^2 + \alpha_{21}^2}{c^2},$$

$$\alpha_{14} = \max\left\{\left|\frac{\bar{n}^{k+1} - \bar{n}^k}{\Delta t}\right| : \ n \in \left[\epsilon_1, \frac{1}{b} - \epsilon_1\right]\right\}, \quad \alpha_{17} = \frac{\alpha_{12}\alpha_{14} + \alpha_{22}\alpha_{14}}{c},$$

$$\alpha_{16} = \frac{\alpha_{11}^2 + \alpha_{21}^2 + \alpha_{12}\alpha_{14} + \alpha_{22}\alpha_{14}}{c}, \quad \alpha_{18} = 16\alpha_{15} + \frac{2}{c} + 4,$$

$$\alpha_{19} = \max\left\{4\alpha_{13}\left(4\alpha_{15} + 1\right) + 4\alpha_{17}, 4\alpha_{16}\right\}, \quad C_{11} = \sqrt{\frac{|\Omega|}{\alpha_{13}}} m_1 \exp\left(\alpha_{13} T_m\right),$$

$$C_{12} = \sqrt[4]{\frac{2\alpha_{18}}{\alpha_{13}\alpha_{19}} k_0^2 \left|\Omega\right|^2} \exp\left(\left(\frac{\alpha_{13}}{2} + \frac{\alpha_{19}}{4}\right)(k+1)\Delta t\right) m_1.$$

Theorem 2.3. *(Error estimate.) Suppose the unique, smooth, periodic solution for the original fourth order equation (2.1.4a) is given by $\bar{n}(x, y, t)$ on Ω for $0 < t \le T_m$ for some $T_m < \infty$ with initial data $\bar{n}(x, y, 0)$. As for $k = 0, 1, ..., K-1$, define*

$$\bar{n}_{i,j}^k := \bar{n}(x_i, y_j, k\Delta t), \tag{2.3.14}$$

and $e_{i,j}^k = \bar{n}_{i,j}^k - n_{i,j}^k$, where $n_{i,j}^k$ is the k-th periodic solution of (2.3.9)-(2.3.10) with $n_{i,j}^0 = \bar{n}_{i,j}^0$. Then if $\Delta t < \dfrac{c}{2(\alpha_{11}^2 + c)}$, we have

$$\left\|e^K\right\| \le C_{11}(h_1^2 + h_2^2 + \Delta t).$$

If $\Delta t < \min\left\{\dfrac{c}{2(\alpha_{11}^2 + c)}, \dfrac{c}{2\alpha_{12}\alpha_{14}}\right\}$, the L^∞ error estimation could be given as

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

Proof. The continuous function $\bar{n}$ solves the discrete equations

$$\frac{\bar{n}_{ij}^{k+1} - \bar{n}_{ij}^k}{\Delta t} = \Delta_h \tilde{\mu}(\bar{n}_{ij}^{k+1}, \bar{n}_{ij}^k) + R_{ij}^{k+1}, \tag{2.3.15}$$

where R_{ij}^{k+1} is the local truncation error, which satisfies

$$|R_{ij}^{k+1}| \le m_1(h_1^2 + h_2^2 + \Delta t), \tag{2.3.16}$$

for all i, j, and k for some $m_1 \geq 0$ that depends only on T_m, L_x, L_y.

Subtracting (2.3.10) from (2.3.15), we have

$$\frac{e_{ij}^{k+1} - e_{ij}^{k}}{\Delta t} = \triangle_h \tilde{\mu}\left(\bar{n}_{ij}^{k+1}, \bar{n}_{ij}^{k}\right) - \triangle_h \tilde{\mu}\left(n_{ij}^{k+1}, n_{ij}^{k}\right) + R_{ij}^{k+1},$$

$$1 \leq i \leq M_1, \quad 1 \leq j \leq M_2, \quad 0 \leq k \leq K-1. \tag{2.3.17}$$

$$e_{ij}^{0} = 0, \qquad 1 \leq i \leq M_1, \quad 1 \leq j \leq M_2. \tag{2.3.18}$$

Taking inner product of (2.4.10) with $2\Delta t e^{k+1}$ yields

$$\begin{aligned} &\left\|e^{k+1}\right\|^2 - \left\|e^{k}\right\|^2 + \left\|e^{k+1} - e^{k}\right\|^2 \\ &= 2\Delta t \left\langle \Delta_h \tilde{\mu}\left(\bar{n}^{k+1}, \bar{n}^{k}\right) - \Delta_h \tilde{\mu}\left(n^{k+1}, n^{k}\right), e^{k+1}\right\rangle + 2\Delta t \left\langle R^{k+1}, e^{k+1}\right\rangle. \end{aligned} \tag{2.3.19}$$

According to Lemma 2.3, we have

$$\begin{aligned} &2\Delta t \left\langle \triangle_h \tilde{\mu}\left(\bar{n}^{k+1}, \bar{n}^{k}\right) - \triangle_h \tilde{\mu}\left(n^{k+1}, n^{k}\right), e^{k+1}\right\rangle \\ &= -2\Delta t \Big\langle - c\Delta_h^2 e^{k+1} + \triangle_h \mu_{01}\left(\bar{n}^{k+1}\right) - \triangle_h \mu_{01}\left(n^{k+1}\right) \\ &\quad - \left[\triangle_h \mu_{02}\left(\bar{n}^{k}\right) - \triangle_h \mu_{02}\left(n^{k}\right)\right], e^{k+1} \Big\rangle \\ &= -2c\Delta t \left\|\Delta_h e^{k+1}\right\|^2 + 2\Delta t \left\langle \mu_{01}\left(\bar{n}^{k+1}\right) - \mu_{01}\left(n^{k+1}\right), \triangle_h e^{k+1}\right\rangle \\ &\quad - 2\Delta t \left\langle \mu_{02}\left(\bar{n}^{k}\right) - \mu_{02}\left(n^{k}\right), \triangle_h e^{k+1}\right\rangle \\ &= -2c\Delta t \left\|\Delta_h e^{k+1}\right\|^2 + 2\Delta t \left\langle \mu_{01}'(\xi_1^{k+1}) e^{k+1}, \Delta_h e^{k+1}\right\rangle - 2\Delta t \left\langle \mu_{02}'(\xi_2^{k}) e^{k}, \Delta_h e^{k+1}\right\rangle \\ &\leq -2c\Delta t \left\|\Delta_h e^{k+1}\right\|^2 + 2\alpha_{11}\Delta t \left\|e^{k+1}\right\| \left\|\Delta_h e^{k+1}\right\| + 2\alpha_{21}\Delta t \left\|e^{k}\right\| \left\|\Delta_h e^{k+1}\right\| \\ &\leq -2c\Delta t \left\|\Delta_h e^{k+1}\right\|^2 + \frac{\alpha_{11}^2 \Delta t}{c} \left\|e^{k+1}\right\|^2 + c\Delta t \left\|\triangle_h e^{k+1}\right\|^2 \\ &\quad + \frac{\alpha_{21}^2 \Delta t}{c} \left\|e^{k}\right\|^2 + c\Delta t \left\|\triangle_h e^{k+1}\right\|^2 \\ &\leq \frac{\alpha_{11}^2 \Delta t}{c} \left\|e^{k+1}\right\|^2 + \frac{a(T)^2 \Delta t}{c} \left\|e^{k}\right\|^2, \end{aligned}$$

and

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

Combining all the above results and ignoring the nonnegative term $\left\| e^{k+1} - e^k \right\|^2$ in (2.3.19), we obtain

$$\begin{aligned} \left\| e^{k+1} \right\|^2 - \left\| e^k \right\|^2 \leq & \left(\frac{\alpha_{11}^2}{c} + 1 \right) \Delta t \left\| e^{k+1} \right\|^2 + \frac{a(T)^2 \Delta t}{c} \left\| e^k \right\|^2 \\ & + m_1^2|\Omega|\Delta t(h_1^2 + h_2^2 + \Delta t)^2. \end{aligned} \tag{2.3.20}$$

Therefore,

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

$$\begin{aligned} \left\| e^{k+1} \right\|^2 \leq & \frac{1 + \frac{a(T)^2 \Delta t}{c}}{1 - \frac{\alpha_{11}^2 \Delta t}{c} - \Delta t} \left\| e^k \right\|^2 + \frac{m_1^2|\Omega|\Delta t(h_1^2 + h_2^2 + \Delta t)^2}{1 - \frac{\alpha_{11}^2 \Delta t}{c} - \Delta t} \\ = & \left(1 + \frac{\frac{c + \alpha_{11}^2 + a(T)^2}{c}}{1 - \frac{\alpha_{11}^2 + c}{c} \Delta t} \Delta t \right) \left\| e^k \right\|^2 + \frac{m_1^2|\Omega|\Delta t(h_1^2 + h_2^2 + \Delta t)^2}{1 - \frac{\alpha_{11}^2 + c}{c} \Delta t}. \end{aligned}$$

If $\frac{\alpha_{11}^2 + c}{c} \Delta t < \frac{1}{2}$, then

$$\begin{aligned} \left\| e^{k+1} \right\|^2 \leq & \left(1 + 2\frac{c + \alpha_{11}^2 + a(T)^2}{c} \Delta t \right) \left\| e^k \right\|^2 + 2m_1^2|\Omega|\Delta t(h_1^2 + h_2^2 + \Delta t)^2 \\ = & (1 + 2\alpha_{13}\Delta t) \left\| e^k \right\|^2 + 2m_1^2|\Omega|\Delta t(h_1^2 + h_2^2 + \Delta t)^2. \end{aligned}$$

According to Gronwall inequality given by Lemma 2.6, we can get

$$\begin{aligned} \left\| e^{k+1} \right\|^2 \leq & \frac{2m_1^2|\Omega|}{2\alpha_{13}} \exp\left(2\alpha_{13}(k+1)\Delta t\right) \left(h_1^2 + h_2^2 + \Delta t \right)^2 \\ \leq & \frac{m_1^2|\Omega|}{\alpha_{13}} \exp\left(2\alpha_{13} T_m\right) \left(h_1^2 + h_2^2 + \Delta t \right)^2, \end{aligned} \tag{2.3.21}$$

$$\left\| e^{k+1} \right\| \leq \sqrt{\frac{|\Omega|}{\alpha_{13}}} m_1 \exp\left(\alpha_{13} T_m\right) \left(h_1^2 + h_2^2 + \Delta t \right) = C_{11} \left(h_1^2 + h_2^2 + \Delta t \right).$$

Replacing k in the inequality (2.3.20) by l and summing l from 0 to k, we obtain

$$\begin{aligned}
\left\|e^{k+1}\right\|^2 =& \sum_{l=0}^{k}\left(\left\|e^{l+1}\right\|^2-\left\|e^{l}\right\|^2\right)\\
&\leq \left(\frac{\alpha_{11}^2}{c}+1\right)\Delta t\sum_{l=0}^{k}\left\|e^{l+1}\right\|^2+\frac{a(T)^2\Delta t}{c}\sum_{l=0}^{k}\left\|e^{l}\right\|^2\\
&\quad + m_1^2|\Omega|(h_1^2+h_2^2+\Delta t)^2(k+1)\Delta t\\
&\leq \left(\frac{\alpha_{11}^2}{c}+1\right)\Delta t\left\|e^{k+1}\right\|^2+\left(\frac{\alpha_{11}^2}{c}+1+\frac{a(T)^2}{c}\right)\Delta t\sum_{l=0}^{k}\left\|e^{l}\right\|^2\\
&\quad + m_1^2|\Omega|(h_1^2+h_2^2+\Delta t)^2(k+1)\Delta t.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\left[1-\left(\frac{\alpha_{11}^2}{c}+1\right)\Delta t\right]\left\|e^{k+1}\right\|^2 \leq& \left(\frac{\alpha_{11}^2}{c}+1+\frac{a(T)^2}{c}\right)\Delta t\sum_{l=0}^{k}\left\|e^{l}\right\|^2\\
&+4m_1^2|\Omega|(h_1^2+h_2^2+\Delta t)^2(k+1)\Delta t,
\end{aligned}$$

$$\begin{aligned}
\left\|e^{k+1}\right\|^2 \leq& \frac{\frac{\alpha_{11}^2}{c}+1+\frac{a(T)^2}{c}}{1-\left(\frac{\alpha_{11}^2}{c}+1\right)\Delta t}\Delta t\sum_{l=0}^{k}\left\|e^{l}\right\|^2\\
&+\frac{m_1^2|\Omega|}{1-\left(\frac{\alpha_{11}^2}{c}+1\right)\Delta t}(h_1^2+h_2^2+\Delta t)^2(k+1)\Delta t.
\end{aligned}$$

If $\left(\frac{\alpha_{11}^2}{c}+1\right)\Delta t\leq\frac{1}{2}$, we have

$$\begin{aligned}
\left\|e^{k+1}\right\|^2 \leq& \left(\frac{2\alpha_{11}^2}{c}+2+\frac{2a(T)^2}{c}\right)\Delta t\sum_{l=0}^{k}\left\|e^{l}\right\|^2+2m_1^2|\Omega|(h_1^2+h_2^2+\Delta t)^2(k+1)\Delta t\\
=&2\alpha_{13}\Delta t\sum_{l=0}^{k}\left\|e^{l}\right\|^2+2m_1^2|\Omega|(h_1^2+h_2^2+\Delta t)^2(k+1)\Delta t. \qquad (2.3.22)
\end{aligned}$$

The Gronwall inequality yields

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

To derive the estimation of $\left\|\Delta_h e^{k+1}\right\|$, the equation (2.4.10) is taken inner product with $\delta_t e^{k+\frac{1}{2}} = \dfrac{e^{k+1}-e^k}{\Delta t}$,

$$\left\|\frac{e^{k+1}-e^k}{\Delta t}\right\|^2 = \left\langle \triangle_h \tilde{\mu}\left(\bar{n}^{k+1}, \bar{n}^k\right) - \triangle_h \tilde{\mu}\left(n^{k+1}, n^k\right), \delta_t e^{k+\frac{1}{2}} \right\rangle$$
$$+ \left\langle R^{k+1}, \frac{e^{k+1}-e^k}{\Delta t} \right\rangle. \tag{2.3.23}$$

The last term of the above equation satisfies

$$\left\langle R^{k+1}, \frac{e^{k+1}-e^k}{\Delta t} \right\rangle \leq \frac{m_1^2|\Omega|}{2}(h_1^2+h_2^2+\Delta t)^2 + \frac{1}{2}\left\|\frac{e^{k+1}-e^k}{\Delta t}\right\|^2. \tag{2.3.24}$$

And for the first term of the right hand side of (2.3.23), we have

$$\begin{aligned}
&\left\langle \Delta_h \tilde{\mu}\left(\bar{n}^{k+1}, \bar{n}^k\right) - \Delta_h \tilde{\mu}\left(n^{k+1}, n^k\right), \delta_t e^{k+\frac{1}{2}} \right\rangle \\
&= \Bigg\langle -c\Delta_h^2 e^{k+1} + \triangle_h \mu_{01}\left(\bar{n}^{k+1}\right) - \Delta_h \mu_{01}\left(n^{k+1}\right) \\
&\quad - \left[\triangle_h \mu_{02}\left(\bar{n}^k\right) - \triangle_h \mu_{02}\left(n^k\right)\right], \delta_t e^{k+\frac{1}{2}} \Bigg\rangle \\
&= \frac{1}{\Delta t}\left\langle -c\Delta_h e^{k+1}, \Delta_h e^{k+1} - \Delta_h e^k \right\rangle + \left\langle \mu_{01}\left(\bar{n}^{k+1}\right) - \mu_{01}\left(n^{k+1}\right), \delta_t \Delta_h e^{k+\frac{1}{2}} \right\rangle \\
&\quad - \left\langle \mu_{02}\left(\bar{n}^k\right) - \mu_{02}\left(n^k\right), \delta_t \Delta_h e^{k+\frac{1}{2}} \right\rangle \\
&= -\frac{c}{2\Delta t}\left(\left\|\Delta_h e^{k+1}\right\|^2 - \left\|\Delta_h e^k\right\|^2 + \left\|\Delta_h e^{k+1} - \Delta_h e^k\right\|^2\right) \\
&\quad + \left\langle \mu_{01}\left(\bar{n}^{k+1}\right) - \mu_{01}\left(n^{k+1}\right), \delta_t \Delta_h e^{k+\frac{1}{2}} \right\rangle - \left\langle \mu_{02}\left(\bar{n}^k\right) - \mu_{02}\left(n^k\right), \delta_t \Delta_h e^{k+\frac{1}{2}} \right\rangle \\
&\leq -\frac{c}{2\Delta t}\left(\left\|\Delta_h e^{k+1}\right\|^2 - \left\|\Delta_h e^k\right\|^2\right) + \left\langle \mu_{01}\left(\bar{n}^{k+1}\right) - \mu_{01}\left(n^{k+1}\right), \delta_t \Delta_h e^{k+\frac{1}{2}} \right\rangle \\
&\quad - \left\langle \mu_{02}\left(\bar{n}^k\right) - \mu_{02}\left(n^k\right), \delta_t \Delta_h e^{k+\frac{1}{2}} \right\rangle.
\end{aligned} \tag{2.3.25}$$

Combination of (2.3.23), (2.3.24) and (2.3.25) leads to

$$
\begin{aligned}
&\left\|\frac{e^{k+1}-e^k}{\Delta t}\right\|^2 \\
&\quad \leq \frac{m_1^2|\Omega|}{2}(h_1^2+h_2^2+\Delta t)^2+\frac{1}{2}\left\|\frac{e^{k+1}-e^k}{\Delta t}\right\|^2-\frac{c}{2\Delta t}\left(\left\|\Delta_h e^{k+1}\right\|^2-\left\|\Delta_h e^k\right\|^2\right) \\
&\quad +\left\langle\mu_{01}\left(\bar{n}^{k+1}\right)-\mu_{01}\left(n^{k+1}\right), \delta_t\Delta_h e^{k+\frac{1}{2}}\right\rangle-\left\langle\mu_{02}\left(\bar{n}^{k}\right)-\mu_{02}\left(n^{k}\right), \delta_t\Delta_h e^{k+\frac{1}{2}}\right\rangle,
\end{aligned}
$$

from which, we have

$$
\begin{aligned}
&\frac{c}{2\Delta t}\left(\left\|\Delta_h e^{k+1}\right\|^2-\left\|\Delta_h e^k\right\|^2\right) \\
&\quad \leq \left\langle\mu_{01}\left(\bar{n}^{k+1}\right)-\mu_{01}\left(n^{k+1}\right), \delta_t\Delta_h e^{k+\frac{1}{2}}\right\rangle-\left\langle\mu_{02}\left(\bar{n}^{k}\right)-\mu_{02}\left(n^{k}\right), \delta_t\Delta_h e^{k+\frac{1}{2}}\right\rangle \\
&\qquad -\frac{1}{2}\left\|\frac{e^{k+1}-e^k}{\Delta t}\right\|^2+\frac{m_1^2|\Omega|}{2}(h_1^2+h_2^2+\Delta t)^2.
\end{aligned}
$$

Accordingly,

$$
\begin{aligned}
&\left\|\Delta_h e^{k+1}\right\|^2-\left\|\Delta_h e^k\right\|^2 \\
&\quad \leq \frac{2\Delta t}{c}\left\langle\mu_{01}\left(\bar{n}^{k+1}\right)-\mu_{01}\left(n^{k+1}\right), \delta_t\Delta_h e^{k+\frac{1}{2}}\right\rangle-\frac{2\Delta t}{c}\left\langle\mu_{02}\left(\bar{n}^{k}\right)-\mu_{02}\left(n^{k}\right), \delta_t\Delta_h e^{k+\frac{1}{2}}\right\rangle \\
&\qquad -\frac{\Delta t}{c}\left\|\frac{e^{k+1}-e^k}{\Delta t}\right\|^2+\frac{m_1^2|\Omega|}{c}\Delta t(h_1^2+h_2^2+\Delta t)^2.
\end{aligned}
$$

Replacing k in the last inequality above by l and summing l from 0 to k, we can get

$$
\begin{aligned}
&\left\|\Delta_h e^{k+1}\right\|^2 \\
&\quad =\sum_{l=0}^{k}\left(\left\|\Delta_h e^{l+1}\right\|^2-\left\|\Delta_h e^l\right\|^2\right) \\
&\quad \leq -\frac{2\Delta t}{c}\sum_{l=0}^{k}\left\langle\mu_{02}\left(\bar{n}^{l}\right)-\mu_{02}\left(n^{l}\right), \delta_t\Delta_h e^{l+\frac{1}{2}}\right\rangle+\frac{m_1^2|\Omega|}{c}(k+1)\Delta t(h_1^2+h_2^2+\Delta t)^2 \\
&\qquad +\frac{2\Delta t}{c}\sum_{l=0}^{k}\left\langle\mu_{01}\left(\bar{n}^{l+1}\right)-\mu_{01}\left(n^{l+1}\right), \delta_t\Delta_h e^{l+\frac{1}{2}}\right\rangle-\frac{\Delta t}{c}\sum_{l=0}^{k}\left\|\frac{e^{l+1}-e^l}{\Delta t}\right\|^2.
\end{aligned}
\tag{2.3.26}
$$

Using Lemma 2.7 and Lemma 2.8, we have

$$\frac{2\Delta t}{c}\sum_{l=0}^{k}\left\langle\mu_{01}\left(\bar{n}^{l+1}\right)-\mu_{01}\left(n^{l+1}\right),\delta_t\Delta_h e^{k+\frac{1}{2}}\right\rangle$$

$$=\frac{2}{c}\left[\left\langle\mu_{01}\left(\bar{n}^{k+1}\right)-\mu_{01}\left(n^{k+1}\right),\Delta_h e^{k+1}\right\rangle-\left\langle\mu_{01}\left(\bar{n}^{1}\right)-\mu_{01}\left(n^{1}\right),\Delta_h e^{0}\right\rangle\right]$$

$$-\frac{2\Delta t}{c}\sum_{l=1}^{k}\left\langle\delta_t\left[\mu_{01}\left(\bar{n}^{l+\frac{1}{2}}\right)-\mu_{01}\left(n^{l+\frac{1}{2}}\right)\right],\Delta_h e^{l}\right\rangle$$

$$=\frac{2}{c}\left\langle\mu_{01}'\left(\xi_{11}^{k+1}\right)e^{k+1},\Delta_h e^{k+1}\right\rangle-\frac{2\Delta t}{c}\sum_{l=1}^{k}\left\langle\delta_t\left[\mu_{01}\left(\bar{n}^{l+\frac{1}{2}}\right)-\mu_{01}\left(n^{l+\frac{1}{2}}\right)\right],\Delta_h e^{l}\right\rangle$$

$$\leq-\frac{2\Delta t}{c}\sum_{l=1}^{k}\left\langle\mu_{01}'\left(\rho_{11}^{l+\frac{1}{2}}n^{l+1}+(1-\rho_{11}^{l+\frac{1}{2}})n^{l}\right)\delta_t\left(\bar{n}^{l+\frac{1}{2}}-n^{l+\frac{1}{2}}\right),\Delta_h e^{l}\right\rangle$$

$$-\frac{2\Delta t}{c}\sum_{l=1}^{k}\left\langle\mu_{01}''\left(\xi_{12}^{l+\frac{1}{2}}\right)\left(\rho_{11}^{l+\frac{1}{2}}\left(\bar{n}^{l+1}-n^{l+1}\right)+(1-\rho_{11}^{l+\frac{1}{2}})\left(\bar{n}^{l}-n^{l}\right)\right)\delta_t\bar{n}^{l+\frac{1}{2}},\Delta_h e^{l}\right\rangle$$

$$+\frac{2\alpha_{11}}{c}\left\|e^{k+1}\right\|\left\|\Delta_h e^{k+1}\right\|$$

$$\leq\frac{2\alpha_{11}}{c}\left\|e^{k+1}\right\|\left\|\Delta_h e^{k+1}\right\|+\frac{2\alpha_{11}\Delta t}{c}\sum_{l=1}^{k}\left\|\delta_t e^{l+\frac{1}{2}}\right\|\left\|\Delta_h e^{l}\right\|$$

$$+\frac{2\alpha_{12}\alpha_{14}\Delta t}{c}\sum_{l=1}^{k}\left(\left\|e^{l+1}\right\|+\left\|e^{l}\right\|\right)\left\|\Delta_h e^{l}\right\|$$

$$\leq\frac{1}{4}\left\|\Delta_h e^{k+1}\right\|^2+\frac{4\alpha_{11}^2}{c^2}\left\|e^{k+1}\right\|^2+\frac{\Delta t}{2c}\sum_{l=1}^{k}\left\|\delta_t e^{l+\frac{1}{2}}\right\|^2+\frac{2\alpha_{11}^2\Delta t}{c}\sum_{l=1}^{k}\left\|\Delta_h e^{l}\right\|^2$$

$$+\frac{\alpha_{12}\alpha_{14}\Delta t}{c}\left\|e^{k+1}\right\|^2+\frac{2\alpha_{12}\alpha_{14}\Delta t}{c}\sum_{l=1}^{k}\left\|e^{l}\right\|^2+\frac{2\alpha_{12}\alpha_{14}\Delta t}{c}\sum_{l=1}^{k}\left\|\Delta_h e^{l}\right\|^2. \tag{2.3.27}$$

And

$$-\frac{2\Delta t}{c}\sum_{l=0}^{k}\left\langle\mu_{02}\left(\bar{n}^{k}\right)-\mu_{02}\left(n^{k}\right),\delta_t\Delta_h e^{k+\frac{1}{2}}\right\rangle$$

$$
\begin{aligned}
&= -\frac{2}{c}\left[\left\langle \mu_{02}\left(\bar{n}^{k}\right)-\mu_{02}\left(n^{k}\right), \Delta_h e^{k+1}\right\rangle - \left\langle \mu_{02}\left(\bar{n}^{0}\right)-\mu_{02}\left(n^{0}\right), \Delta_h e^{0}\right\rangle\right] \\
&\quad + \frac{2\Delta t}{c}\sum_{l=1}^{k}\left\langle \frac{\mu_{02}\left(\bar{n}^{l}\right)-\mu_{02}\left(n^{l}\right)-\left[\mu_{02}\left(\bar{n}^{l-1}\right)-\mu_{02}\left(n^{l-1}\right)\right]}{\Delta t}, \Delta_h e^{l}\right\rangle \\
&= -\frac{2}{c}\left\langle \mu_{02}'\left(\xi_{21}^{k}\right)e^{k}, \Delta_h e^{k+1}\right\rangle + \frac{2\Delta t}{c}\sum_{l=1}^{k}\left\langle \delta_t\left[\mu_{02}\left(\bar{n}^{l-\frac{1}{2}}\right)-\mu_{02}\left(n^{l-\frac{1}{2}}\right)\right], \Delta_h e^{l}\right\rangle \\
&\le \frac{2\Delta t}{c}\sum_{l=1}^{k}\left\langle \mu_{02}'\left(\rho_{12}^{l-\frac{1}{2}}n^{l}+(1-\rho_{12}^{l-\frac{1}{2}})n^{l}\right)\delta_t\left(\bar{n}^{l-\frac{1}{2}}-n^{l-\frac{1}{2}}\right), \Delta_h e^{l}\right\rangle \\
&\quad + \frac{2\Delta t}{c}\sum_{l=1}^{k}\left\langle \mu_{02}''\left(\xi_{22}^{l-\frac{1}{2}}\right)\left(\rho_{12}^{l-\frac{1}{2}}\left(\bar{n}^{l}-n^{l}\right)+(1-\rho_{12}^{l-\frac{1}{2}})\left(\bar{n}^{l-1}-n^{l-1}\right)\right)\delta_t\bar{n}^{l-\frac{1}{2}}, \Delta_h e^{l}\right\rangle \\
&\quad + \frac{2\alpha_{21}}{c}\left\|e^{k}\right\|\left\|\Delta_h e^{k+1}\right\| \\
&\le \frac{2\alpha_{21}}{c}\left\|e^{k}\right\|\left\|\Delta_h e^{k+1}\right\| + \frac{2\alpha_{21}\Delta t}{c}\sum_{l=1}^{k}\left\|\delta_t e^{l-\frac{1}{2}}\right\|\left\|\Delta_h e^{l}\right\| \\
&\quad + \frac{2\alpha_{22}\alpha_{14}\Delta t}{c}\sum_{l=1}^{k}\left(\left\|e^{l}\right\|+\left\|e^{l-1}\right\|\right)\left\|\Delta_h e^{l}\right\| \\
&\le \frac{1}{4}\left\|\Delta_h e^{k+1}\right\|^2 + \frac{4\alpha_{21}^2}{c^2}\left\|e^{k+1}\right\|^2 + \frac{\Delta t}{2c}\sum_{l=1}^{k}\left\|\delta_t e^{l-\frac{1}{2}}\right\|^2 + \frac{2\alpha_{21}^2\Delta t}{c}\sum_{l=1}^{k}\left\|\Delta_h e^{l}\right\|^2 \\
&\quad + \frac{2\alpha_{22}\alpha_{14}\Delta t}{c}\sum_{l=1}^{k}\left\|e^{l}\right\|^2 + \frac{2\alpha_{22}\alpha_{14}\Delta t}{c}\sum_{l=1}^{k}\left\|\Delta_h e^{l}\right\|^2. \qquad (2.3.28)
\end{aligned}
$$

Combining (2.3.26), (2.3.27) with (2.3.28), we can obtain

$$
\begin{aligned}
&\left\|\Delta_h e^{k+1}\right\|^2 \\
&\quad \le \frac{1}{4}\left\|\Delta_h e^{k+1}\right\|^2 + \frac{4\alpha_{11}^2}{c^2}\left\|e^{k+1}\right\|^2 + \frac{\Delta t}{2c}\sum_{l=1}^{k}\left\|\delta_t e^{l+\frac{1}{2}}\right\|^2 + \frac{2\alpha_{11}^2\Delta t}{c}\sum_{l=1}^{k}\left\|\Delta_h e^{l}\right\|^2 \\
&\qquad + \frac{\alpha_{12}\alpha_{14}\Delta t}{c}\left\|e^{k+1}\right\|^2 + \frac{2\alpha_{12}\alpha_{14}\Delta t}{c}\sum_{l=1}^{k}\left\|e^{l}\right\|^2 + \frac{2\alpha_{12}\alpha_{14}\Delta t}{c}\sum_{l=1}^{k}\left\|\Delta_h e^{l}\right\|^2
\end{aligned}
$$

$$
\begin{aligned}
&+ \frac{1}{4}\left\|\Delta_h e^{k+1}\right\|^2 + \frac{4\alpha_{21}^2}{c^2}\left\|e^{k+1}\right\|^2 + \frac{\Delta t}{2c}\sum_{l=1}^{k}\left\|\delta_t e^{l-\frac{1}{2}}\right\|^2 + \frac{2\alpha_{21}^2\Delta t}{c}\sum_{l=1}^{k}\left\|\Delta_h e^l\right\|^2 \\
&+ \frac{2\alpha_{22}\alpha_{14}\Delta t}{c}\sum_{l=1}^{k}\left\|e^l\right\|^2 + \frac{2\alpha_{22}\alpha_{14}\Delta t}{c}\sum_{l=1}^{k}\left\|\Delta_h e^l\right\|^2 \\
&- \frac{\Delta t}{c}\sum_{l=0}^{k}\left\|\frac{e^{l+1}-e^l}{\Delta t}\right\|^2 + \frac{2m_1^2|\Omega|}{c}(k+1)\Delta t(h_1^2+h_2^2+\Delta t)^2 \\
\le\ & \frac{1}{2}\left\|\Delta_h e^{k+1}\right\|^2 + \frac{4\alpha_{11}^2+4\alpha_{21}^2}{c^2}\left\|e^{k+1}\right\|^2 + \frac{\alpha_{12}\alpha_{14}\Delta t}{c}\left\|e^{k+1}\right\|^2 \\
&+ \frac{2\alpha_{11}^2+2\alpha_{21}^2+2\alpha_{12}\alpha_{14}+2\alpha_{22}\alpha_{14}}{c}\Delta t\sum_{l=1}^{k}\left\|\Delta_h e^l\right\|^2 \\
&+ \frac{2\alpha_{12}\alpha_{14}+2\alpha_{22}\alpha_{14}}{c}\Delta t\sum_{l=1}^{k}\left\|e^l\right\|^2 + \frac{m_1^2|\Omega|}{c}(k+1)\Delta t(h_1^2+h_2^2+\Delta t)^2 \\
\le\ & \frac{1}{2}\left\|\Delta_h e^{k+1}\right\|^2 + 4\alpha_{15}\left\|e^{k+1}\right\|^2 + 2\alpha_{16}\Delta t\sum_{l=1}^{k}\left\|\Delta_h e^l\right\|^2 + \frac{\alpha_{12}\alpha_{14}\Delta t}{c}\left\|e^{k+1}\right\|^2 \\
&+ 2\alpha_{17}\Delta t\sum_{l=1}^{k}\left\|e^l\right\|^2 + \frac{m_1^2|\Omega|}{c}(k+1)\Delta t(h_1^2+h_2^2+\Delta t)^2. \qquad (2.3.29)
\end{aligned}
$$

Using the inequality (2.3.22) under the condition $\left(\frac{\alpha_{11}^2}{c}+1\right)\Delta t \le \frac{1}{2}$, we have

$$
\begin{aligned}
&\frac{1}{2}\left\|\Delta_h e^{k+1}\right\|^2 + \left\|e^{k+1}\right\|^2 \\
&\quad\le (4\alpha_{15}+1)\left[2\alpha_{13}\Delta t\sum_{l=0}^{k}\left\|e^l\right\|^2 + 2m_1^2|\Omega|(h_1^2+h_2^2+\Delta t)^2(k+1)\Delta t\right] \\
&\quad+ \frac{\alpha_{12}\alpha_{14}\Delta t}{c}\left\|e^{k+1}\right\|^2 + 2\alpha_{16}\Delta t\sum_{l=1}^{k}\left\|\Delta_h e^l\right\|^2 + 2\alpha_{17}\Delta t\sum_{l=1}^{k}\left\|e^l\right\|^2 \\
&\quad+ \frac{2m_1^2|\Omega|}{c}(k+1)\Delta t(h_1^2+h_2^2+\Delta t)^2
\end{aligned}
$$

$$= \left[2\alpha_{13}\left(4\alpha_{15}+1\right)+2\alpha_{17}\right]\Delta t\sum_{l=0}^{k}\left\|e^{l}\right\|^{2}+\frac{\alpha_{12}\alpha_{14}\Delta t}{c}\left\|e^{k+1}\right\|^{2}+2\alpha_{16}\Delta t\sum_{l=1}^{k}\left\|\Delta_{h}e^{l}\right\|^{2}$$
$$+\left(8\alpha_{15}+2+\frac{1}{c}\right)m_1^2|\Omega|(k+1)\Delta t(h_1^2+h_2^2+\Delta t)^2. \tag{2.3.30}$$

If $\frac{\alpha_{12}\alpha_{14}\Delta t}{c}\leq\frac{1}{2}$, then

$$\frac{1}{2}\left\|\Delta_{h}e^{k+1}\right\|^{2}+\frac{1}{2}\left\|e^{k+1}\right\|^{2}$$
$$\leq\left[2\alpha_{13}\left(4\alpha_{15}+1\right)+2\alpha_{17}\right]\Delta t\sum_{l=0}^{k}\left\|e^{l}\right\|^{2}+2\alpha_{16}\Delta t\sum_{l=1}^{k}\left\|\Delta_{h}e^{l}\right\|^{2}$$
$$+\left(8\alpha_{15}+\frac{1}{c}+2\right)m_1^2|\Omega|(k+1)\Delta t(h_1^2+h_2^2+\Delta t)^2. \tag{2.3.31}$$

Therefore,

$$\left\|\Delta_{h}e^{k+1}\right\|^{2}+\left\|e^{k+1}\right\|^{2}$$
$$\leq\left[4\alpha_{13}\left(4\alpha_{15}+1\right)+4\alpha_{17}\right]\Delta t\sum_{l=0}^{k}\left\|e^{l}\right\|^{2}+4\alpha_{16}\Delta t\sum_{l=1}^{k}\left\|\Delta_{h}e^{l}\right\|^{2}$$
$$+\left(16\alpha_{15}+\frac{2}{c}+4\right)m_1^2|\Omega|(k+1)\Delta t(h_1^2+h_2^2+\Delta t)^2$$
$$\leq\alpha_{19}\Delta t\sum_{l=0}^{k}\left(\left\|e^{l}\right\|^{2}+\left\|\Delta_{h}e^{l}\right\|^{2}\right)+\alpha_{18}m_1^2|\Omega|(k+1)\Delta t(h_1^2+h_2^2+\Delta t)^2. \tag{2.3.32}$$

Gronwall inequality yields

$$\left\|e^{k+1}\right\|^{2}+\left\|\Delta_{h}e^{k+1}\right\|^{2}\leq\frac{\alpha_{18}}{\alpha_{19}}\exp\left(\alpha_{19}(k+1)\Delta t\right)\cdot|\Omega|\left[m_1\left(h_1^2+h_2^2+\Delta t\right)\right]^2. \tag{2.3.33}$$

where $k=0,1,...,K-1$. With the help of Lemma 2.4 and (2.4.14), we can get

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

$$\leq k_0 \sqrt{\frac{2\alpha_{18}}{\alpha_{13}\alpha_{19}}} \exp\left(\left(\alpha_{13} + \frac{\alpha_{19}}{2}\right)(k+1)\Delta t\right) m_1^2 |\Omega| \left(h_1^2 + h_2^2 + \triangle t\right)^2.$$

Therefore,

$$\begin{aligned}\left\|e^{k+1}\right\|_\infty \leq & \sqrt[4]{\frac{2\alpha_{18}}{\alpha_{13}\alpha_{19}} k_0^2 |\Omega|^2} \exp\left(\left(\frac{\alpha_{13}}{2} + \frac{\alpha_{19}}{4}\right)(k+1)\Delta t\right) m_1 \left(h_1^2 + h_2^2 + \triangle t\right) \\ \leq & C_{12}\left(h_1^2 + h_2^2 + \triangle t^2\right).\end{aligned}$$

This completes the proof. $\square$

2.4 The Crank-Nicolson scheme for the fourth-order parabolic equation

Applying Taylor expansion to (2.1.4a), (2.1.5), we have

$$\begin{gathered}\frac{\bar{n}_{ij}^{k+1} - \bar{n}_{ij}^k}{\triangle t} + c\triangle_h^2 \bar{n}_{ij}^{k+\frac{1}{2}} - \triangle_h \mu_0 \left(\bar{n}_{ij}^{k+\frac{1}{2}}\right) = R_{ij}^{k+\frac{1}{2}}, \\ 1 \leq i \leq M_1, \quad 1 \leq i \leq M_2, \quad 0 \leq k \leq K-1,\end{gathered} \tag{2.4.1a}$$

$$\begin{gathered}\frac{(\bar{f}_0)_{ij}^{k+1} - (\bar{f}_0)_{ij}^k}{\triangle t} = \mu_0 \left(\bar{n}^{k+\frac{1}{2}}\right) \frac{\bar{n}_{ij}^{k+1} - \bar{n}_{ij}^k}{\triangle t} + S_{ij}^{k+\frac{1}{2}}, \\ 1 \leq i \leq M_1, \quad 1 \leq j \leq M_2, \quad 0 \leq k \leq K-1.\end{gathered} \tag{2.4.1b}$$

where there exists a constant m_2, such that

$$\begin{gathered}\left|R_{ij}^{k+\frac{1}{2}}\right| \leq m_2 \left(h_1^2 + h_2^2 + \triangle t^2\right), \\ 1 \leq i \leq M_1, \quad 1 \leq j \leq M_2, \quad 0 \leq k \leq K-1,\end{gathered} \tag{2.4.2a}$$

$$\begin{gathered}\left|S_{ij}^{k+\frac{1}{2}}\right| \leq m_2 \left(h_1^2 + h_2^2 + \triangle t^2\right), \\ 1 \leq i \leq M_1, \quad 1 \leq j \leq M_2, \quad 0 \leq k \leq K-1,\end{gathered} \tag{2.4.2b}$$

with the initial conditions

$$\bar{n}_{ij}^0 = n_0(x_i, y_j), \quad 1 \leq i \leq M_1, \quad 1 \leq j \leq M_2, \tag{2.4.3a}$$

$$\bar{f}^0_{ij} = f_0\left(\bar{n}^0_{ij}\right), \qquad 1 \le i \le M_1, \quad 1 \le j \le M_2. \tag{2.4.3b}$$

Omitting the small terms in (2.4.1a) and (2.4.1b), we can derive the Crank-Nicolson scheme of the fourth-order parabolic equation (2.1.4a) and (2.1.5) as follows,

$$\begin{aligned} &\frac{n^{k+1}_{ij} - n^k_{ij}}{\triangle t} + c\triangle_h^2 n^{k+\frac{1}{2}}_{ij} - \triangle_h \mu_0\left(n^{k+\frac{1}{2}}_{ij}\right) = 0, \\ &\qquad\qquad 1 \le i \le M_1, \quad 1 \le j \le M_2, \quad 0 \le k \le K-1, \end{aligned} \tag{2.4.4a}$$

$$\begin{aligned} &\frac{(f_0)^{k+1}_{ij} - (f_0)^k_{ij}}{\triangle t} = \mu_0\left(n^{k+\frac{1}{2}}_{ij}\right)\frac{n^{k+1}_{ij} - n^k_{ij}}{\triangle t}, \\ &\qquad\qquad 1 \le i \le M_1, \quad 1 \le j \le M_2, \quad 0 \le k \le K-1. \end{aligned} \tag{2.4.4b}$$

2.4.1 Mass conservation and energy stability

Lemma 2.12. *The solution of the discrete equation (2.4.4a) satisfies the mass conservation, that is, for any* $0 \le k \le K-1$*,*

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

Proof. Multiplying $h_1 h_2 \triangle t$ to both sides of (2.4.4a) and summing for $i = 1, ..., M_1$, $j = 1, ..., M_2$, with the periodic boundary condition, we obtain

$$h_1 h_2 \sum_{i=1}^{M_1}\sum_{j=1}^{M_2}\left(n^{k+1}_{ij} - n^k_{ij}\right) = -h_1 h_2 \triangle t \sum_{i=1}^{M_1}\sum_{j=1}^{M_2} \triangle_h\left[c\triangle_h n^{k+\frac{1}{2}}_{ij} - \mu_0\left(n^{k+\frac{1}{2}}_{ij}\right)\right].$$

Let

$$c\triangle_h n^{k+\frac{1}{2}}_{ij} - \mu_0\left(n^{k+\frac{1}{2}}_{ij}\right) = w^{k+\frac{1}{2}}_{ij}, \tag{2.4.5}$$

then

$$h_1 h_2 \sum_{i=1}^{M_1}\sum_{j=1}^{M_2}\left(n^{k+1}_{ij} - n^k_{ij}\right)$$

$$
\begin{aligned}
&= -h_1 h_2 \triangle t \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} \triangle_h w_{ij}^{k+\frac{1}{2}} \\
&= -h_1 h_2 \triangle t \sum_{j=1}^{M_2} \frac{1}{h_1^2} \sum_{i=1}^{M_1} \left[\left(w_{i+1,j}^{k+\frac{1}{2}} - w_{ij}^{k+\frac{1}{2}} \right) - \left(w_{ij}^{k+\frac{1}{2}} - w_{i-1,j}^{k+\frac{1}{2}} \right) \right] \\
&\quad - h_1 h_2 \triangle t \sum_{i=1}^{M_1} \frac{1}{h_2^2} \sum_{j=1}^{M_2} \left[\left(w_{i,j+1}^{k+\frac{1}{2}} - w_{ij}^{k+\frac{1}{2}} \right) - \left(w_{ij}^{k+\frac{1}{2}} - w_{i,j-1}^{k+\frac{1}{2}} \right) \right] \\
&= 0.
\end{aligned}
$$

This completes the proof. □

Theorem 2.4. *If the total discrete free energy at $k\Delta t$, $k = 0, 1, ...K$, is defined by (2.3.7), the discrete scheme provided by (2.4.4a)-(2.4.4b) can guarantee the following energy identity for any time step $\Delta t > 0$ as follows,*

$$
\frac{F_h^{k+1} - F_h^k}{\triangle t} + \left\| -\nabla w^{k+\frac{1}{2}} \right\|^2 = 0. \tag{2.4.6}
$$

Proof. Taking the inner product of (2.4.4a) with $-w^{k+\frac{1}{2}}$ defined by (2.4.5), we can get

$$
\left\langle -c\triangle_h n^{k+\frac{1}{2}} + \mu_0 \left(n^{k+\frac{1}{2}} \right), \frac{n^{k+1} - n^k}{\triangle t} \right\rangle + \left\| -\nabla w^{k+\frac{1}{2}} \right\|^2 = 0,
$$

which is equivalent to

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

Noticing the relation given by (2.4.4b), we have

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

Recombining the terms in the above formula, we can get

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

which is an expanded form of (2.4.6). This completes the proof. $\square$

2.4.2 The unique solvability

In this subsection, we consider the existence of the solution of (2.4.4a).

Theorem 2.5. *The discrete scheme (2.4.4a) has at least one solution if* $\Delta t<\dfrac{c}{4a(T)}$.

Proof. The scheme (2.4.4a) can be written as

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

$$1\le i\le M_1,\quad 1\le j\le M_2,\quad 0\le k\le K-1,$$

or

$$\begin{aligned}&(w_{ij}-n_{ij}^k)+\frac{c\triangle t}{2}\triangle_h^2 w_{ij}-\frac{\triangle t}{2}\triangle_h\mu_0\left(w_{ij}\right)=0,\\ &1\le i\le M_1,\quad 1\le j\le M_2,\quad 0\le k\le K-1,\end{aligned}\tag{2.4.7}$$

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

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

then

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

Here,

$$\begin{aligned}
\mu_0\left(w\right) = {} & RT\ln\frac{w}{1-bw} + RT\frac{bw}{1-bw} + \frac{a(T)}{2\sqrt{2}b}\ln\left(\frac{1+(1-\sqrt{2})bw}{1+(1+\sqrt{2})bw}\right) \\
& - \frac{a(T)w}{1+2bw-b^2w^2} \\
& \geq RT\ln w + RTbw + \frac{a(T)}{2\sqrt{2}b}\ln\left(\frac{1+(1-\sqrt{2})bw}{4}\right) - \frac{a(T)w}{2bw} \\
& = RT\ln w + RTbw + \frac{a(T)}{2\sqrt{2}b}\ln\left(\frac{1+(1-\sqrt{2})bw}{4}\right) - \frac{a(T)}{2b},
\end{aligned}$$

which yields

$$\mu_0'(w) = \frac{RT}{w(1-bw)^2} - \frac{2a(T)(1+bw)}{(1+2bw-b^2w^2)^2} > -\frac{2a(T)(1+bw)}{(1+2bw-b^2w^2)^2} > -4a(T).$$

Therefore,

$$\begin{aligned}
\langle g(w), w\rangle > {} & \left[\|w\|^2 - \left\langle n^k, w\right\rangle\right] + \frac{c\triangle t}{2}\|\triangle_h w\|^2 - 2a(T)\triangle t\,\|\nabla_h w\|^2 \\
& \geq \left[\|w\|^2 - \left\langle n^k, w\right\rangle\right] + \frac{c\triangle t}{2}\|\triangle_h w\|^2 - 2a(T)\triangle t\,\|w\|\,\|\triangle_h w\| \\
& \geq \left[\|w\|^2 - \left\|n^k\right\|\|w\|\right] + \frac{c\triangle t}{2}\|\triangle_h w\|^2 \\
& \quad - \left(\frac{c\triangle t}{2}\|\triangle_h w\|^2 + \frac{2a^2(T)\triangle t}{c}\|w\|^2\right) \\
& = \left(1 - \frac{2a^2(T)\triangle t}{c}\right)\|w\|^2 - \left\|n^k\right\|\|w\| \\
& \geq \left[\left(1 - \frac{2a^2(T)\triangle t}{c}\right)\|w\| - \left\|n^k\right\|\right]\|w\|.
\end{aligned}$$

When $\triangle t < \dfrac{c}{4a^2(T)}$, $\dfrac{2a^2(T)\triangle t}{c} < \dfrac{1}{2}$, it follows that

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

If $\|w\| = 2\left\|n^k\right\|$, we have $\langle g(w), w\rangle \geq 0$. By Lemma 2.5, there is at least one solution w satisfying $\|w\| \leq 2\left\|n^k\right\|$. The solvability of the Crank-Nicolson scheme is proved. $\square$

Now we present the uniqueness of the solution of (2.4.4a).

Theorem 2.6. *The discrete scheme (2.4.4a) has at most one solution in the region* $\left[\theta_0, \frac{1}{b} - \theta_0\right]$ *for any* $\theta_0 \in \left(0, \frac{1}{b}\right)$ *if* $\Delta t < \frac{2c}{M^2}$. *Here* $M = \max\left\{|\mu'(n)| : n \in \left[\theta_0, \frac{1}{b} - \theta_0\right]\right\}$.

Proof. Suppose (2.4.7) has another solution z, and $w_{ij} \in \left[\theta_0, \frac{1}{b} - \theta_0\right]$ and $z_{ij} \in \left[\theta_0, \frac{1}{b} - \theta_0\right]$ for all $1 \leq i \leq M_1$, $1 \leq j \leq M_2$, then

$$(z_{ij} - n_{ij}^k) + \frac{c\triangle t}{2}\triangle_h^2 z_{ij} - \frac{\triangle t}{2}\triangle_h \mu_0\left(z_{ij}\right) = 0, \quad 0 \leq k \leq K-1. \tag{2.4.8}$$

Let $\epsilon_{ij} = w_{ij} - z_{ij}$. Subtracting (2.4.8) from (2.4.7), we have

$$\epsilon_{ij} + \frac{c\triangle t}{2}\triangle_h^2 \epsilon_{ij} - \frac{\triangle t}{2}\left[\triangle_h \mu_0(w_{ij}) - \triangle_h \mu_0(z_{ij})\right] = 0. \tag{2.4.9}$$

Taking the inner product of (2.4.9) with ϵ, we obtain

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

According to the Lemma 2.3, we have

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

Then

$$\begin{aligned}\|\epsilon\|^2 + \frac{c\triangle t}{2}\left\|\triangle_h \epsilon\right\|^2 =& \frac{\triangle t}{2}\left\langle \mu_0\left(w\right) - \mu_0\left(z\right), \triangle_h \epsilon\right\rangle = \left\langle \frac{\partial \mu_0}{\partial n}(\xi)\epsilon, \Delta_h \epsilon\right\rangle \\ \leq& M\left\|\epsilon\right\|\left\|\Delta \epsilon\right\| \leq \frac{\Delta t M^2}{2c}\left\|\epsilon\right\|^2 + \frac{c\Delta t}{2}\left\|\Delta_h \epsilon\right\|^2.\end{aligned}$$

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

$$\|\epsilon\|^2 + \frac{c\triangle t}{2}\|\triangle_h \epsilon\|^2 \le \frac{\Delta t M^2}{2c}\|\epsilon\|^2 + \frac{c\triangle t}{2}\|\triangle_h \epsilon\|^2,$$

which finally yields

$$\|\epsilon\|^2 \le \frac{\Delta t M^2}{2c}\|\epsilon\|^2.$$

If $\Delta t < \dfrac{2c}{M^2}$, we get $\epsilon = 0$. This completes the proof. □

2.4.3 Convergence

To derive (2.2.6), we also apply the differential mid-value theorem. This completes the proof. Denote

$$\alpha_{01} = \max\left\{|\mu_0'(n)| : \ n \in \left[\epsilon_1, \frac{1}{b} - \epsilon_1\right]\right\}, \quad \alpha_{02} = \max\left\{|\mu_0''(n)| : \ n \in \left[\epsilon_1, \frac{1}{b} - \epsilon_1\right]\right\},$$

$$\alpha_{23} = \frac{\alpha_{01}^2}{4c} + \frac{1}{2}, \quad \alpha_{24} = \max\left\{\left|\frac{\bar{n}^{k+1} - \bar{n}^k}{\Delta t}\right|, k = 1, 2, ...K-1.\right\}$$

$$\alpha_{28} = 2 + \frac{8\alpha_{01}^2}{c^2} + \frac{4\alpha_{02}^2\alpha_{24}^2}{c} + \frac{2}{c}, \quad \alpha_{29} = \max\left\{1 + \frac{4\alpha_{01}^2}{c^2} + \frac{2\alpha_{02}^2\alpha_{24}^2}{c}, \frac{4}{c} + \frac{2\alpha_{01}^2}{c}\right\}.$$

$$C_{21} = \sqrt{\frac{|\Omega|}{4\alpha_{23}}} \exp\left(2\alpha_{23}(k+1)\Delta t\right) m_2,$$

$$C_{22} = \sqrt[4]{\frac{\alpha_{28}}{2\alpha_{23}\alpha_{29}} k_0^2 |\Omega|^2} \exp\left(\left(\alpha_{23} + \frac{\alpha_{29}}{4}\right)(k+1)\Delta t\right) m_2.$$

Theorem 2.7. *Suppose the solution of the original fourth order equation (2.1.4a)-(2.1.4b) is sufficiently smooth, and there exists* ϵ_1 *such that for any* $k = 0, 1, ..., K-1$, *the solution of the Crank-Nicolson scheme (2.4.4a), we have* $n^k \in \left[\epsilon_1, \frac{1}{b} - \epsilon_1\right]$. *If* $\alpha_{23}\Delta t < \frac{1}{2}$, *then*

$$\left\|e^{k+1}\right\| \le C_{21}\left(h_1^2 + h_2^2 + \Delta t^2\right);$$

if $\alpha_{28}\Delta t < \dfrac{1}{2}$*, we can obtain*

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

Proof. Define $\bar{n}(x, y, t)$ as the exact solution of (2.1.4a). $\bar{n}_{ij}^{k+1} = \bar{n}(x_i, y_j, t_k)$ is the solution of (2.4.1a), and n_{ij}^{k+1} is the solution of (2.4.4a), Let $e_{ij}^k = \bar{n}_{ij}^k - n_{ij}^k$. Subtracting (2.4.4a) from (2.4.1a), we have

$$\frac{e_{ij}^{k+1} - e_{ij}^k}{\triangle t} + c\triangle_h^2 e_{ij}^{k+\frac{1}{2}} - \triangle_h\mu_0\left(\bar{n}_{ij}^{k+\frac{1}{2}}\right) + \triangle_h\mu_0\left(n_{ij}^{k+\frac{1}{2}}\right) = R_{ij}^{k+\frac{1}{2}}, \tag{2.4.10}$$

$$1 \le i \le M_1, \quad 1 \le j \le M_2, \quad 0 \le k \le K-1.$$

$$e_{ij}^0 = 0, \quad 1 \le i \le M_1, \quad 1 \le j \le M_2. \tag{2.4.11}$$

Taking inner product of (2.4.10) with $e^{k+\frac{1}{2}} = \dfrac{e^{k+1} + e^k}{2}$, then

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

For convenience, we use its equivalent form as

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

According to Lemma 2.3, we have

$$\left\langle \triangle_h\mu_0\left(\bar{n}^{k+\frac{1}{2}}\right) - \triangle_h\mu_0\left(n^{k+\frac{1}{2}}\right), e^{k+\frac{1}{2}}\right\rangle$$
$$= \left\langle \mu_0\left(\bar{n}^{k+\frac{1}{2}}\right) - \mu_0\left(n^{k+\frac{1}{2}}\right), \triangle_h e^{k+\frac{1}{2}}\right\rangle = \left\langle \mu_0(\xi^{k+\frac{1}{2}})e^{k+\frac{1}{2}}, \Delta_h e^{k+\frac{1}{2}}\right\rangle$$
$$\le \alpha_{01}\left\|e^{k+\frac{1}{2}}\right\|\left\|\Delta_h e^{k+\frac{1}{2}}\right\| \le \frac{\alpha_{01}^2}{4c}\left\|e^{k+\frac{1}{2}}\right\|^2 + c\left\|\triangle_h e^{k+\frac{1}{2}}\right\|^2.$$

Using (2.4.2a), we have

$$\left\langle R^{k+\frac{1}{2}}, e^{k+\frac{1}{2}} \right\rangle = \left\langle R^{k+\frac{1}{2}}, \frac{e^{k+1}+e^k}{2} \right\rangle \le \left\| R^{k+\frac{1}{2}} \right\| \left\| \frac{e^{k+1}+e^k}{2} \right\|$$

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

$$\le \frac{|\Omega|}{2} m_2^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2 + \frac{\left\|e^{k+1}\right\|^2 + \left\|e^k\right\|^2}{4}.$$

Combining all the above results, we obtain

$$\frac{\left\|e^{k+1}\right\|^2 - \left\|e^k\right\|^2}{2\triangle t} + c \left\| \triangle_h e^{k+\frac{1}{2}} \right\|^2 \le \frac{\alpha_{01}^2}{4c} \left\| e^{k+\frac{1}{2}} \right\|^2 + c \left\| \triangle_h e^{k+\frac{1}{2}} \right\|^2 + \frac{\left\|e^{k+1}\right\|^2 + \left\|e^k\right\|^2}{4}$$
$$+ \frac{|\Omega|}{2} m_2^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2,$$

$$\frac{\left\|e^{k+1}\right\|^2 - \left\|e^k\right\|^2}{2\triangle t}$$
$$\le \frac{\alpha_{01}^2}{4c} \left\| e^{k+\frac{1}{2}} \right\|^2 + \frac{|\Omega|}{2} m_2^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2 + \frac{\left\|e^{k+1}\right\|^2 + \left\|e^k\right\|^2}{4}, \tag{2.4.12}$$
$$\le \left(\frac{\alpha_{01}^2}{8c} + \frac{1}{4}\right) \left(\left\|e^{k+1}\right\|^2 + \left\|e^k\right\|^2\right) + \frac{|\Omega|}{2} m_2^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2.$$

Therefore,

$$\left\|e^{k+1}\right\|^2 \le \left\|e^k\right\|^2 + \left(\frac{\alpha_{01}^2}{4c} + \frac{1}{2}\right) \Delta t \left(\left\|e^{k+1}\right\|^2 + \left\|e^k\right\|^2\right) + |\Omega| \, \Delta t m_2^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2$$
$$= \left\|e^k\right\|^2 + \alpha_{23} \Delta t \left(\left\|e^{k+1}\right\|^2 + \left\|e^k\right\|^2\right) + |\Omega| \, \Delta t m_2^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2. \tag{2.4.13}$$

$$(1 - \alpha_{23} \Delta t) \left\|e^{k+1}\right\|^2 \le (1 + \alpha_{23} \Delta t) \left\|e^k\right\|^2 + |\Omega| \, \Delta t m_2^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2.$$

If $\alpha_{23} \Delta t < \dfrac{1}{2}$, then

$$\left\|e^{k+1}\right\|^2 \le (1 + 4\alpha_{23} \Delta t) \left\|e^k\right\|^2 + 2 \, |\Omega| \, \Delta t m_2^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2.$$

According to Gronwall inequality given by Lemma 2.6, we can get

$$\left\|e^{k+1}\right\|^2 \leq \frac{|\Omega|}{2\alpha_{23}} \exp\left(4\alpha_{23}(k+1)\Delta t\right) m_2^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2, \tag{2.4.14}$$

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

From (2.4.12), we also can obtain

$$\begin{aligned}\left\|e^{k+1}\right\|^2 - \left\|e^k\right\|^2 \leq & \left(\frac{\alpha_{01}^2}{4c} + \frac{1}{2}\right)\left(\left\|e^{k+1}\right\|^2 + \left\|e^k\right\|^2\right)\Delta t \\ & + |\Omega|\, m_2^2 \left(h_1^2 + h_2^2 + \Delta t^2\right)^2 \Delta t. \end{aligned} \tag{2.4.15}$$

Replacing the superscript k by l in (2.4.15) and summing up for l from 0 to k leads to

$$\begin{aligned}\left\|e^{k+1}\right\|^2 &= \sum_{l=0}^{k}\left[\left\|e^{l+1}\right\|^2 - \left\|e^l\right\|^2\right] \\ &\leq \sum_{l=0}^{k}\left(\frac{\alpha_{01}^2}{4c} + \frac{1}{2}\right)\left(\left\|e^{l+1}\right\|^2 + \left\|e^l\right\|^2\right)\Delta t + (k+1)\,|\Omega|\, m_2^2\left(h_1^2 + h_2^2 + \Delta t^2\right)^2 \Delta t.\end{aligned}$$

Putting all terms for $\left\|e^{k+1}\right\|$ on the left hand side, we have

$$\begin{aligned}&\left[1 - \left(\frac{\alpha_{01}^2}{4c} + \frac{1}{2}\right)\Delta t\right]\left\|e^{k+1}\right\|^2 \\ &\quad\leq \left(\frac{\alpha_{01}^2}{2c} + 1\right)\Delta t \sum_{l=0}^{k}\left\|e^l\right\|^2 + (k+1)\,|\Omega|\, m_2^2\left(h_1^2 + h_2^2 + \Delta t^2\right)^2 \Delta t,\end{aligned}$$

$$\left\|e^{k+1}\right\|^2 \leq \frac{\left(\frac{\alpha_{01}^2}{2c} + 1\right)\Delta t}{1 - \left(\frac{\alpha_{01}^2}{4c} + \frac{1}{2}\right)\Delta t}\sum_{l=0}^{k}\left\|e^l\right\|^2 + \frac{(k+1)\,|\Omega|\, m_2^2}{1 - \left(\frac{\alpha_{01}^2}{4c} + \frac{1}{2}\right)\Delta t}\left(h_1^2 + h_2^2 + \Delta t^2\right)^2 \Delta t.$$

If $\Delta t \leq 1/\left(\frac{\alpha_{01}^2}{2c} + 1\right)$, $\left(\frac{\alpha_{01}^2}{4c} + \frac{1}{2}\right)\Delta t \leq \frac{1}{2}$, and

$$\left\|e^{k+1}\right\|^2 \leq \left(\frac{\alpha_{01}^2}{c} + 2\right)\Delta t \sum_{l=0}^{k}\left\|e^l\right\|^2 + 2(k+1)\,|\Omega|\, m_2^2\left(h_1^2 + h_2^2 + \Delta t^2\right)^2 \Delta t. \tag{2.4.16}$$

Gronwall inequality leads to

$$\left\|e^{k+1}\right\|^2 \leq \frac{|\Omega|}{2\alpha_{23}} \exp\left[\left(\frac{\alpha_{01}^2}{c}+2\right)(k+1)\Delta t\right] |\Omega| \, m_2^2 \left(h_1^2+h_2^2+\Delta t^2\right)^2. \qquad (2.4.17)$$

For estimating $\left\|\Delta e^{k+1}\right\|$, we take inner product of (2.4.10) with $\delta_t e^{k+\frac{1}{2}} = \dfrac{e^{k+1}-e^k}{\Delta t}$. With the help of Lemma 2.3, we have

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

The last term of above formula satisfies

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

Therefore,

$$\begin{aligned}
&\frac{1}{2}\left\|\frac{e^{k+1}-e^k}{\Delta t}\right\|^2 + \frac{c}{2\Delta t}\left(\left\|\triangle_h e^{k+1}\right\|^2 - \left\|\triangle_h e^k\right\|^2\right) \\
&\quad \leq \left\langle \mu_0\left(\bar{n}^{k+\frac{1}{2}}\right) - \mu_0\left(n^{k+\frac{1}{2}}\right), \delta_t \triangle_h e^{k+\frac{1}{2}} \right\rangle + \frac{|\Omega|}{2} m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2. \qquad (2.4.18)
\end{aligned}$$

Replacing the superscript k by l in (2.4.18) and summing up for l from 0 to k and using Lemma 2.7, we can obtain

$$\begin{aligned}
&\frac{1}{2}\sum_{l=0}^{k}\left\|\frac{e^{l+1}-e^l}{\Delta t}\right\|^2 + \frac{c}{2\Delta t}\sum_{l=0}^{k}\left(\left\|\triangle_h e^{l+1}\right\|^2 - \left\|\triangle_h e^l\right\|^2\right) \\
&\quad \leq \sum_{l=0}^{k}\left\langle \mu_0\left(\bar{n}^{l+\frac{1}{2}}\right) - \mu_0\left(n^{l+\frac{1}{2}}\right), \delta_t \Delta_h e^{l+\frac{1}{2}} \right\rangle + \frac{|\Omega|}{2}(k+1) m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2
\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{\Delta t}\left\langle \mu_0\left(\bar{n}^{k+\frac{1}{2}}\right) - \mu_0\left(n^{k+\frac{1}{2}}\right), \Delta_h e^{k+1}\right\rangle - \frac{1}{\Delta t}\left\langle \mu_0\left(\bar{n}^{\frac{1}{2}}\right) - \mu_0\left(n^{\frac{1}{2}}\right), \Delta_h e^{0}\right\rangle \\
&\quad + \sum_{l=1}^{k}\left\langle \delta_t\left[\mu_0\left(\bar{n}^{l+\frac{1}{2}}\right) - \mu_0\left(n^{l+\frac{1}{2}}\right)\right], \Delta_h e^{l}\right\rangle + \frac{|\Omega|}{2}(k+1)m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2 \\
&= \frac{1}{\Delta t}\left\langle \mu_0\left(\bar{n}^{k+\frac{1}{2}}\right) - \mu_0\left(n^{k+\frac{1}{2}}\right), \Delta_h e^{k+1}\right\rangle + \frac{|\Omega|}{2}(k+1)m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2 \\
&\quad + \sum_{l=1}^{k}\left\langle \delta_t\left[\mu_0\left(\bar{n}^{l+\frac{1}{2}}\right) - \mu_0\left(n^{l+\frac{1}{2}}\right)\right], \Delta_h e^{l}\right\rangle \\
&= \frac{1}{\Delta t}\left\langle \mu_0'\left(\xi_1^{k+\frac{1}{2}}\right) e^{k+\frac{1}{2}}, \Delta_h e^{k+1}\right\rangle - \sum_{l=1}^{k}\left\langle \delta_t\left[\mu_0\left(\bar{n}^{l+\frac{1}{2}}\right) - \mu_0\left(n^{l+\frac{1}{2}}\right)\right], \Delta_h e^{l}\right\rangle \\
&\quad + \frac{|\Omega|}{2}(k+1)m_2^2\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}}, \Delta_h e^{k+1}\right\rangle + \frac{|\Omega|}{2}(k+1)m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2 \\
&\quad - \sum_{l=1}^{k}\left\langle \mu_0''\left(\xi_2^{l+\frac{1}{2}}\right)\left(\rho^{l+\frac{1}{2}}\left(\bar{n}^{l+1}-n^{l+1}\right) + (1-\rho^{l+\frac{1}{2}})\left(\bar{n}^{l}-n^{l}\right)\right)\delta_t \bar{n}^{l+\frac{1}{2}}, \Delta_h e^{l}\right\rangle \\
&\quad + \sum_{l=1}^{k}\left\langle \mu_0'\left(\rho^{l+\frac{1}{2}}n^{l+1} + (1-\rho^{k+\frac{1}{2}})n^{l}\right)\delta_t\left(\bar{n}^{l+\frac{1}{2}} - n^{l+\frac{1}{2}}\right), \Delta_h e^{l}\right\rangle \\
&\le \frac{\alpha_{01}}{\Delta t}\left\|e^{k+\frac{1}{2}}\right\|\left\|\Delta_h e^{k+1}\right\| + \frac{|\Omega|}{2}(k+1)m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2 \\
&\quad + \alpha_{02}\alpha_{24}\sum_{l=1}^{k}\left(\left\|e^{l+1}\right\| + \left\|e^{l}\right\|\right)\left\|\Delta_h e^{l}\right\| + \alpha_{01}\sum_{l=1}^{k}\left\|\frac{e^{l+1}-e^{l}}{\Delta t}\right\|\left\|\Delta_h e^{l}\right\| \\
&\le \frac{c}{4\Delta t}\left\|\Delta_h e^{k+1}\right\|^2 + \frac{\alpha_{01}^2}{2c\Delta t}\left(\left\|e^{k+1}\right\|^2 + \left\|e^{k}\right\|^2\right) + \frac{|\Omega|}{2}(k+1)m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2 \\
&\quad + \sum_{l=1}^{k}\left(\frac{\alpha_{02}^2\alpha_{24}^2}{2}\left\|e^{l+1}\right\|^2 + \frac{\alpha_{02}^2\alpha_{24}^2}{2}\left\|e^{l}\right\|^2 + \left\|\Delta_h e^{l}\right\|^2\right) \\
&\quad + \sum_{l=1}^{k}\left(\frac{1}{2}\left\|\frac{e^{l+1}-e^{l}}{\Delta t}\right\|^2 + \frac{\alpha_{01}^2}{2}\left\|\Delta_h e^{l}\right\|\right)
\end{aligned}
$$

Spontaneously,

$$\begin{aligned}\frac{c}{4\Delta t}\left\|\Delta_h e^{k+1}\right\|^2 \leq & \frac{\alpha_{01}^2}{2c\Delta t}\left(\left\|e^{k+1}\right\|^2+\left\|e^k\right\|^2\right)+\frac{|\Omega|}{2}(k+1)m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2 \\ & +\sum_{l=1}^{k}\left(\frac{\alpha_{02}^2\alpha_{24}^2}{2}\left\|e^{l+1}\right\|^2+\frac{\alpha_{02}^2\alpha_{24}^2}{2}\left\|e^l\right\|^2+\left\|\Delta_h e^l\right\|^2\right)+\frac{\alpha_{01}^2}{2}\sum_{l=1}^{k}\left\|\Delta_h e^l\right\|^2.\end{aligned}$$

It naturally gives

$$\begin{aligned}\left\|\Delta_h e^{k+1}\right\|^2 \leq & \frac{2\alpha_{01}^2}{c^2}\left(\left\|e^{k+1}\right\|^2+\left\|e^k\right\|^2\right)+\frac{2|\Omega|}{c}(k+1)m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2\Delta t \\ & +\sum_{l=1}^{k}\left(\frac{2\alpha_{02}^2\alpha_{24}^2}{c}\left\|e^{l+1}\right\|^2+\frac{2\alpha_{02}^2\alpha_{24}^2}{c}\left\|e^l\right\|^2\right)\Delta t \\ & +\left(\frac{4}{c}+\frac{2\alpha_{01}^2}{c}\right)\sum_{l=1}^{k}\left\|\Delta_h e^l\right\|^2\Delta t. \qquad (2.4.19)\end{aligned}$$

The inequality (2.4.16) provides

$$\left\|e^k\right\|^2 \leq \left(\frac{\alpha_{01}^2}{c}+2\right)\Delta t\sum_{l=0}^{k-1}\left\|e^l\right\|^2+2k|\Omega|m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2\Delta t. \qquad (2.4.20)$$

Combining (2.4.16), (2.4.20) and (2.3.21), we can obtain

$$\begin{aligned}&\left\|\Delta_h e^{k+1}\right\|^2+\left\|e^{k+1}\right\|^2 \\ &\leq \left(1+\frac{2\alpha_{01}^2}{c^2}+\frac{2\alpha_{02}^2\alpha_{24}^2}{c}\right)\left\|e^{k+1}\right\|^2+\frac{2\alpha_{01}^2}{c^2}\left\|e^k\right\|^2+\frac{4\alpha_{02}^2\alpha_{24}^2}{c}\Delta t\sum_{l=1}^{k}\left\|e^l\right\|^2 \\ &\quad +\frac{2|\Omega|}{c}(k+1)m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2\Delta t+\left(\frac{4}{c}+\frac{2\alpha_{01}^2}{c}\right)\sum_{l=1}^{k}\left\|\Delta_h e^l\right\|^2\Delta t \\ &\leq \left(1+\frac{2\alpha_{01}^2}{c^2}+\frac{2\alpha_{02}^2\alpha_{24}^2}{c}\right)\Bigg[\left(\frac{\alpha_{01}^2}{c}+2\right)\Delta t\sum_{l=0}^{k}\left\|e^l\right\|^2 \\ &\quad +2(k+1)|\Omega|m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2\Delta t\Bigg]\end{aligned}$$

$$
\begin{aligned}
&+\frac{2\alpha_{01}^2}{c^2}\left[\left(\frac{\alpha_{01}^2}{c}+2\right)\Delta t\sum_{l=0}^{k-1}\left\|e^l\right\|^2+2k\left|\Omega\right|m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2\Delta t\right]\\
&+\frac{4\alpha_{02}^2\alpha_{24}^2}{c}\Delta t\sum_{l=1}^{k}\left\|e^l\right\|^2+\left(\frac{4}{c}+\frac{2\alpha_{01}^2}{c}\right)\sum_{l=1}^{k}\left\|\Delta_h e^l\right\|^2\Delta t\\
&+\frac{2\left|\Omega\right|}{c}(k+1)m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2\Delta t\\
\leq&\frac{\alpha_{01}^2+4c}{c}\left(1+\frac{4\alpha_{01}^2}{c^2}+\frac{2\alpha_{02}^2\alpha_{24}^2}{c}\right)\Delta t\sum_{l=0}^{k}\left\|e^l\right\|^2+\frac{4+2\alpha_{01}^2}{c}\sum_{l=1}^{k}\left\|\Delta_h e^l\right\|^2\Delta t\\
&+\left(2+\frac{8\alpha_{01}^2}{c^2}+\frac{4\alpha_{02}^2\alpha_{24}^2}{c}+\frac{2}{c}\right)(k+1)\left|\Omega\right|m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2\Delta t\\
\leq&\max\left\{1+\frac{4\alpha_{01}^2}{c^2}+\frac{2\alpha_{02}^2\alpha_{24}^2}{c},\frac{4}{c}+\frac{2\alpha_{01}^2}{c}\right\}\Delta t\sum_{l=0}^{k}\left(\left\|e^l\right\|^2+\left\|\Delta_h e^l\right\|^2\right)\\
&+\left(2+\frac{8\alpha_{01}^2}{c^2}+\frac{4\alpha_{02}^2\alpha_{24}^2}{c}+\frac{2}{c}\right)(k+1)\left|\Omega\right|m_2^2\left(h_1^2+h_2^2+\Delta t^2\right)^2\Delta t\\
\leq&\alpha_{29}\Delta t\sum_{l=1}^{k}\left(\left\|e^l\right\|^2+\left\|\Delta_h e^l\right\|^2\right)+(k+1)\alpha_{28}\left|\Omega\right|m_2^2(h_1^2+h_2^2+\Delta t^2)^2\Delta t.
\end{aligned}
$$

Gronwall inequality yields

$$
\left\|e^{k+1}\right\|^2+\left\|\Delta_h e^{k+1}\right\|^2\leq\frac{\alpha_{28}}{\alpha_{29}}\exp\left(\alpha_{29}(k+1)\Delta t\right)\cdot\left|\Omega\right|\left[m_2\left(h_1^2+h_2^2+\triangle t^2\right)\right]^2,
$$

where $k=0,1,...,K-1$. Using Lemma 2.4 and (2.4.14), we can get

$$
\begin{aligned}
\left\|e^{k+1}\right\|_\infty^2\leq&k_0\left\|e^{k+1}\right\|\left(\left\|\triangle_h e^{k+1}\right\|+\left\|e^{k+1}\right\|\right)\\
\leq&k_0\sqrt{2\left\|e^{k+1}\right\|^2\left(\left\|e^{k+1}\right\|^2+\left\|\triangle_h e^{k+1}\right\|^2\right)}\\
\leq&k_0\sqrt{\frac{\alpha_{28}}{2\alpha_{23}\alpha_{29}}}\exp\left(\left(2\alpha_{23}+\frac{\alpha_{29}}{2}\right)(k+1)\Delta t\right)m_2^2\left|\Omega\right|\left(h_1^2+h_2^2+\triangle t^2\right)^2.
\end{aligned}
$$

Therefore,

$$
\left\|e^{k+1}\right\|_\infty\leq\sqrt[4]{\frac{\alpha_{28}}{2\alpha_{23}\alpha_{29}}k_0^2\left|\Omega\right|^2}\exp\left(\left(\alpha_{23}+\frac{\alpha_{29}}{4}\right)(k+1)\Delta t\right)m_2\left(h_1^2+h_2^2+\triangle t^2\right)
$$

$$\leq C_{22}\left(h_1^2+h_2^2+\triangle t^2\right).$$

Using Lemma 2.4 and (2.4.17), we can obtain

$$\begin{aligned}\left\|e^{k+1}\right\|_\infty^2 \leq & k_0\left\|e^{k+1}\right\|\left(\left\|\triangle_h e^{k+1}\right\|+\left\|e^{k+1}\right\|\right)\\ \leq & k_0\sqrt{2\left\|e^{k+1}\right\|^2\left(\left\|e^{k+1}\right\|^2+\left\|\triangle_h e^{k+1}\right\|^2\right)}\\ \leq & k_0\sqrt{\frac{\alpha_{28}}{2\alpha_{23}\alpha_{29}}}\exp\left(\left(2\alpha_{23}+\frac{\alpha_{29}}{2}\right)(k+1)\Delta t\right)m_2^2\left|\Omega\right|\left(h_1^2+h_2^2+\triangle t^2\right)^2.\end{aligned}$$

Therefore,

$$\begin{aligned}\left\|e^{k+1}\right\|_\infty \leq & \sqrt[4]{\frac{\alpha_{28}}{2\alpha_{23}\alpha_{29}}k_0^2\left|\Omega\right|^2}\exp\left(\left(\alpha_{23}+\frac{\alpha_{29}}{4}\right)(k+1)\Delta t\right)m_2\left(h_1^2+h_2^2+\triangle t^2\right)\\ \leq & C_{22}\left(h_1^2+h_2^2+\triangle t^2\right).\end{aligned}$$

This completes the proof. □

2.5 A second order linearization scheme for the fourth-order parabolic equation

In this section, we also use $\bar{n}_{ij}^k$ to denote the exact discrete solution of the proposed scheme. As an element in the function space $\mathcal{W}_\tau$, $\hat{\bar{n}}_{ij}^{k+\frac{1}{2}}$ is also defined by (2.2.2). Applying Taylor expansion to (2.1.4a), (2.1.5), we have

$$\frac{\bar{n}_{ij}^{k+1}-\bar{n}_{ij}^k}{\triangle t}+c\triangle_h^2\bar{n}_{ij}^{k+\frac{1}{2}}-\triangle_h\mu_0\left(\hat{\bar{n}}_{ij}^{k+\frac{1}{2}}\right)=\hat{R}_{ij}^{k+\frac{1}{2}}, \tag{2.5.1a}$$

$$1\leq i\leq M_1,\quad 1\leq j\leq M_2,\quad 0\leq k\leq K-1,$$

$$\frac{(\bar{f}_0)_{ij}^{k+1}-(\bar{f}_0)_{ij}^k}{\triangle t}=\mu_0\left(\hat{\bar{n}}^{k+\frac{1}{2}}\right)\frac{\bar{n}_{ij}^{k+1}-\bar{n}_{ij}^k}{\triangle t}+\hat{S}_{ij}^{k+\frac{1}{2}}, \tag{2.5.1b}$$

$$1\leq i\leq M_1,\quad 1\leq j\leq M_2,\quad 0\leq k\leq K-1,$$

with following initial conditions

$$\bar{n}_{ij}^0=n_0(\mathbf{x}_{ij}),\quad 1\leq i\leq M_1,\quad 1\leq j\leq M_2, \tag{2.5.2a}$$

$$(\bar{f}_0)_{ij}^0 = \bar{f}_0(n(\mathbf{x}_{ij})), \quad 1 \le i \le M_1, \quad 1 \le j \le M_2, \tag{2.5.2b}$$

where there exists a constant m_3 such that

$$\begin{aligned} \left|\hat{R}_{ij}^{k+\frac{1}{2}}\right| \le & m_3 \left(h_1^2 + h_2^2 + \triangle t^2\right), \\ & 1 \le i \le M_1, \quad 1 \le j \le M_2, \quad 0 \le k \le K-1, \end{aligned} \tag{2.5.3a}$$

$$\begin{aligned} \left|\hat{S}_{ij}^{k+\frac{1}{2}}\right| \le & m_3 \left(h_1^2 + h_2^2 + \triangle t^2\right), \\ & 1 \le i \le M_1, \quad 1 \le j \le M_2, \quad 0 \le k \le K-1. \end{aligned} \tag{2.5.3b}$$

The difference scheme is constructed by omitting the small terms in the above two equations as follows,

$$\begin{aligned} & \frac{n_{ij}^{k+1} - n_{ij}^k}{\triangle t} + c\triangle_h^2 n_{ij}^{k+\frac{1}{2}} - \triangle_h \mu_0 \left(\hat{n}_{ij}^{k+\frac{1}{2}}\right) = 0, \\ & \qquad 1 \le i \le M_1, \quad 1 \le j \le M_2, \quad 0 \le k \le K-1, \end{aligned} \tag{2.5.4a}$$

subject to the initial condition

$$n_{ij}^0 = n_0(\mathbf{x}_{ij}), \quad 1 \le i \le M_1, \quad 1 \le j \le M_2. \tag{2.5.4b}$$

The discrete energy density $(f_0)_{ij}^{k+1}$ is computed by

$$\begin{aligned} & \frac{(f_0)_{ij}^{k+1} - (f_0)_{ij}^k}{\triangle t} = \mu_0 \left(\hat{n}_{ij}^{k+\frac{1}{2}}\right) \frac{n_{ij}^{k+1} - n_{ij}^k}{\triangle t}, \\ & \qquad 1 \le i \le M_1, \quad 1 \le j \le M_2, \quad 0 \le k \le K-1, \end{aligned} \tag{2.5.5a}$$

with initial value

$$(f_0)_{ij}^0 = f_0(n_0(\mathbf{x}_{ij})), \quad 1 \le i \le M_1, \quad 1 \le j \le M_2. \tag{2.5.5b}$$

2.5.1 Mass conservation and energy stability

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

Lemma 2.13. *The solution of the discrete equation (2.5.4a)-(2.5.4b) satisfies the mass conservation if periodic boundary condition is given, which means that for any* $0 \le k \le K-1$,

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

Lemma 2.14. *If the discrete total energy at* $k\Delta t$, $k = 0, 1, ...K$, *is defined as (2.3.7), then the discrete scheme provided by (2.5.4a)-(2.5.5a) can guarantee the following energy identity for any time step* $\Delta t > 0$ *as follows,*

$$\frac{F_h^{k+1} - F_h^k}{\triangle t} + \left\| -\nabla \hat{w}^{k+\frac{1}{2}} \right\|^2 = 0, \tag{2.5.6}$$

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

2.5.2 The unique solvability and convergence

Theorem 2.8. *The linearization scheme (2.5.4a)-(2.5.4b) is uniquely solvable.*

Proof. The scheme (2.5.4a) can be written as

$$\begin{gathered} n_{ij}^{k+1} + \frac{c\triangle t}{2} \triangle_h^2 n_{ij}^{k+1} = n_{ij}^k - \frac{c\triangle t}{2} \triangle_h^2 n_{ij}^k + \Delta t \triangle_h \mu_0 \left(\hat{n}_{ij}^{k+\frac{1}{2}} \right), \\ 1 \le i \le M_1, \quad 1 \le j \le M_2, \quad 0 \le k \le K-1. \end{gathered} \tag{2.5.7}$$

Suppose n^k, $\hat{n}^{k+\frac{1}{2}}$ have been determined. Then (2.5.7) is a linear equation about n^{k+1}. Consider its homogenous system as follows,

$$n_{ij}^{k+1} + \frac{c\triangle t}{2} \triangle_h^2 n_{ij}^{k+1} = 0, \quad 1 \le i \le M_1, \quad 1 \le j \le M_2. \tag{2.5.8}$$

Taking inner product of (2.5.8) with n^{k+1}, we have

$$\left\|n^{k+1}\right\|^2 + \frac{c\triangle t}{2}\left\|\triangle_h n^{k+1}\right\|^2 = 0. \tag{2.5.9}$$

It requires $n^{k+1} = 0$. Therefore (2.5.7) has a unique solution. This completes the proof. □

We also provide a lemma which is similar to Lemma 2.8 as an auxiliary to derive the convergence of the linearization scheme.

Lemma 2.15. *Denote* $e^k_{ij} = \bar{n}^k_{ij} - n^k_{ij}$, $\hat{n} = (\hat{n}^{\frac{1}{2}}, \hat{n}^{\frac{3}{2}}, ..., \hat{n}^{K-\frac{1}{2}})$, $\hat{\hat{n}} = (\hat{\hat{n}}^{\frac{1}{2}}, \hat{\hat{n}}^{\frac{3}{2}}, ..., \hat{\hat{n}}^{K-\frac{1}{2}})$. *For* $\hat{n},\ \hat{\hat{n}} \in \mathcal{V}_h$, *there exists* $\hat{\rho}^l \in (0,1)$ *and* $\gamma_1 = \hat{\rho}^l\hat{n}^{l+\frac{1}{2}} + (1-\hat{\rho}^l)\hat{n}^{l-\frac{1}{2}}$, $\gamma_2 = \hat{\rho}^l\hat{\hat{n}}^{l+\frac{1}{2}} + (1-\hat{\rho}^l)\hat{\hat{n}}^{l-\frac{1}{2}}$, $\hat{\xi}^l \in (\min\{\gamma_1,\gamma_2\}, \max\{\gamma_1,\gamma_2\})$, $k,\ l = 0,1,2,...,K-1$, *such that*

$$\begin{aligned}
&\frac{1}{\Delta t}\left[\mu_0(\hat{\hat{n}}^{l+\frac{1}{2}}) - \mu_0(\hat{n}^{l+\frac{1}{2}}) - \left(\mu_0(\hat{\hat{n}}^{l-\frac{1}{2}}) - \mu_0(\hat{n}^{l-\frac{1}{2}})\right)\right] \\
&= \mu_0'(\hat{\rho}^l\hat{n}^{l+\frac{1}{2}} + (1-\hat{\rho}^l)\hat{n}^{l-\frac{1}{2}})\frac{\hat{e}^{l+\frac{1}{2}} - \hat{e}^{l-\frac{1}{2}}}{\Delta t} \\
&\quad + \mu_0''(\xi^l)\left(\hat{\rho}^l\hat{e}^{l+\frac{1}{2}} + (1-\hat{\rho}^l)\hat{e}^{l-\frac{1}{2}}\right)\frac{\hat{\hat{n}}^{l+\frac{1}{2}} - \hat{\hat{n}}^{l-\frac{1}{2}}}{\Delta t}.
\end{aligned}$$

Proof.

$$\begin{aligned}
&\frac{1}{\Delta t}\left[\mu_0(\hat{\hat{n}}^{l+\frac{1}{2}}) - \mu_0(\hat{n}^{l+\frac{1}{2}}) - \left(\mu_0(\hat{\hat{n}}^{l-\frac{1}{2}}) - \mu_0(\hat{n}^{l-\frac{1}{2}})\right)\right] \\
&= \mu_0'\left(\rho^l\hat{\hat{n}}^{l+\frac{1}{2}} + (1-\rho^l)\hat{\hat{n}}^{l-\frac{1}{2}}\right)\frac{\hat{\hat{n}}^{l+\frac{1}{2}} - \hat{\hat{n}}^{l-\frac{1}{2}}}{\Delta t} \\
&\quad - \mu_0'\left(\rho^l\hat{n}^{l+\frac{1}{2}} + (1-\rho^l)\hat{n}^{l-\frac{1}{2}}\right)\frac{\hat{n}^{l+\frac{1}{2}} - \hat{n}^{l-\frac{1}{2}}}{\Delta t} \\
&= \left[\mu_0'\left(\rho^l\hat{\hat{n}}^{l+\frac{1}{2}} + (1-\rho^l)\hat{\hat{n}}^{l-\frac{1}{2}}\right) - \mu_0'\left(\rho^l\hat{n}^{l+\frac{1}{2}} + (1-\rho^l)\hat{n}^{l-\frac{1}{2}}\right)\right]\frac{\hat{\hat{n}}^{l+\frac{1}{2}} - \hat{\hat{n}}^{l-\frac{1}{2}}}{\Delta t} \\
&\quad + \mu_0'\left(\rho^l\hat{n}^{l+\frac{1}{2}} + (1-\rho^l)\hat{n}^{l-\frac{1}{2}}\right)\left[\frac{\hat{\hat{n}}^{l+\frac{1}{2}} - \hat{\hat{n}}^{l-\frac{1}{2}}}{\Delta t} - \frac{\hat{n}^{l+\frac{1}{2}} - \hat{n}^{l-\frac{1}{2}}}{\Delta t}\right] \\
&= \mu_0'(\hat{\rho}^l\hat{n}^{l+\frac{1}{2}} + (1-\hat{\rho}^l)\hat{n}^{l-\frac{1}{2}})\frac{\hat{e}^{l+\frac{1}{2}} - \hat{e}^{l-\frac{1}{2}}}{\Delta t}
\end{aligned}$$

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

This completes the proof. $\square$

Let

$$\hat{c}_1=\max\left\{|\mu_0'(n)|:\ n\in\left[\frac{\hat{\theta}}{2},\frac{1}{b}-\frac{\hat{\theta}}{2}\right]\right\},\quad \hat{c}_2=\max\left\{|\mu_0''(n)|:\ n\in\left[\frac{\hat{\theta}}{2},\frac{1}{b}-\frac{\hat{\theta}}{2}\right]\right\},$$

$$\hat{c}_3=\frac{9\hat{c}_1^2}{4c}+1,\quad \hat{c}_4=\max\left\{\left|\frac{\bar{n}^{k+1}-\bar{n}^k}{\Delta t}\right|,k=0,1,...K-1.\right\},\quad \hat{c}_8=\frac{12\hat{c}_1^2+1}{c}+1,$$

$$\hat{c}_7=\max\left\{\frac{13\hat{c}_3^2}{4},2\hat{c}_1^2+4\right\},\quad \hat{c}_9=\max\left\{\hat{c}_3+\frac{12\hat{c}_3\hat{c}_1^2}{c^2}+\frac{5\hat{c}_2^2\hat{c}_4^2}{c},\frac{2\hat{c}_7}{c}\right\},$$

$$\tilde{c}=\exp\left(\hat{c}_3T_m\right)\sqrt{\frac{|\Omega|}{\hat{c}_3}}m_3,\quad \hat{c}=\sqrt[4]{\frac{2\hat{c}_8}{\hat{c}_3\hat{c}_9}k_0^2\left|\Omega\right|^2}\exp\left(\left(\frac{\hat{c}_3+\hat{c}_9}{2}\right)T_m\right)m_3.$$

Theorem 2.9. *Suppose the solution $\bar{n}(\mathbf{x},t)$ to the fourth order equation (2.1.4a)-(2.1.4b) is sufficiently smooth, and there is a $\hat{\theta}\in(0,1)$, such that $\bar{n}_{ij}^k\in[\hat{\theta},\frac{1}{b}-\hat{\theta}]$ for all $1\le i\le M_1$, $1\le j\le M_2$, $k=0,1,..K$. If*

$$\hat{c}(h_1^2+h_2^2+\Delta t^2)\le\frac{\hat{\theta}}{2},\tag{2.5.10}$$

then the difference scheme (2.5.4a)-(2.5.4b) is convergent with second order in both time and space in the following detailed form

$$\left\|e^{k+1}\right\|\le\tilde{c}\left(h_1^2+h_2^2+\triangle t^2\right),\quad \left\|e^{k+1}\right\|_\infty\le\hat{c}\left(h_1^2+h_2^2+\triangle t^2\right).\tag{2.5.11}$$

Proof. Since

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

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

we have

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

Subtracting (2.5.4a) from (2.5.1a), we have

$$\begin{aligned} &\frac{e_{ij}^{k+1}-e_{ij}^{k}}{\triangle t}+c\left(\triangle_h^2 e_{ij}^{k+\frac{1}{2}}\right)=\hat{R}_{ij}^{k+\frac{1}{2}}, \\ &\qquad 1\le i\le M_1, \quad 1\le j\le M_2, \quad k=0,1. \end{aligned} \tag{2.5.12}$$

$$\begin{aligned} &\frac{e_{ij}^{k+1}-e_{ij}^{k}}{\triangle t}+\left[c\left(\triangle_h^2 e^{k+\frac{1}{2}}\right)_{ij}-\triangle_h\mu_0\left(\hat{\hat{n}}_{ij}^{k+\frac{1}{2}}\right)+\triangle_h\mu_0\left(\hat{n}_{ij}^{k+\frac{1}{2}}\right)\right]=\hat{R}_{ij}^{k+\frac{1}{2}}, \\ &\qquad 1\le i\le M_1, \quad 1\le j\le M_2, \quad 2\le k\le K-1. \end{aligned} \tag{2.5.13}$$

$$e_{ij}^0=0, \qquad 1\le i\le M_1, \quad 1\le j\le M_2. \tag{2.5.14}$$

For the first step, taking inner product of (2.5.12) at $k=0$ with $e^{\frac{1}{2}}=\dfrac{e^0+e^1}{2}$ yields

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

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

$$\frac{\|e^1\|^2}{2\triangle t}+c\left\|\triangle_h\frac{e^1}{2}\right\|^2=\left\langle \hat{R}^{\frac{1}{2}},\frac{e^1}{2}\right\rangle, \quad 1\le i\le M_1, \quad 1\le j\le M_2. \tag{2.5.15}$$

Using (2.5.3a), we can get

$$\frac{\|e^1\|^2}{2\triangle t}+\frac{c}{4}\left\|\triangle_h e^1\right\|^2\le\frac{\|e^1\|^2}{4\triangle t}+\frac{\triangle t\,|\Omega|\,c_2^2\left(h_1^2+h_2^2+\triangle t^2\right)^2}{4}, \tag{2.5.16}$$

which gives

$$\frac{\|e^1\|^2}{2\triangle t}\le\frac{\|e^1\|^2}{4\triangle t}+\frac{|\Omega|\,\triangle t m_3^2\left(h_1^2+h_2^2+\triangle t^2\right)^2}{4}, \tag{2.5.17a}$$

$$\frac{\|e^1\|^2}{4\triangle t}\le\frac{|\Omega|\,m_3^2\triangle t\left(h_1^2+h_2^2+\triangle t^2\right)^2}{4}. \tag{2.5.17b}$$

$$\frac{\|e^1\|^2}{2\triangle t} \leq \frac{|\Omega|\, m_3^2 \triangle t \left(h_1^2 + h_2^2 + \triangle t^2\right)^2}{2}. \tag{2.5.17c}$$

$$\left\|e^1\right\|^2 \leq |\Omega|\, m_3^2 \triangle t^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2, \tag{2.5.17d}$$

$$\left\|e^1\right\| \leq \sqrt{|\Omega|} m_3 \triangle t \left(h_1^2 + h_2^2 + \triangle t^2\right), \tag{2.5.17e}$$

and

$$\frac{c}{4} \left\|\triangle_h e^1\right\|^2 \leq \frac{|\Omega| \triangle t m_3^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2}{4}. \tag{2.5.18}$$

From (2.5.18),

$$\frac{c}{4} \left\|\triangle_h e^1\right\|^2 \leq \frac{|\Omega| \triangle t m_3^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2}{4}, \tag{2.5.19a}$$

$$\frac{c}{2\Delta t} \left\|\triangle_h e^1\right\|^2 \leq \frac{|\Omega|\, m_3^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2}{2}, \tag{2.5.19b}$$

$$\left\|\triangle_h e^1\right\| \leq \sqrt{\frac{|\Omega| \triangle t}{c}} m_3 \left(h_1^2 + h_2^2 + \triangle t^2\right). \tag{2.5.19c}$$

According to Lemma 2.4,

$$\left\|e^1\right\|_\infty^2 \tag{2.5.20}$$

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

$$\leq k_0 \left[\sqrt{\frac{\triangle t}{c}} \hat{c}_2^2 \,|\Omega| \triangle t \left(h_1^2 + h_2^2 + \triangle t^2\right)^2 + |\Omega|\, m_3^2 \triangle t^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2\right]. \tag{2.5.21}$$

If $\Delta t < \dfrac{1}{c}$, then

$$\left\|e^1\right\|_\infty^2 \leq \frac{2\,|\Omega|\, k_0 \triangle t}{c} \hat{c}_2^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2. \tag{2.5.22}$$

Besides, from (2.5.15) we can also obtain

$$\frac{\|e^1\|^2}{2\triangle t} + \frac{c}{4} \left\|\triangle_h e^1\right\|^2 \leq \frac{\|e^1\|^2}{4} + \frac{|\Omega|\, m_3^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2}{4}. \tag{2.5.23}$$

Therefore,

$$\frac{\|e^1\|^2}{2\triangle t} \le \frac{\|e^1\|^2}{4} + \frac{|\Omega|\, m_3^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2}{4}. \tag{2.5.24}$$

Secondly, to get the error at second time step $\|e^2\|_\infty$, we take the inner product of (2.5.12) when $k = 1$ with $e^{\frac{3}{2}} = \dfrac{e^1 + e^2}{2}$,

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

Applying (2.5.3a), we have

$$\frac{\|e^2\|^2 - \|e^1\|^2}{2\triangle t} + c\left\|\triangle_h\left(\frac{e^1+e^2}{2}\right)\right\|^2 \le \frac{\|e^1\|^2 + \|e^2\|^2}{4\triangle t} + \frac{|\Omega|\,\triangle t}{2} m_3^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2.$$

$$\frac{\|e^2\|^2 - \|e^1\|^2}{2\triangle t} \le \frac{\|e^1\|^2 + \|e^2\|^2}{4} + \frac{|\Omega|}{2} m_3^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2, \tag{2.5.25}$$

or

$$\frac{\|e^2\|^2 - \|e^1\|^2}{2\triangle t} \le \frac{\|e^1\|^2 + \|e^2\|^2}{4\triangle t} + \frac{|\Omega|\,\triangle t}{2} m_3^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2. \tag{2.5.26}$$

From (2.5.26) and the estimation of $\left\|e^1\right\|^2$ by (2.5.17e), we can get

$$\frac{\|e^2\|^2}{4\triangle t} \le \frac{|\Omega|\,\triangle t}{2} m_3^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2 + \frac{3\,\|e^1\|^2}{4\triangle t}.$$

$$\frac{\|e^2\|^2}{4\triangle t} \le \frac{5}{4}\,|\Omega|\, m_3^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2, \tag{2.5.27a}$$

$$\left\|e^2\right\|^2 \le 5\,|\Omega|\, m_3^2 \triangle t^2 \left(h_1^2 + h_2^2 + \triangle t^2\right)^2, \tag{2.5.27b}$$

$$\left\|e^2\right\| \le \sqrt{5\,|\Omega|}\, m_3 \triangle t \left(h_1^2 + h_2^2 + \triangle t^2\right). \tag{2.5.27c}$$

To get the estimation of $\left\|\Delta e^2\right\|$, taking the inner product of (2.5.12) when $k = 1$ with $\dfrac{e^2 - e^1}{\Delta t}$, we have

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

$$= \left\langle \hat{R}^{\frac{3}{2}}, \frac{e^2 - e^1}{\Delta t} \right\rangle \leq \left\| \frac{e^2 - e^1}{\triangle t} \right\|^2 + \frac{|\Omega|}{4} \hat{c}_2^2 \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2.$$

Accordingly,

$$\frac{c}{2\Delta t} \left(\left\| \triangle_h e^2 \right\|^2 - \left\| \triangle_h e^1 \right\|^2 \right) \leq \frac{|\Omega|}{4} \hat{c}_2^2 \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2, \tag{2.5.28}$$

$$\frac{c}{2\Delta t} \left\| \triangle_h e^2 \right\|^2 \leq \frac{c}{2\Delta t} \left\| \triangle_h e^1 \right\|^2 + \frac{|\Omega|}{4} \hat{c}_2^2 \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2, \tag{2.5.29}$$

$$\left\| \triangle_h e^2 \right\|^2 \leq \left\| \triangle_h e^1 \right\|^2 + \frac{|\Omega| \, \Delta t}{2c} \hat{c}_2^2 \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2.$$

Combining the above equation with (2.5.19c), we can get

$$\left\| \triangle_h e^2 \right\|^2 \leq \frac{3 \, |\Omega| \, \Delta t}{2c} \hat{c}_2^2 \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2.$$

Similar to the first case,

$$\begin{aligned} & \left\| e^2 \right\|_\infty^2 \\ & \leq k_0 \left(\left\| \triangle_h e^2 \right\| \left\| e^2 \right\| + \left\| e^2 \right\|^2 \right) \\ & \leq k_0 \left[\sqrt{\frac{3\triangle t}{2c}} \, |\Omega| \, \hat{c}_2^2 \triangle t \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2 + 5 \, |\Omega| \, m_3^2 \triangle t^2 \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2 \right]. \end{aligned} \tag{2.5.30}$$

If $\Delta t < \dfrac{1}{c}$, then

$$\left\| e^2 \right\|_\infty^2 \leq \frac{25 k_0 \, |\Omega| \, \triangle t}{4c} \hat{c}_2^2 \left(h_1^2 + h_2^2 + \triangle t^2 \right)^2. \tag{2.5.31}$$

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 (2.5.11) is true for l from 0 to k ($0 \leq k \leq K-1$). Then if (2.5.10) is satisfied, we have

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

Then it follows that

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

Taking inner product of (2.5.13) with $e^{k+\frac{1}{2}} = \dfrac{e^k + e^{k+1}}{2}$, we obtain

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

Because

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

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 $\hat{\xi}^{k+\frac{1}{2}} = \hat{\lambda}^{k+\frac{1}{2}}\hat{\bar{n}}^{k+\frac{1}{2}} + (1 - \hat{\lambda}^{k+\frac{1}{2}})\hat{n}^{k+\frac{1}{2}}$, $\hat{\lambda}^{k+\frac{1}{2}} \in [0, 1]$. Therefore, according to Lemma 2.3, we can get

$$\begin{aligned}
&\left\langle \triangle_h \mu_0\left(\hat{\bar{n}}^{k+\frac{1}{2}}\right) - \triangle_h \mu_0\left(\hat{n}^{k+\frac{1}{2}}\right), e^{k+\frac{1}{2}} \right\rangle \\
&= \left\langle \mu_0\left(\hat{\bar{n}}^{k+\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{k+\frac{1}{2}}\right), \triangle_h e^{k+\frac{1}{2}} \right\rangle \\
&\le \left\|\mu'(\hat{\xi}^{k+\frac{1}{2}})\left(e^k + \frac{1}{2}e^{k-1} - \frac{1}{2}e^{k-2}\right)\right\| \left\|\triangle_h e^{k+\frac{1}{2}}\right\| \\
&\le \hat{c}_1\left[\left\|e^k\right\| + \frac{1}{2}\left\|e^{k-1}\right\| + \frac{1}{2}\left\|e^{k-2}\right\|\right]\left\|\triangle_h e^{k+\frac{1}{2}}\right\|.
\end{aligned} \tag{2.5.32}$$

Whereupon

$$
\begin{aligned}
&\frac{\left\|e^{k+1}\right\|^2-\left\|e^k\right\|^2}{2\triangle t}+c\left\|\triangle_h\left(\frac{e^k+e^{k+1}}{2}\right)\right\|^2 \\
&\quad\le \hat{c}_1\left(\left\|e^k\right\|+\frac{1}{2}\left\|e^{k-1}\right\|+\frac{1}{2}\left\|e^{k-2}\right\|\right)\left\|\triangle_h\left(\frac{e^k+e^{k+1}}{2}\right)\right\|+\left\langle \hat{R}^{k+\frac{1}{2}},\frac{e^k+e^{k+1}}{2}\right\rangle \\
&\quad\le \frac{3\hat{c}_1^2}{4c}\left(\left\|e^k\right\|^2+\frac{1}{4}\left\|e^{k-1}\right\|^2+\frac{1}{4}\left\|e^{k-2}\right\|^2\right)+c\left\|\triangle_h\left(\frac{e^k+e^{k+1}}{2}\right)\right\|^2 \\
&\qquad+\frac{\left\|e^k\right\|^2+\left\|e^{k+1}\right\|^2}{4}+\frac{|\Omega|}{2}m_3^2\left(h_1^2+h_2^2+\triangle t^2\right)^2.
\end{aligned}
$$

Accordingly,

$$
\begin{aligned}
\frac{\left\|e^{k+1}\right\|^2-\left\|e^k\right\|^2}{2\triangle t}\le&\frac{3\hat{c}_1^2}{4c}\left(\left\|e^k\right\|^2+\frac{1}{4}\left\|e^{k-1}\right\|^2+\frac{1}{4}\left\|e^{k-2}\right\|^2\right) \\
&+\frac{\left\|e^k\right\|^2+\left\|e^{k+1}\right\|^2}{4}+\frac{|\Omega|}{2}m_3^2\left(h_1^2+h_2^2+\triangle t^2\right)^2.
\end{aligned}
\tag{2.5.33}
$$

Replacing the superscript k by l in (2.5.33) and summing up for l from 2 to k, we can get

$$
\begin{aligned}
&\sum_{l=2}^{k}\frac{\left\|e^{l+1}\right\|^2-\left\|e^l\right\|^2}{2\triangle t} \\
&\quad\le \frac{3\hat{c}_1^2}{4c}\sum_{l=2}^{k}\left(\left\|e^l\right\|^2+\frac{1}{4}\left\|e^{l-1}\right\|^2+\frac{1}{4}\left\|e^{l-2}\right\|^2\right)+\sum_{l=2}^{k}\frac{\left\|e^l\right\|^2+\left\|e^{l+1}\right\|^2}{4} \\
&\qquad+\frac{|\Omega|}{2}\sum_{l=2}^{k}m_3^2\left(h_1^2+h_2^2+\triangle t^2\right)^2 \\
&\quad=\frac{3\hat{c}_1^2}{4c}\left(\sum_{l=2}^{k}\left\|e^l\right\|^2+\frac{1}{4}\sum_{l=1}^{k-1}\left\|e^l\right\|^2+\frac{1}{4}\sum_{l=1}^{k-2}\left\|e^l\right\|^2\right)+\frac{\left(\sum_{l=2}^{k}\left\|e^l\right\|^2+\sum_{l=3}^{k+1}\left\|e^l\right\|^2\right)}{4} \\
&\qquad+\frac{|\Omega|}{2}\sum_{l=2}^{k}m_3^2\left(h_1^2+h_2^2+\triangle t^2\right)^2.
\end{aligned}
\tag{2.5.34}
$$

Combining (2.5.24), (2.5.25) with (2.5.34), we obtain

$$
\begin{aligned}
&\left(1-\frac{\Delta t}{2}\right)\left\|e^{k+1}\right\|^2 \\
&\leq \frac{3\hat{c}_1^2}{2c}\left(\sum_{l=2}^{k}\left\|e^l\right\|^2+\frac{1}{4}\sum_{l=1}^{k-1}\left\|e^l\right\|^2+\frac{1}{4}\sum_{l=1}^{k-2}\left\|e^l\right\|^2\right)\Delta t \\
&\quad+\frac{\Delta t}{2}\left(\sum_{l=2}^{k}\left\|e^l\right\|^2+\sum_{l=3}^{k}\left\|e^l\right\|^2\right)+|\Omega|\,\Delta t\sum_{l=2}^{k}m_3^2\left(h_1^2+h_2^2+\triangle t^2\right)^2 \\
&\quad+\frac{\left\|e^2\right\|^2+\left\|e^1\right\|^2}{2}\Delta t+|\Omega|\,\Delta t m_3^2\left(h_1^2+h_2^2+\triangle t^2\right)^2 \\
&\quad+\frac{\left\|e^1\right\|^2\Delta t}{2}+\frac{|\Omega|\,m_3^2\left(h_1^2+h_2^2+\triangle t^2\right)^2}{2}\Delta t \\
&\leq \frac{3\hat{c}_1^2}{2c}\cdot\frac{3}{2}\Delta t\sum_{l=1}^{k}\left\|e^l\right\|^2+\Delta t\sum_{l=1}^{k}\left\|e^l\right\|^2+(k+1)\,|\Omega|\,\Delta t m_3^2\left(h_1^2+h_2^2+\triangle t^2\right)^2 \\
&=\left(\frac{9\hat{c}_1^2}{4c}+1\right)\Delta t\sum_{l=1}^{k}\left\|e^l\right\|^2+(k+1)\,|\Omega|\,m_3^2\triangle t\left(h_1^2+h_2^2+\triangle t^2\right)^2 \\
&=\hat{c}_3\Delta t\sum_{l=1}^{k}\left\|e^l\right\|^2+(k+1)\,|\Omega|\,m_3^2\triangle t\left(h_1^2+h_2^2+\triangle t^2\right)^2.
\end{aligned}
$$

If $\Delta t<1$, then

$$
\left\|e^{k+1}\right\|^2\leq 2\hat{c}_3\Delta t\sum_{l=1}^{k}\left\|e^l\right\|^2+2(k+1)\,|\Omega|\,m_3^2\triangle t\left(h_1^2+h_2^2+\triangle t^2\right)^2. \tag{2.5.35}
$$

The Gronwall inequality yields

$$
\left\|e^{k+1}\right\|^2\leq\exp\left(2\hat{c}_3(k+1)\Delta t\right)\frac{|\Omega|}{\hat{c}_3}m_3^2\left(h_1^2+h_2^2+\triangle t^2\right)^2. \tag{2.5.36}
$$

Therefore,

$$
\left\|e^{k+1}\right\|\leq\exp\left(\hat{c}_3(k+1)\Delta t\right)\sqrt{\frac{|\Omega|}{\hat{c}_3}}m_3\left(h_1^2+h_2^2+\triangle t^2\right)=\tilde{c}\left(h_1^2+h_2^2+\triangle t^2\right).
$$

For estimating $\left\|\Delta e^{k+1}\right\|$, we take inner product of (2.5.13) with $\delta_t e^{k+\frac{1}{2}} = \dfrac{e^{k+1}-e^k}{\Delta t}$, then

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

Similar to the derivation of (2.5.32), we have

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

Also, we can obtain

$$\left\langle \hat{R}^{k+\frac{1}{2}}, \frac{e^{k+1}-e^k}{\Delta t}\right\rangle \leq \frac{|\Omega|\,\hat{c}_2^2(h_1^2+h_2^2+\Delta t^2)^2}{2} + \frac{1}{2}\left\|\frac{e^{k+1}-e^k}{\triangle t}\right\|^2.$$

Therefore, we have

$$\begin{aligned}
&\frac{1}{2}\left\|\frac{e^{k+1}-e^k}{\triangle t}\right\|^2 + \frac{c}{2\Delta t}\left(\left\|\triangle_h e^{k+1}\right\|^2 - \left\|\triangle_h e^k\right\|^2\right)\\
&\quad \leq \left\langle \mu_0\left(\hat{\hat{n}}^{k+\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{k+\frac{1}{2}}\right), \delta_t \Delta_h e^{k+\frac{1}{2}}\right\rangle + \frac{|\Omega|\,\hat{c}_2^2(h_1^2+h_2^2+\Delta t^2)^2}{2}. \qquad (2.5.37)
\end{aligned}$$

Replacing the superscript k by l in (2.5.37) and summing up for l from 0 to k, we can get

$$\begin{aligned}
&\frac{1}{2}\sum_{l=0}^{k}\left\|\frac{e^{l+1}-e^l}{\triangle t}\right\|^2 + \frac{c}{2\Delta t}\left\|\triangle_h e^{k+1}\right\|^2\\
&\quad \leq \sum_{l=0}^{k}\left\langle \mu_0\left(\hat{\hat{n}}^{l+\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{l+\frac{1}{2}}\right), \delta_t \Delta_h e^{l+\frac{1}{2}}\right\rangle + \sum_{l=0}^{k}\frac{|\Omega|\,\hat{c}_2^2(h_1^2+h_2^2+\Delta t^2)^2}{2}. \quad (2.5.38)
\end{aligned}$$

According to Lemma 2.7, we have

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

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

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

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

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

Here,

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

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

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

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

$$\mu_0\left(\hat{\hat{u}}^{\frac{5}{2}}\right) - \mu_0\left(\hat{u}^{\frac{5}{2}}\right)$$

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

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

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

and

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

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

$$\leq \frac{c}{4\Delta t}\left\|\Delta_h e^{k+1}\right\|^2 + \frac{2\hat{c}_1^2}{c\Delta t}\left(\left\|e^k\right\|^2 + \frac{1}{4}\left\|e^{k-1}\right\|^2 + \frac{1}{4}\left\|e^{k-2}\right\|^2\right).$$

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

$$= -\frac{1}{\Delta t}\left\langle \mu_0'(\hat{\rho}^{\frac{5}{2}}\hat{\bar{n}}^{\frac{5}{2}} + (1-\hat{\rho}^{\frac{5}{2}})\hat{n}^{\frac{5}{2}})\left(e^2 - e^1 + \frac{3}{2}e^1 - \frac{3}{2}e^0\right), \Delta_h e^2\right\rangle$$

$$\leq \hat{c}_1\left\|\frac{e^2-e^1}{\Delta t} + \frac{3}{2}\frac{e^1-e^0}{\Delta t}\right\|\left\|\Delta_h e^2\right\| \leq \hat{c}_1\left\|\frac{e^2-e^1}{\Delta t}\right\|\left\|\Delta_h e^2\right\| + \frac{3\hat{c}_1}{2}\left\|\frac{e^1-e^0}{\Delta t}\right\|\left\|\Delta_h e^2\right\|$$

$$\leq \frac{1}{4}\left\|\frac{e^2-e^1}{\Delta t}\right\|^2 + \hat{c}_1^2\left\|\Delta_h e^2\right\|^2 + \frac{1}{4}\left\|\frac{e^1-e^0}{\Delta t}\right\|^2 + \frac{9}{4}\hat{c}_1^2\left\|\Delta_h e^2\right\|^2$$

$$\leq \frac{1}{4}\left[\left\|\frac{e^2-e^1}{\Delta t}\right\|^2 + \left\|\frac{e^1-e^0}{\Delta t}\right\|^2\right] + \frac{13\hat{c}_1^2}{4}\left\|\Delta_h e^2\right\|^2.$$

For the term $\frac{1}{\Delta t}\left[\mu_0\left(\hat{\bar{n}}^{l+\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{l+\frac{1}{2}}\right) - \left(\mu_0\left(\hat{\bar{n}}^{l-\frac{1}{2}}\right) - \mu_0\left(\hat{n}^{l-\frac{1}{2}}\right)\right)\right]$, using Lemma 2.15, we can get

$$\frac{1}{\Delta t}\left[\mu_0(\hat{\bar{n}}^{l+\frac{1}{2}}) - \mu_0(\hat{n}^{l+\frac{1}{2}}) - \left(\mu_0(\hat{\bar{n}}^{l-\frac{1}{2}}) - \mu_0(\hat{n}^{l-\frac{1}{2}})\right)\right]$$

$$= \mu_0'(\hat{\rho}^l\hat{n}^{l+\frac{1}{2}} + (1-\hat{\rho}^l)\hat{n}^{l-\frac{1}{2}})\frac{\hat{e}^{l+\frac{1}{2}} - \hat{e}^{l-\frac{1}{2}}}{\Delta t}$$

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

$$= \mu_0'(\hat{\rho}^l\hat{n}^{l+\frac{1}{2}} + (1-\hat{\rho}^l)\hat{n}^{l-\frac{1}{2}})\frac{e^l - e^{l-1} + \frac{1}{2}(e^{l-1}-e^{l-2}) - \frac{1}{2}(e^{l-2}-e^{l-3})}{\Delta t}$$

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

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

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

$$
\begin{aligned}
&= -\sum_{l=3}^{k}\left\langle \mu_0'(\hat{\rho}^l\hat{n}^{l+\frac{1}{2}}+(1-\hat{\rho}^l)\hat{n}^{l-\frac{1}{2}})\frac{e^l-e^{l-1}+\frac{1}{2}(e^{l-1}-e^{l-2})-\frac{1}{2}(e^{l-2}-e^{l-3})}{\Delta t},\Delta_h e^l\right\rangle \\
&\quad -\sum_{l=3}^{k}\left\langle \mu_0''(\xi^l)\left(\hat{\rho}^l\hat{e}^{l+\frac{1}{2}}+(1-\hat{\rho}^l)\hat{e}^{l-\frac{1}{2}}\right)\frac{\bar{n}^l-\bar{n}^{l-1}+\frac{\bar{n}^{l-1}-\bar{n}^{l-2}}{2}-\frac{\bar{n}^{l-2}-\bar{n}^{l-3}}{2}}{\Delta t},\Delta_h e^l\right\rangle.
\end{aligned} \tag{2.5.39}
$$

The first term of the right hand side of (2.5.39) satisfies

$$
\begin{aligned}
&-\sum_{l=3}^{k}\left\langle \mu_0'(\hat{\rho}^l\hat{n}^{l+\frac{1}{2}}+(1-\hat{\rho}^l)\hat{n}^{l-\frac{1}{2}})\frac{e^l-e^{l-1}+\frac{1}{2}(e^{l-1}-e^{l-2})-\frac{1}{2}(e^{l-2}-e^{l-3})}{\Delta t},\Delta_h e^l\right\rangle \\
&\leq \frac{1}{4}\sum_{l=3}^{k}\left\|\frac{e^l-e^{l-1}}{\Delta t}\right\|^2+\hat{c}_1^2\sum_{l=3}^{k}\left\|\Delta_h e^l\right\|^2+\frac{1}{8}\sum_{l=3}^{k}\left\|\frac{e^{l-1}-e^{l-2}}{\Delta t}\right\|^2+\frac{\hat{c}_1^2}{2}\sum_{l=3}^{k}\left\|\Delta_h e^l\right\|^2 \\
&\quad +\frac{1}{8}\sum_{l=3}^{k}\left\|\frac{e^{l-2}-e^{l-3}}{\Delta t}\right\|^2+\frac{\hat{c}_1^2}{2}\sum_{l=3}^{k}\left\|\Delta_h e^l\right\|^2.
\end{aligned} \tag{2.5.40}
$$

And for the second term of (2.5.39), we have

$$
\begin{aligned}
&\left|\sum_{l=3}^{k}\left\langle \mu_0''(\xi^l)\left(\hat{\rho}^l\hat{e}^{l+\frac{1}{2}}+(1-\hat{\rho}^l)\hat{e}^{l-\frac{1}{2}}\right)\frac{\bar{n}^l-\bar{n}^{l-1}+\frac{\bar{n}^{l-1}-\bar{n}^{l-2}}{2}-\frac{\bar{n}^{l-2}-\bar{n}^{l-3}}{2}}{\Delta t},\Delta_h e^l\right\rangle\right| \\
&\leq 2\sum_{l=3}^{k}\hat{c}_2\hat{c}_4\left\|\hat{\rho}e^{l+\frac{1}{2}}+(1-\hat{\rho})e^{l-\frac{1}{2}}\right\|\left\|\Delta_h e^l\right\| \\
&= 2\sum_{l=3}^{k}\hat{c}_2\hat{c}_4\left\|\hat{\rho}\left(e^l+\frac{1}{2}e^{l-1}-\frac{1}{2}e^{l-2}\right)+(1-\hat{\rho})\left(e^{l-1}+\frac{1}{2}e^{l-2}-\frac{1}{2}e^{l-3}\right)\right\|\left\|\Delta_h e^l\right\| \\
&= 2\sum_{l=3}^{k}\hat{c}_2\hat{c}_4\left\|\hat{\rho}e^l+\left(1-\frac{\hat{\rho}}{2}\right)e^{l-1}+\left(\frac{1}{2}-\hat{\rho}\right)e^{l-2}+\frac{1-\hat{\rho}}{2}e^{l-3}\right\|\left\|\Delta_h e^l\right\| \\
&\leq 2\sum_{l=3}^{k}\hat{c}_2\hat{c}_4\left[\left\|\hat{\rho}e^l\right\|+\left\|\left(1-\frac{\hat{\rho}}{2}\right)e^{l-1}\right\|+\left\|\left(\frac{1}{2}-\hat{\rho}\right)e^{l-2}\right\|+\left\|\frac{1-\hat{\rho}}{2}e^{l-3}\right\|\right]\left\|\Delta_h e^l\right\| \\
&\leq 2\sum_{l=3}^{k}\hat{c}_2\hat{c}_4\left[\left\|e^l\right\|^2+\left\|e^{l-1}\right\|+\frac{1}{2}\left\|e^{l-2}\right\|+\frac{1}{2}\left\|e^{l-3}\right\|\right]\left\|\Delta_h e^l\right\|
\end{aligned}
$$

$$\leq \sum_{l=3}^{k}\left[\hat{c}_2^2\hat{c}_4^2\left\|e^l\right\| + \hat{c}_2^2\hat{c}_4^2\left\|e^{l-1}\right\|^2 + \frac{\hat{c}_2^2\hat{c}_4^2}{4}\left\|e^{l-2}\right\|^2 + \frac{\hat{c}_2^2\hat{c}_4^2}{4}\left\|e^{l-3}\right\|^2 + 4\left\|\Delta_h e^l\right\|^2\right]$$

$$= \sum_{l=3}^{k}\hat{c}_2^2\hat{c}_4^2\left\|e^l\right\|^2 + \sum_{l=2}^{k-1}\hat{c}_2^2\hat{c}_4^2\left\|e^l\right\|^2 + \sum_{l=1}^{k-2}\frac{\hat{c}_2^2\hat{c}_4^2}{4}\left\|e^l\right\|^2 + \sum_{l=1}^{k-3}\frac{\hat{c}_2^2\hat{c}_4^2}{4}\left\|e^l\right\|^2 + 4\sum_{l=3}^{k}\left\|\Delta_h e^l\right\|^2.$$

Hence,

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

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

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

$$\leq \frac{c}{4\Delta t}\left\|\Delta_h e^{k+1}\right\|^2 + \frac{2\hat{c}_1^2}{c\Delta t}\left(\left\|e^k\right\|^2 + \frac{1}{4}\left\|e^{k-1}\right\|^2 + \frac{1}{4}\left\|e^{k-2}\right\|^2\right)$$

$$+ \frac{1}{4}\left[\left\|\frac{e^2 - e^1}{\Delta t}\right\|^2 + \left\|\frac{e^1 - e^0}{\Delta t}\right\|^2\right] + \frac{13\hat{c}_3^2}{4}\left\|\Delta_h e^2\right\|^2 + (2\hat{c}_1^2 + 4)\sum_{l=3}^{k}\left\|\Delta_h e^l\right\|^2$$

$$+ \frac{1}{4}\sum_{l=2}^{k-1}\left\|\frac{e^{l+1} - e^l}{\Delta t}\right\|^2 + \frac{1}{8}\sum_{l=1}^{k-2}\left\|\frac{e^{l+1} - e^l}{\Delta t}\right\|^2 + \frac{1}{8}\sum_{l=0}^{k-3}\left\|\frac{e^{l+1} - e^l}{\Delta t}\right\|^2$$

$$+ \sum_{l=3}^{k}\hat{c}_2^2\hat{c}_4^2\left\|e^l\right\|^2 + \sum_{l=2}^{k-1}\hat{c}_2^2\hat{c}_4^2\left\|e^l\right\|^2 + \sum_{l=1}^{k-2}\frac{\hat{c}_2^2\hat{c}_4^2}{4}\left\|e^l\right\|^2 + \sum_{l=1}^{k-3}\frac{\hat{c}_2^2\hat{c}_4^2}{4}\left\|e^l\right\|^2$$

$$\leq \frac{c}{4\Delta t}\left\|\Delta_h e^{k+1}\right\|^2 + \frac{2\hat{c}_1^2}{c\Delta t}\left(\left\|e^k\right\|^2 + \frac{1}{4}\left\|e^{k-1}\right\|^2 + \frac{1}{4}\left\|e^{k-2}\right\|^2\right)$$

$$+ \frac{1}{2}\sum_{l=0}^{k-1}\left\|\frac{e^{l+1} - e^l}{\Delta t}\right\|^2 + \max\left\{\frac{13\hat{c}_3^2}{4}, 2\hat{c}_1^2 + 4\right\}\sum_{l=2}^{k}\left\|\Delta_h e^l\right\|^2$$

$$+ \sum_{l=3}^{k}\hat{c}_2^2\hat{c}_4^2\left\|e^l\right\|^2 + \sum_{l=2}^{k-1}\hat{c}_2^2\hat{c}_4^2\left\|e^l\right\|^2 + \sum_{l=1}^{k-2}\frac{\hat{c}_2^2\hat{c}_4^2}{4}\left\|e^l\right\|^2 + \sum_{l=1}^{k-3}\frac{\hat{c}_2^2\hat{c}_4^2}{4}\left\|e^l\right\|^2$$

$$
\begin{aligned}
&\leq \frac{c}{4\Delta t}\left\|\Delta_h e^{k+1}\right\|^2 + \frac{2\hat{c}_1^2}{c\Delta t}\left(\left\|e^k\right\|^2 + \frac{1}{4}\left\|e^{k-1}\right\|^2 + \frac{1}{4}\left\|e^{k-2}\right\|^2\right) \\
&\quad + \frac{1}{2}\sum_{l=0}^{k-1}\left\|\frac{e^{l+1}-e^l}{\Delta t}\right\|^2 + \hat{c}_7\sum_{l=2}^{k}\left\|\Delta_h e^l\right\|^2 + \sum_{l=3}^{k}\hat{c}_2^2\hat{c}_4^2\left\|e^l\right\|^2 \\
&\quad + \sum_{l=2}^{k-1}\hat{c}_2^2\hat{c}_4^2\left\|e^l\right\|^2 + \sum_{l=1}^{k-2}\frac{\hat{c}_2^2\hat{c}_4^2}{4}\left\|e^l\right\|^2 + \sum_{l=1}^{k-3}\frac{\hat{c}_2^2\hat{c}_4^2}{4}\left\|e^l\right\|^2. \qquad (2.5.41)
\end{aligned}
$$

Combining (2.5.41) with (2.5.38), we can get

$$
\begin{aligned}
&\frac{1}{2}\sum_{l=0}^{k}\left\|\frac{e^{l+1}-e^l}{\triangle t}\right\|^2 + \frac{c}{2\Delta t}\left\|\triangle_h e^{k+1}\right\|^2 \\
&\quad \leq \frac{c}{4\Delta t}\left\|\Delta_h e^{k+1}\right\|^2 + \frac{2\hat{c}_1^2}{c\Delta t}\left(\left\|e^k\right\|^2 + \frac{1}{4}\left\|e^{k-1}\right\|^2 + \frac{1}{4}\left\|e^{k-2}\right\|^2\right) \\
&\quad\quad + \frac{1}{2}\sum_{l=0}^{k-1}\left\|\frac{e^{l+1}-e^l}{\Delta t}\right\|^2 + \hat{c}_7\sum_{l=2}^{k}\left\|\Delta_h e^l\right\|^2 + \sum_{l=3}^{k}\hat{c}_2^2\hat{c}_4^2\left\|e^l\right\|^2 + \sum_{l=2}^{k-1}\hat{c}_2^2\hat{c}_4^2\left\|e^l\right\|^2 \\
&\quad\quad + \sum_{l=1}^{k-2}\frac{\hat{c}_2^2\hat{c}_4^2}{4}\left\|e^l\right\|^2 + \sum_{l=1}^{k-3}\frac{\hat{c}_2^2\hat{c}_4^2}{4}\left\|e^l\right\|^2 + \sum_{l=0}^{k}\frac{|\Omega|\,\hat{c}_2^2(h_1^2+h_2^2+\Delta t^2)^2}{2}. \qquad (2.5.42)
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\frac{c}{4\Delta t}\left\|\triangle_h e^{k+1}\right\|^2 \leq & \frac{2\hat{c}_1^2}{c\Delta t}\left(\left\|e^k\right\|^2 + \frac{1}{4}\left\|e^{k-1}\right\|^2 + \frac{1}{4}\left\|e^{k-2}\right\|^2\right) + \hat{c}_7\sum_{l=2}^{k}\left\|\Delta_h e^l\right\|^2 \\
& + \sum_{l=3}^{k}\hat{c}_2^2\hat{c}_4^2\left\|e^l\right\|^2 + \sum_{l=2}^{k-1}\hat{c}_2^2\hat{c}_4^2\left\|e^l\right\|^2 + \sum_{l=1}^{k-2}\frac{\hat{c}_2^2\hat{c}_4^2}{4}\left\|e^l\right\|^2 + \sum_{l=1}^{k-3}\frac{\hat{c}_2^2\hat{c}_4^2}{4}\left\|e^l\right\|^2 \\
& + \sum_{l=0}^{k}\frac{|\Omega|\,\hat{c}_2^2(h_1^2+h_2^2+\Delta t^2)^2}{2}. \qquad (2.5.43)
\end{aligned}
$$

Accordingly,

$$
\left\|\triangle_h e^{k+1}\right\|^2 \leq \frac{8\hat{c}_1^2}{c^2}\left(\left\|e^k\right\|^2 + \frac{1}{4}\left\|e^{k-1}\right\|^2 + \frac{1}{4}\left\|e^{k-2}\right\|^2\right) + \frac{4\hat{c}_7}{c}\Delta t\sum_{l=2}^{k}\left\|\Delta_h e^l\right\|^2
$$

$$+\sum_{l=3}^{k}\frac{4\hat{c}_2^2\hat{c}_4^2}{c}\Delta t\left\|e^l\right\|^2+\sum_{l=2}^{k-1}\frac{4\hat{c}_2^2\hat{c}_4^2}{c}\Delta t\left\|e^l\right\|^2+\sum_{l=1}^{k-2}\frac{\hat{c}_2^2\hat{c}_4^2}{c}\Delta t\left\|e^l\right\|^2$$

$$+\sum_{l=1}^{k-3}\frac{\hat{c}_2^2\hat{c}_4^2}{c}\Delta t\left\|e^l\right\|^2+\sum_{l=0}^{k}\frac{2\left|\Omega\right|\hat{c}_2^2(h_1^2+h_2^2+\Delta t^2)^2}{c}\Delta t. \qquad (2.5.44)$$

According to (2.5.35), if $\Delta t<1$, we can get

$$\left\|e^{k+1}\right\|^2\le 2\hat{c}_3\Delta t\sum_{l=1}^{k}\left\|e^l\right\|^2+2(k+1)\left|\Omega\right|m_3^2\triangle t\left(h_1^2+h_2^2+\triangle t^2\right)^2,$$

$$\left\|e^{k}\right\|^2\le 2\hat{c}_3\Delta t\sum_{l=1}^{k-1}\left\|e^l\right\|^2+2k\left|\Omega\right|m_3^2\triangle t\left(h_1^2+h_2^2+\triangle t^2\right)^2,$$

$$\left\|e^{k-1}\right\|^2\le 2\hat{c}_3\Delta t\sum_{l=1}^{k-2}\left\|e^l\right\|^2+2(k-1)\left|\Omega\right|m_3^2\triangle t\left(h_1^2+h_2^2+\triangle t^2\right)^2,$$

$$\left\|e^{k-2}\right\|^2\le 2\hat{c}_3\Delta t\sum_{l=1}^{k-3}\left\|e^l\right\|^2+2(k-2)\left|\Omega\right|m_3^2\triangle t\left(h_1^2+h_2^2+\triangle t^2\right)^2.$$

Synthesizing the above results, (2.5.35) with (2.5.44), we have

$$\begin{aligned}
&\left\|e^{k+1}\right\|^2+\left\|\triangle_h e^{k+1}\right\|^2\\
&\le 2\hat{c}_3\Delta t\sum_{l=1}^{k}\left\|e^l\right\|^2+2(k+1)\left|\Omega\right|m_3^2\triangle t\left(h_1^2+h_2^2+\triangle t^2\right)^2+\frac{4\hat{c}_7}{c}\Delta t\sum_{l=2}^{k}\left\|\Delta_h e^l\right\|^2\\
&\quad+\frac{8\hat{c}_1^2}{c^2}\left[2\hat{c}_3\Delta t\sum_{l=1}^{k-1}\left\|e^l\right\|^2+2k\left|\Omega\right|m_3^2\triangle t\left(h_1^2+h_2^2+\triangle t^2\right)^2\right]\\
&\quad+\frac{2\hat{c}_1^2}{c^2}\left[2\hat{c}_3\Delta t\sum_{l=1}^{k-2}\left\|e^l\right\|^2+2(k-1)\left|\Omega\right|m_3^2\triangle t\left(h_1^2+h_2^2+\triangle t^2\right)^2\right]\\
&\quad+\frac{2\hat{c}_1^2}{c^2}\left[2\hat{c}_3\Delta t\sum_{l=1}^{k-3}\left\|e^l\right\|^2+2(k-2)\left|\Omega\right|m_3^2\triangle t\left(h_1^2+h_2^2+\triangle t^2\right)^2\right]\\
&\quad+\sum_{l=3}^{k}\frac{4\hat{c}_2^2\hat{c}_4^2}{c}\Delta t\left\|e^l\right\|^2+\sum_{l=2}^{k-1}\frac{4\hat{c}_2^2\hat{c}_4^2}{c}\Delta t\left\|e^l\right\|^2+\sum_{l=1}^{k-2}\frac{\hat{c}_2^2\hat{c}_4^2}{c}\Delta t\left\|e^l\right\|^2
\end{aligned}$$

$$
\begin{aligned}
&+\sum_{l=1}^{k-3}\frac{\hat{c}_2^2\hat{c}_4^2}{c}\Delta t\left\|e^l\right\|^2+\sum_{l=0}^{k}\frac{2\left|\Omega\right|\hat{c}_2^2(h_1^2+h_2^2+\Delta t^2)^2}{c}\Delta t\\
\leq&\left(2\hat{c}_3+\frac{24\hat{c}_3\hat{c}_1^2}{c^2}+\frac{10\hat{c}_2^2\hat{c}_4^2}{c}\right)\Delta t\sum_{l=1}^{k}\left\|e^l\right\|^2+\frac{4\hat{c}_7}{c}\Delta t\sum_{l=1}^{k}\left\|\Delta_h e^l\right\|^2\\
&+(k+1)\left(2+\frac{24\hat{c}_1^2}{c^2}+\frac{2}{c}\right)\left|\Omega\right|\hat{c}_2^2(h_1^2+h_2^2+\Delta t^2)^2\Delta t\\
\leq&\max\left\{2\hat{c}_3+\frac{24\hat{c}_3\hat{c}_1^2}{c^2}+\frac{10\hat{c}_2^2\hat{c}_4^2}{c},\frac{4\hat{c}_7}{c}\right\}\Delta t\sum_{l=1}^{k}\left(\left\|e^l\right\|^2+\left\|\Delta_h e^l\right\|^2\right)\\
&+(k+1)\left(2+\frac{24\hat{c}_1^2}{c^2}+\frac{2}{c}\right)\left|\Omega\right|\hat{c}_2^2(h_1^2+h_2^2+\Delta t^2)^2\Delta t\\
\leq&\,2\hat{c}_9\Delta t\sum_{l=1}^{k}\left(\left\|e^l\right\|^2+\left\|\Delta_h e^l\right\|^2\right)+2(k+1)\hat{c}_8\left|\Omega\right|\hat{c}_2^2(h_1^2+h_2^2+\Delta t^2)^2\Delta t.
\end{aligned}
$$

Gronwall inequality yields

$$
\left\|e^{k+1}\right\|^2+\left\|\triangle_h e^{k+1}\right\|^2\leq\frac{\hat{c}_8}{\hat{c}_9}\exp\left(\hat{c}_9(k+1)\Delta t\right)\cdot\left|\Omega\right|\left[\hat{c}_2\left(h_1^2+h_2^2+\triangle t^2\right)\right]^2,
$$

where $k=0,1,...,K-1$. Using Lemma 2.4 and (2.5.36), we can get

$$
\begin{aligned}
\left\|e^{k+1}\right\|_\infty^2\leq&k_0\left\|e^{k+1}\right\|\left(\left\|\triangle_h e^{k+1}\right\|+\left\|e^{k+1}\right\|\right)\\
\leq&k_0\sqrt{2\left\|e^{k+1}\right\|^2\left(\left\|e^{k+1}\right\|^2+\left\|\triangle_h e^{k+1}\right\|^2\right)}\\
\leq&k_0\sqrt{\frac{2\hat{c}_8}{\hat{c}_3\hat{c}_9}}\exp\left(\left(\hat{c}_3+\hat{c}_9\right)(k+1)\Delta t\right)m_3^2\left|\Omega\right|\left(h_1^2+h_2^2+\triangle t^2\right)^2.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\left\|e^{k+1}\right\|_\infty\leq&\sqrt[4]{\frac{2\hat{c}_8}{\hat{c}_3\hat{c}_9}k_0^2\left|\Omega\right|^2}\exp\left(\left(\frac{\hat{c}_3+\hat{c}_9}{2}\right)(k+1)\Delta t\right)m_3\left(h_1^2+h_2^2+\triangle t^2\right)\\
\leq&\,\hat{c}\left(h_1^2+h_2^2+\triangle t^2\right).
\end{aligned}
$$

This completes the proof. □

Table 2.1: Critical properties (Data from the Table 3.1 on Page 141 of the book by Firoozabadi [36]), ω and m (our computed results) of isobutane (nC_4).

symbol	T_c, K	P_c, MPa	T_b, K	ω	m
nC_4	425.18	3.797	3.797	0.1990	0.6709

2.6 Numerical Examples

In this section, all the above three schemes are used to obtain the steady state and the evolution history of the solution of the fourth order equations (2.1.4a)-(2.1.4b).

In our numerical experiments, we also consider the substance of isobutane(nC_4) at the temperature of 350 K for comparing with the results of the second-order parabolic equation provided in [85]. At this time, the values of parameters are $a = 1.6977$, $b = 7.2442e - 5$, $c = 2.08869e - 19$. The critical properties and the normal boiling point of nC_4 are provided in Table 2.1.

For comparing with the results in [85], we also consider the problem of our fourth order equation on the two-dimensional domain $\Omega = [0, L]^2$ with $L = 2 \times 10^{-8}$ meters. The initial condition is also set as: the molar density equals the liquid isobutane (nC_4) under a saturated pressure in the region $[0.3L, 0.7L]$, the rest of the domain and a saturated isobutane gas fills the rest of the region. The periodic boundary condition is imposed. This original domain Ω is projected to its normalized map $\hat{\Omega} = [0, \hat{L}]^2$, where $\hat{L} = 10^8 \times L$, to simplify the computational process. The whole discrete domain $\hat{\Omega}$ has 200×200 uniform rectangular meshes. Newton iterative method has been used to obtain the solution at every temporal step, and the resulted linear systems are solved by an algebraic multigrid (AMG) solver. The tolerances for the Newton iteration and AMG solver are set to be 10^{-5} and 10^{-6}, respectively.

2.6.1 Spatial distribution of molar density and other chemical properties

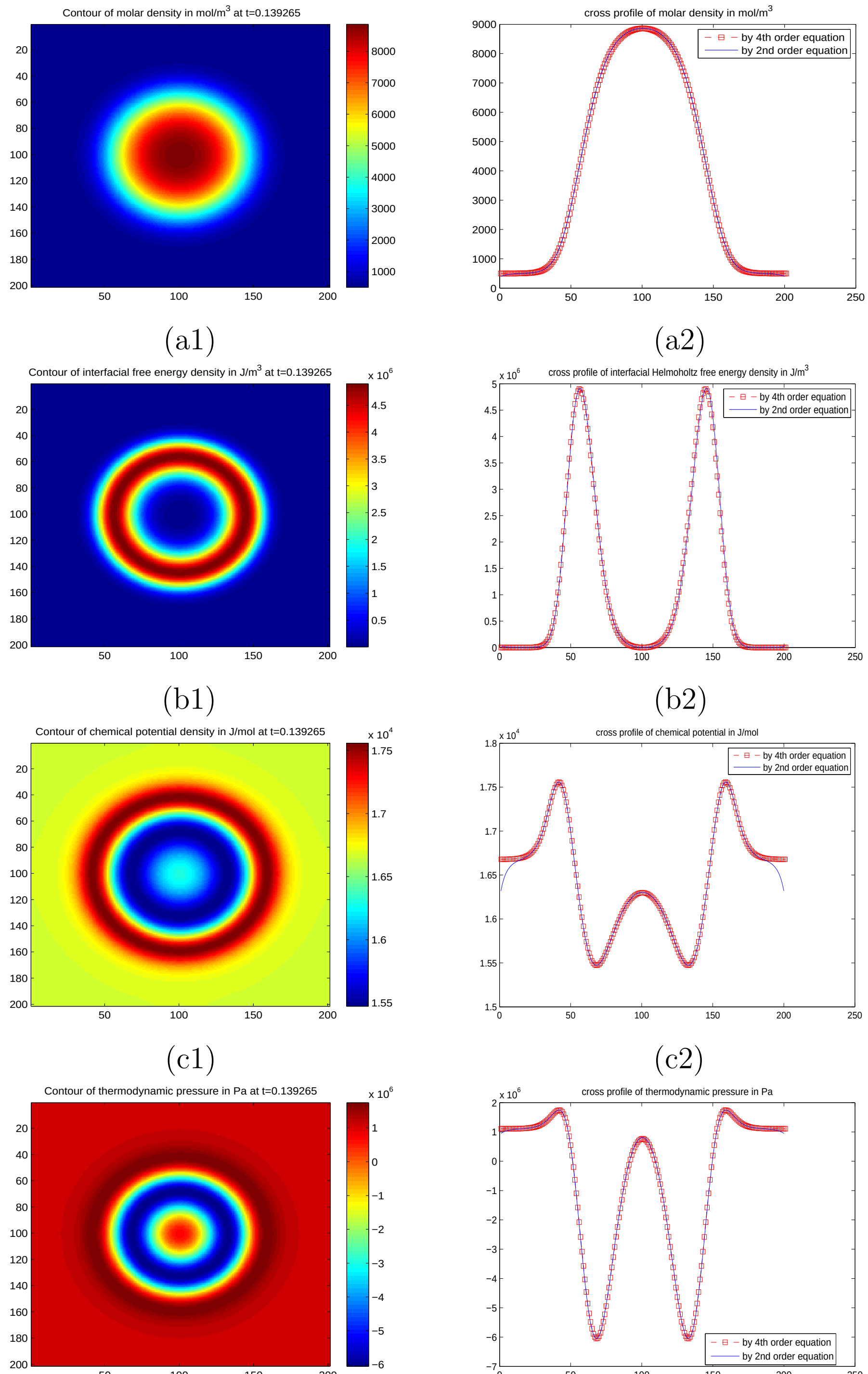
In this part, we provide comparisons of the numerical results of our fourth-order parabolic equation with the second-order parabolic equation provided by Qiao and Sun's previous work [85] based on the same equation of state. We note that, all these three numerical schemes have been applied to solve the above initial and boundary problem. Since the evolution history and steady state obtained from these schemes are quite similar, only the results provided by the convex-splitting scheme is presented for our demonstration.

The molar density, homogeneous chemical potential density and the thermodynamic pressure at the steady state are our concerned variables for this comparison. Here, the homogeneous contribution of chemical potential μ_0 is defined as (2.1.3). The surface tension contribution to the Helmholtz free energy density, $f_{intfTens}$, and the thermodynamic pressure, p_0, have the same expressions as those presented in Qiao and Sun's paper [85] as follows,

$$f_{intfTens} = 2f_{\nabla}(n) = c\nabla n \cdot \nabla n. \tag{2.6.1}$$

$$\begin{aligned} p_0 = n\left(\frac{\partial f_0}{\partial n}\right) - f_0 = n\mu_0 - f_0 = \frac{nRT}{1-bn} - \frac{n^2 a(T)}{1+2bn-b^2n^2} \\ = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)+b(v-b)}. \end{aligned} \tag{2.6.2}$$

The corresponding results are depicted in Fig. 2.1. We can see that, the fourth-order parabolic equation has similar equilibrium state with the second-order parabolic equation, and both these two equations indicate that all these three variables experience a sharp variation at the interface at the the steady state. As shown in Fig. 2.2 (a1), (a2), the total Helmholtz free energy has a clear dissipative trend during the whole evolution history, and it decays rapidly initially and slows down within later time.



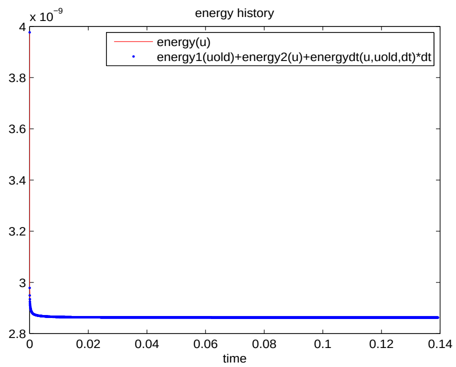
(a1) (a2)

(b1) (b2)

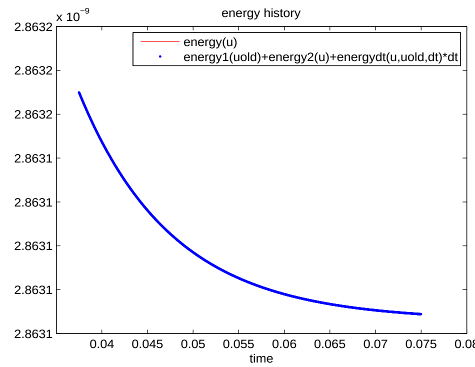
(c1) (c2)

(d1) (d2)

Figure 2.1: Numerical results given by the fourth-order parabolic equation obtained from convex-splitting scheme at steady state: (a1) molar density; (b1) interfacial Helmholtz free energy density; (c1) chemical potential density; (d1) thermodynamic pressure density; cross profile of (a2) molar density; (b2) interfacial Helmholtz free energy; (c2) chemical potential; (d2) thermodynamic pressure density provided by the fourth-order and second-order parabolic equations.



(a1)



(a2)

Figure 2.2: Energy evolution history of the fourth-order parabolic equation obtained from convex-splitting scheme.

2.6.2 Calculation of interface tension and verification against Young-Laplace equation

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 we also use the formula [36, 85]

$$\sigma = \frac{\partial F}{\partial A} = \frac{F(n) - F_0(n_{init})}{A}$$

with the assumption that σ is spatially constant within the interface for the given system.

In our simulation, the contribution of the surface tension to the total free energy at equilibrium state is defined as $\Delta F = F(n) - F_0(n_{init})$. We also assume that the volume of the liquid droplet does not change with time and the steady state has a perfect circular shape. 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 equals $2\pi \times 4,514 \times 10^{-9}$ meters. For example, at temperature $T = 350K$, $F(n) - F_0(n_{init}) \cong 1.774 \times 10^{-10} J$, the surface tension is derived by $\sigma = 1.774 \times 10^{-10}/A = 6.2578 \times 10^{-3} J/m^2$. The surface tension ranging from $250K$ to $350K$ are obtained in the same way. The results are plotted in Fig. 2.3 with the laboratory results provided in Table 2 of [67]. 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, which comes mainly from modeling errors [85], is acceptable from the engineering point of view. Therefore, it is reasonable for us to calculate another physically concerned quality, capillary pressure, based on the value of surface tension provided by the fourth-order parabolic equation.

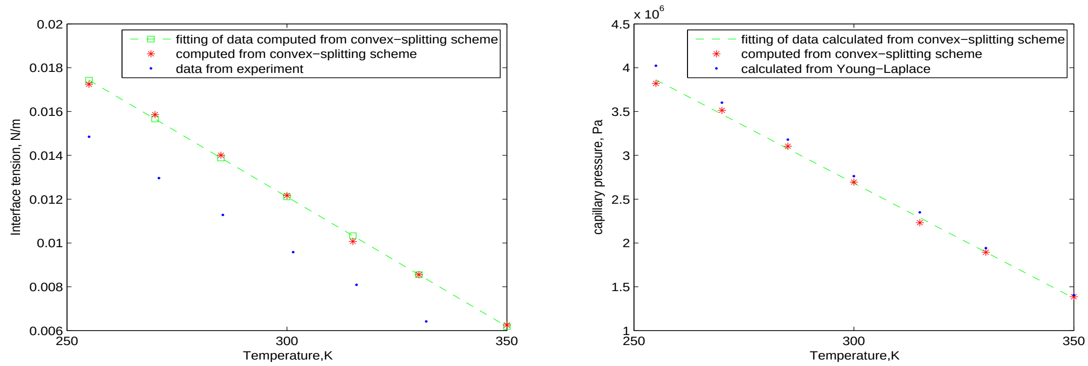
The capillary pressure, P_c, relates to the surface tension, σ, through the well-known Young-Laplace equation in the form of [36, 85]

$$P_c = P_{liquid} - P_{gas} = \frac{\sigma}{r}.$$

Based on this formula, two different approaches have been used to calculate the capillary pressure based on our numerical results for the fourth-order parabolic equation. On the one hand, it is viewed as the difference of the liquid drop pressure, P_{liquid}, and the pressure of the gas phase, P_{gas}. In our numerical example, the pressure in the center of the liquid drop, P_{liquid}, is picked from the grid point $(101, 101)$ and the pressure in the bulk gas region P_{gas} is picked from the point $(51, 51)$. All the variables are projected from $\hat{\Omega}$ to the original domain Ω. The capillary pressure is calculated by $P_{c1} = P_{liquid} - P_{gas}$. On the other hand, the capillary pressure could be obtained by applying the previously calculated value of the surface tension, σ, by the relation $P_{c2} = \sigma/r$. The capillary pressure P_c from temperature $250K$ to $350K$ are given by these two methods respectively, and depicted by Fig.2.3. It could be observed that, the capillary pressure obtained from these two different methods based on the numerical results of the fourth-order parabolic equation are in nice agreement. This guarantees the reliability of the fourth-order equation and its numerical schemes.

2.6.3 Predictions under a special initial condition

From the numerical results demonstrated in the above paragraphs, we can see that the fourth-order parabolic equation is reliable to be used to approach the steady



(a) (b)

Figure 2.3: Comparison of (a) the surface tension (N/m) obtained by Convex-splitting scheme and laboratory data; (b) capillary pressure calculated from the numerical results of the fourth-order equation by two methods: $P_{c1} = P_{liquid} - P_{gas}$ (red stars) and $P_{c2} = \sigma/r$ (blue dots).

state of the single-component, two phase fluids for the substance isobutane (nC4). Here, we use the convex-splitting scheme to predict the solution evolution history under a specific initial condition. Fig. 2.4 depicts the molar density distribution at several different points of time: and the energy evolution history during the whole process. The initial data is set by putting four commensurate square bubbles around the center of the domain symmetrically. From this group of pictures, we can see that, a gas-liquid interface is formed around every single bubble during initial time as showed in Fig. 2.4 (a2), (a3). These bubbles get rounded separately at early stage during time slot $[0.0005, 0.01]$. At time $0.01s$, these nearly circular bubbles touch their neighboring bubbles. After that stage, the contact areas between contiguous droplets increase gradually, then, the bubbles become a unit ring. Finally, this single ring becomes a circular droplet at the center of the domain at time $T_m = 0.90638$. The total energy is decreasing all the time and decays rapidly when the shape of the liquid bubble changes dramatically.

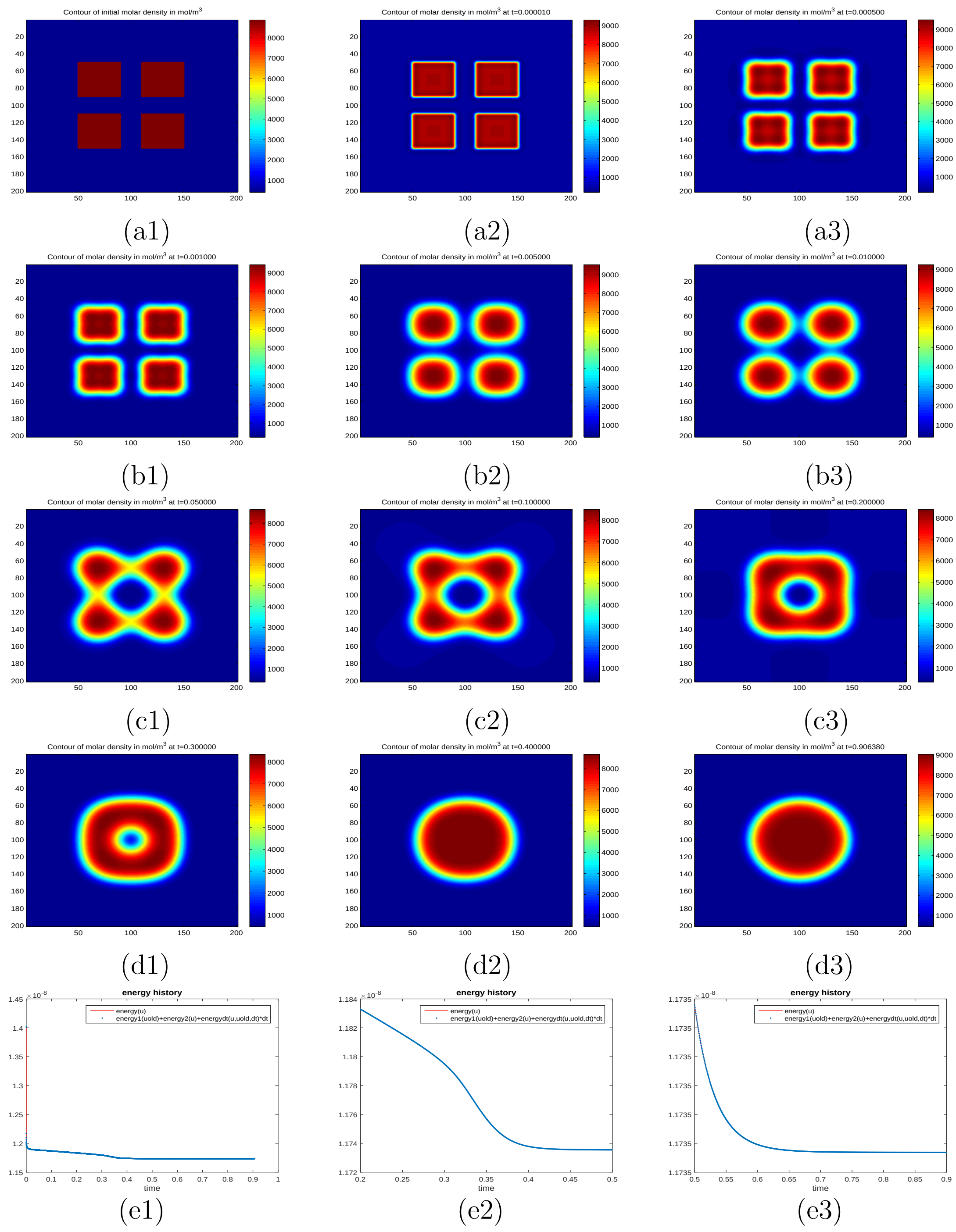


Figure 2.4: Evolution history of solution of the fourth-order parabolic equation and total energy under a specific initial condition. Subfigures (a1)-(d3) depict the molar density distribution at different points of time during the whole evolution history. The subfigure (e1) describes the whole total Helmoltz energy evolution history; subfigure (e2) depicts the energy decreasing process during the time slot $[0.2, 0.5]$; subfigure (e3) describes the energy decaying trend during later period of evolution.

2.7 Chapter summary

In this chapter, we have investigated a fourth-order parabolic equation for a single-component, two-phase substance. For this equation, three numerical schemes have been proposed in order to describe the kinetic and steady state of the molar density distribution. The mass conservation and energy stability of both the original continuous and discrete equation are demonstrated from both theoretical and numerical perspectives. The unique solvability and L^∞ convergence of these schemes are theoretically investigated in detail and guaranteed by numerical experiments. Moreover, the numerical results of these schemes coincide to a great degree with the laboratory experimental results.

Chapter 3

Euler-Lagrange equation for single-component substances and its numerical solutions

In this chapter, we present achievements for the Euler-Lagrange equations derived from the Peng-Robinson EOS. This includes the work of Kou et al. [59, 60] on demonstration and numerical approaches for the Euler-Lagrange equation for multi-component fluids and our work for the iterative methods of the single-component, two-phase case.

The contents of this chapter is organized as follows. In next section, we will present the expressions of the Euler-Lagrange equations for multi-component fluids and achievements on its previous numerical approaches. In section 2, convergence and energy stability of three potential iterative schemes will be analyzed in detail. After that, numerical results obtained from two available iterations for the Euler-Lagrange equation of pure substances will be presented and compared. The concluding remarks will be provided in the last section.

3.1 Euler-Lagrange equations

According to the second law of thermodynamics, the total Helmholtz free energy expressed by (1.2) achieves its minimum at the equilibrium state. Suppose Ω is open, bounded and connected, and has a sufficiently smooth boundary. Let $V = \left(\mathrm{H}^1(\Omega)\right)^M$, associated with the norm

$$\|\mathbf{v}\|_V = \left(\|\mathbf{v}\|^2_{(L^2(\Omega))^M} + \sum_{i=1}^{M} \|\nabla v_i\|^2_{(L^2(\Omega))^d}\right)^{1/2}.$$

To get the equilibrium state, we need to consider the problem of minimizing Helmholtz energy: find $\mathbf{n}$ satisfying

$$F(\mathbf{n}) = \min_{\tilde{\mathbf{n}} \in V} F(\tilde{\mathbf{n}}), \tag{3.1.1}$$

subjected to

$$\int_\Omega \mathbf{n} d\mathbf{x} = \mathbf{n}^t, \tag{3.1.2}$$

where $\mathbf{n}^t = \left(n_1^t, n_2^t, ..., n_M^t\right)^T$ is a given constant vector representing the fixed amount of given substance.

Define

$$F_B(\mathbf{n}_B) = \int_\Omega f_0(\mathbf{n}_B)\, d\mathbf{x},$$

where $\mathbf{n}_B$ is the molar density in the equilibrium bulk phase. We have a similar problem without gradient contribution:

$$F_B(\mathbf{n}_B) = \min_{\tilde{\mathbf{n}}_B \in V} F(\tilde{\mathbf{n}}_B), \tag{3.1.3}$$

subjected to

$$\int_\Omega \mathbf{n}_B d\mathbf{x} = \mathbf{n}^t. \tag{3.1.4}$$

Note: F_B may posses more than one minimizer.

Let us introduce the appropriate admissible class

$$V^C = \left\{ \mathbf{n} \in \left(H^1(\Omega)\right)^N : \int_\Omega \mathbf{n} d\mathbf{x} = \mathbf{n}^t . \right\}$$

and note that V^C is nonempty because $\mathbf{n} = \dfrac{\mathbf{n}^t}{|\Omega|} \in V^C$.

Lemma 3.1. *[59] There exists $\mathbf{n} \in V^C$ such that (3.1.3) and (3.1.4) hold.*

Lemma 3.2. *[59] The equilibrium densities at the interface, minimizers of (3.1.1) constrained with (3.1.2), must satisfy the following Euler-Lagrange equations*

$$\sum_{j=1}^{M} \nabla \cdot c_{ij} \nabla n_j - \frac{1}{2} \sum_{k,j=1}^{M} \frac{\partial c_{kj}}{\partial n_i} \nabla n_k \cdot \nabla n_j = \mu_0^i - \mu_i, \quad i = 1, 2, ..., M,$$

associated with the Dirichlet boundary condition

$$\mathbf{n} = \mathbf{n}_B, \quad at\ \partial\Omega.$$

Here the variable μ_i represents the chemical potential in the equilibrium bulk phase, $\mu_i^0 = \dfrac{\partial f_0(\mathbf{n})}{\partial n_i}$. Neglecting dependence of the influence parameters on density, we have

$$\sum_{j=1}^{M} \nabla \cdot c_{ij} \nabla n_j = \mu_i^0 - \mu_i, \quad i = 1, 2, ..., M.$$

In the recently published work of Kou and Sun [60], these Euler-Lagrange equations were reduced by introducing a well-defined monotonic path function based on a linear transformation. Two efficient algorithms were developed to solve these simplified equations for ternary and five-component mixtures under different temperatures and pressures on one dimensional region. They skipped the difficulties involved in solving and analysis of iterative methods for the discrete differential systems whose gap will be partly made up by our work as follows.

3.2 Iterative methods for the Euler-Lagrange equation

In the present section, we investigate the Euler-Lagrange for one-component, two-phase fluids on a two dimensional domain $\Omega = [0, L_x] \times [0, L_y]$, which is written as follows,

$$-c\Delta n = \mu - \mu_0(n), \tag{3.2.1a}$$

$$\int_\Omega n dx = N^t. \tag{3.2.1b}$$

Here, μ is the Lagrange multiplier and represents the chemical potential at the equilibrium state of this substance. N^t is a given constant representing the fixed amount of the component on the whole domain. $f_0(n)$ and $\mu_0(n)$ have the same expressions as in the previous chapter.

To simplify our demonstration for the discrete case, we employ the following notations. Suppose discrete mesh size is uniformly from both directions with grid's width, h. Let $M_1 = L_x/h$, $M_2 = L_y/h$, $x_{i_1} = (i_1 - 1)h$, $y_{i_2} = (i_2 - 1)h$ for $1 \le i_1 \le M_1 + 1$, $1 \le i_2 \le M_2 + 1$. The discrete counterpart of the original domain is

$$\Omega_h = \left\{(x_{i_1},\ y_{i_2}) \mid 1 \le i_1 \le M_1 + 1,\ 1 \le i_2 \le M_2 + 1\right\}.$$

The space for the discrete functional on Ω_h is defined by

$$\mathcal{V}_h = \left\{n | n = \left\{n_{i_1 i_2}\right\}, 1 \le i_1 \le M_1 + 1, 1 \le i_2 \le M_2 + 1\right\}.$$

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

$$\delta_x n_{i_1+\frac{1}{2},i_2} = \frac{1}{h}\left(n_{i_1+1,i_2} - n_{i_1,i_2}\right), \qquad \delta_y n_{i_1,i_2+\frac{1}{2}} = \frac{1}{h}\left(n_{i_1,i_2+1} - n_{i_1,i_2}\right),$$

$$\delta_x^2 n_{i_1 i_2} = \frac{1}{h^2}\left(n_{i_1+1,i_2} - 2n_{i_1 i_2} + n_{i_1-1,i_2}\right), \qquad \delta_y^2 n_{i_1 i_2} = \frac{1}{h^2}\left(n_{i_1,i_2+1} - 2n_{i_1 i_2} + n_{i_1,i_2-1}\right),$$

$$\nabla_h n_{i_1+\frac{1}{2},i_2+\frac{1}{2}} = \left(\delta_x n_{i_1+\frac{1}{2},i_2}, \delta_y n_{i_1,j+\frac{1}{2}}\right)^T, \qquad \triangle_h n_{i_1 i_2} = \left(\delta_x^2 + \delta_y^2\right) n_{i_1 i_2}. \tag{3.2.2}$$

The inner product for $u, v \in \mathcal{V}_h$ is defined as

$$\langle u, v\rangle = h^2 \sum_{i_1=1}^{M_1+1} \sum_{i_2=1}^{M_2+1} u_{i_1 i_2} v_{i_1 i_2}, \tag{3.2.3}$$

and Sobolev norms are defined as

$$\|u\| = \sqrt{\langle u, u\rangle}, \qquad \|u\|_\infty = \max_{1\le i_1\le M_1+1, 1\le i_2\le M_2+1} |u_{i_1 i_2}|,$$

$$\|\nabla_h u\| = \sqrt{h^2 \sum_{i_1=1}^{M_1} \sum_{i_2=1}^{M_2} \left|\nabla_h u_{i_1+\frac{1}{2}, i_2+\frac{1}{2}}\right|^2}, \qquad \|\triangle_h u\| = \sqrt{h^2 \sum_{i_1=1}^{M_1} \sum_{i_2=1}^{M_2} |\triangle_h u_{i_1 i_2}|^2}.$$

For the $M_t = (M_1+1) \times (M_2+1)$ discrete points, we permutate them in the order of $i = 1, 2, ..., M_t$, where i relates i_1 and i_2 by $i = (i_1 - 1) \times (M_1 + 1) + i_2$, i_2 is the reminder obtained by taking $M_1 + 1$ from i, and $i_1 = \dfrac{i - i_2}{M_1 + 1} + 1$, correspondingly. Hereafter, we use i_1, i_2 to denote the discrete points when norms or inner products are involved, and i to simplify the discrete equations.

The discrete form of the equation (3.2.1a) and (3.2.1b) on Ω_h can be written as

$$-c\Delta_h \mathbf{n} = \mu \mathbf{p}^T - \mu_0(\mathbf{n}), \tag{3.2.4}$$

$$\sum_{i=1}^{M_t} n_i = N^t. \tag{3.2.5}$$

These vectors $\mathbf{n}^{k+1} = (n_1^{k+1}, n_2^{k+1}, ...n_{M_t}^{k+1})$ and $\mathbf{n}^k = (n_1^k, n_2^k, ...n_{M_t}^k)$ represent the values of the n^{k+1} and n^k on mesh points of the discrete domain Ω_h. $\mathbf{p} = (1, 1, ..., 1)$ with M_t elements. N^t denotes the summation of the concentrations on the inner discrete grid points. In addition, $\mathbf{n}^0 = (n_0^0, n_1^0, ...n_{M_t}^0)$ is the initial data for this iteration.

Defining the function of the discrete solution

$$H(\mathbf{n}, \mu) = \begin{bmatrix} -c\Delta_h \mathbf{n} - \mu \mathbf{p}^T + \mu_0(\mathbf{n}) \\ \sum_{i=1}^{M_t} n_i - N^t \end{bmatrix}$$

and supposing $(\mathbf{n}^* = (n_1^*, n_2^*, ..., n_{M_t}^*), \mu^*)$ is the exact solution of discrete equation (3.2.4) and (3.2.5), then we have

$$H(\mathbf{n}^*, \mu^*) = \begin{bmatrix} -c\Delta_h \mathbf{n}^* - \mu^* \mathbf{I} + \mu_0(\mathbf{n}^*) \\ \sum_{i=1}^{M_t} n_i^* - N^t \end{bmatrix} \doteq \begin{bmatrix} H_1(\mathbf{n}^*, \mu^* \mathbf{p}^T) \\ H_2(\mathbf{n}^*, \mu^* \mathbf{p}^T) \end{bmatrix} = 0.$$

3.2.1 Picard iteration

The original Picard iteration of the equation (3.2.4) with molar conservative restriction (3.2.5) is written as

$$c\Delta_h \mathbf{n}^{k+1} = -\mu^{k+1}\mathbf{p}^T + \mu_0(\mathbf{n}^k), \tag{3.2.6}$$

$$\sum_{i=1}^{M_t} n_i^{k+1} = \sum_i n_i^k = N^t. \tag{3.2.7}$$

Here, μ^{k+1} is the updated Lagrangian operator related to the conservative restriction (3.2.7).

Energy stability analysis

Taking the inner product of the equation (3.2.6) with $\mathbf{n}^{k+1} - \mathbf{n}^k$, we have

$$\begin{aligned} &\frac{c}{2}\left[\left\|\nabla_h \mathbf{n}^{k+1}\right\|^2 - \left\|\nabla_h \mathbf{n}^k\right\|^2 + \left\|\nabla_h\left(\mathbf{n}^{k+1} - \mathbf{n}^k\right)\right\|^2\right] + \left\langle f_0(\mathbf{n}^{k+1}) - f_0(\mathbf{n}^k), 1\right\rangle \\ &= \frac{1}{2}\left\langle \frac{\partial \mu_0}{\partial \mathbf{n}}(\xi_0^k)(\mathbf{n}^{k+1} - \mathbf{n}^k)^2, 1\right\rangle + \mu^{k+1}\left\langle \mathbf{n}^{k+1} - \mathbf{n}^k, 1\right\rangle. \end{aligned}$$

With the conservative restriction (3.2.7)

$$\mu^{k+1}\left\langle \mathbf{n}^{k+1} - \mathbf{n}^k, 1\right\rangle = 0, \tag{3.2.8}$$

it is simplified to

$$\begin{aligned} &\frac{c}{2}\left[\left\|\nabla_h \mathbf{n}^{k+1}\right\|^2 - \left\|\nabla_h \mathbf{n}^k\right\|^2 + \left\|\nabla_h\left(\mathbf{n}^{k+1} - \mathbf{n}^k\right)\right\|^2\right] + \left\langle f_0(\mathbf{n}^{k+1}) - f_0(\mathbf{n}^k), 1\right\rangle \\ &= \frac{1}{2}\left\langle \frac{\partial \mu_0}{\partial \mathbf{n}}(\xi_0^k)(\mathbf{n}^{k+1} - \mathbf{n}^k)^2, 1\right\rangle. \end{aligned}$$

From the above equation for the total free energy, we can see that the Picard iteration can not guarantee energy stability by any way since the function $\frac{\partial \mu_0}{\partial n}(\mathbf{n})$ is not nonnegative.

Convergence of the Picard iteration

If we expand $H(\mathbf{n}, \mu)$ at $(\mathbf{n}^k, \mu^k)$ for Picard iteration, then

$$\begin{aligned} H_1(\mathbf{n}, \mu) &= - c\Delta_h \mathbf{n} - \mu \mathbf{p}^T + \mu_0(\mathbf{n}^k) + \frac{\partial \mu_0}{\partial n}(\xi_0^k)(\mathbf{n} - \mathbf{n}^k) \\ &= - \mu \mathbf{p}^T + \mu^{k+1}\mathbf{p}^T - c\Delta_h \mathbf{n} + c\Delta_h \mathbf{n}^{k+1} + \frac{\partial \mu_0}{\partial n}(\xi_0^k)(\mathbf{n} - \mathbf{n}^k). \end{aligned}$$

For the exact solution $(\mathbf{n}^*, \mu^*)$, we have

$$\begin{aligned} &H_1(\mathbf{n}^*, \mu^*) \\ &= -(\mu^* - \mu^{k+1})\mathbf{p}^T - c\Delta_h \left(\mathbf{n}^* - \mathbf{n}^{k+1}\right) + \frac{\partial \mu_0}{\partial \mathbf{n}}(\xi_0^k)(\mathbf{n}^* - \mathbf{n}^k) \\ &= 0. \end{aligned}$$

Therefore, the relationship between errors at $k+1$ step and the k step can be expressed as

$$- c\Delta_h \left(\mathbf{n}^* - \mathbf{n}^{k+1}\right) - (\mu^* - \mu^{k+1})\mathbf{p}^T = -\frac{\partial \mu_0}{\partial \mathbf{n}}(\xi_0^k)(\mathbf{n}^* - \mathbf{n}^k). \tag{3.2.9}$$

Let $-c\Delta_h = \mathbf{A}$, $\frac{\partial \mu_0}{\partial \mathbf{n}}(\xi_0^k) = \mathbf{C}_p^k$, then

$$\begin{bmatrix} \mathbf{A} & \mathbf{p}^T \\ \mathbf{p} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{n}^* - \mathbf{n}^{k+1} \\ \mu^* - \mu^{k+1} \end{bmatrix} = \begin{bmatrix} \mathbf{C}_p^k & 0 \\ \mathbf{0} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{n}^* - \mathbf{n}^k \\ \mu^* - \mu^k \end{bmatrix}. \tag{3.2.10}$$

Multiplying both sides of (3.2.10) with $\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ -\mathbf{p}\mathbf{A}^{-1} & 1 \end{bmatrix}$, we can get

$$\begin{bmatrix} \mathbf{A} & \mathbf{p}^T \\ 0 & -\mathbf{p}\mathbf{A}^{-1}\mathbf{p}^T \end{bmatrix} \begin{bmatrix} \mathbf{n}^* - \mathbf{n}^{k+1} \\ \mu - \mu^{k+1} \end{bmatrix} = \begin{bmatrix} \mathbf{C}_p^k & 0 \\ -\mathbf{p}\mathbf{A}^{-1}\mathbf{C}_p^k & 0 \end{bmatrix} \begin{bmatrix} \mathbf{n}^* - \mathbf{n}^k \\ \mu^* - \mu^k \end{bmatrix}. \tag{3.2.11}$$

Denoting $-\mathbf{p}\mathbf{A}^{-1}\mathbf{p}^T =: \alpha_p$ and multiplying both sides of (3.2.11) with $\begin{bmatrix} \mathbf{I} & \alpha^{-1}\mathbf{p}^T \\ 0 & 1 \end{bmatrix}$, we can get

$$\begin{bmatrix} \mathbf{A} & 0 \\ 0 & -\alpha_p \end{bmatrix} \begin{bmatrix} \mathbf{n}^* - \mathbf{n}^{k+1} \\ \mu - \mu^{k+1} \end{bmatrix} = \begin{bmatrix} \mathbf{C}_p^k - \alpha^{-1}\mathbf{p}^T\mathbf{p}\mathbf{A}^{-1}\mathbf{C}_p^k & 0 \\ -\mathbf{p}\mathbf{A}^{-1}\mathbf{C}_p^k & 0 \end{bmatrix} \begin{bmatrix} \mathbf{n}^* - \mathbf{n}^k \\ \mu^* - \mu^k \end{bmatrix} \tag{3.2.12}$$

$$\mathbf{A}(\mathbf{n}^* - \mathbf{n}^{k+1}) = \left[\mathbf{I} - \alpha^{-1}\mathbf{p}^T\mathbf{p}\mathbf{A}^{-1}\right] \mathbf{C}_p^k(\mathbf{n}^* - \mathbf{n}^k)$$

Therefore,

$$\mathbf{n}^* - \mathbf{n}^{k+1} = \mathbf{A}^{-1}\left[\mathbf{I} - \alpha^{-1}\mathbf{p}^T\mathbf{p}\mathbf{A}^{-1}\right] \mathbf{C}_p^k(\mathbf{n}^* - \mathbf{n}^k) \tag{3.2.13}$$

Convergence of this iteration requires $\left\|\mathbf{A}^{-1}\left[\mathbf{I} - \alpha^{-1}\mathbf{p}^T\mathbf{p}\mathbf{A}^{-1}\right] \mathbf{C}_p^k\right\| \leq 1$ under suitable initial iterative value. However, this requirement could not be satisfied due to the unbound property of the function $\dfrac{\partial \mu_0}{\partial n}(\mathbf{n})$.

3.2.2 The original Newton iteration

The original Newton scheme of the equation (3.2.4) with molar conservative restriction (3.2.5) is written as

$$c\Delta_h \mathbf{n}^{k+1} = -\mu^{k+1}\mathbf{p}^T + \mu_0(\mathbf{n}^k) + \frac{\partial \mu_0}{\partial \mathbf{n}}(\mathbf{n}^k)(\mathbf{n}^{k+1} - \mathbf{n}^k) \tag{3.2.14}$$

$$\sum_{i=1}^{M_t} n_i^{k+1} = \sum_{i=1}^{M_t} n_i^k = N_0^t. \tag{3.2.15}$$

Energy stability analysis

Taking the inner product of the equation (3.2.14) with $n^{k+1} - n^k$, we have

$$\frac{c}{2}\left[\left\|\nabla_h \mathbf{n}^{k+1}\right\|^2 - \left\|\nabla_h \mathbf{n}^k\right\|^2 + \left\|\nabla_h\left(\mathbf{n}^{k+1} - \mathbf{n}^k\right)\right\|^2\right] + \left\langle f_0(\mathbf{n}^{k+1}) - f_0(\mathbf{n}^k), 1\right\rangle$$

$$= -\frac{1}{2}\left\langle \left(\frac{\partial \mu_0}{\partial \mathbf{n}}(\mathbf{n}^k) - \frac{\partial \mu_0}{\partial \mathbf{n}}(\xi_1^k)\right)(\mathbf{n}^{k+1} - \mathbf{n}^k)^2, 1\right\rangle + \mu^{k+1}\left\langle \mathbf{n}^{k+1} - \mathbf{n}^k, 1\right\rangle.$$

With the conservative restriction (3.2.15)

$$\mu^{k+1}\left\langle \mathbf{n}^{k+1}-\mathbf{n}^{k},1\right\rangle = 0, \tag{3.2.16}$$

one can yield

$$\begin{aligned}
&\frac{c}{2}\left[\left\|\nabla_h \mathbf{n}^{k+1}\right\|^2-\left\|\nabla_h \mathbf{n}^{k}\right\|^2+\left\|\nabla_h\left(\mathbf{n}^{k+1}-\mathbf{n}^{k}\right)\right\|^2\right]+\left\langle f_0(\mathbf{n}^{k+1})-f_0(\mathbf{n}^{k}),1\right\rangle \\
&\quad=-\frac{1}{2}\left\langle\left(\frac{\partial\mu_0}{\partial\mathbf{n}}(\mathbf{n}^k)-\frac{\partial\mu_0}{\partial\mathbf{n}}(\xi_1^k)\right)(\mathbf{n}^{k+1}-\mathbf{n}^{k})^2,1\right\rangle.
\end{aligned}$$

From the above formula, we can see that the Newton iteration can also not guarantee energy stability.

Convergence of the Newton iteration

We also expand $H(\mathbf{n},\mu)$ at $(\mathbf{n}^k,\mu^k)$, then

$$\begin{aligned}
H_1(\mathbf{n},\mu)=&-c\Delta_h\mathbf{n}-\mu\mathbf{p}^T+\mu_0(\mathbf{n}^k)+\frac{\partial\mu_0}{\partial n}(\mathbf{n}^k)(\mathbf{n}-\mathbf{n}^k)+\frac{1}{2}\frac{\partial\mu_0}{\partial n}(\xi_1^k)(\mathbf{n}-\mathbf{n}^k)^2 \\
=&-\mu\mathbf{p}^T+\mu^{k+1}\mathbf{p}^T-c\Delta_h\mathbf{n}+c\Delta_h\mathbf{n}^{k+1}+\frac{1}{2}\frac{\partial\mu_0}{\partial n}(\xi_1^k)(\mathbf{n}-\mathbf{n}^k)^2.
\end{aligned}$$

For the exact solution $(\mathbf{n}^*,\mu^*)$, we have

$$\begin{aligned}
&H_1(\mathbf{n}^*,\mu^*) \\
&\quad=-(\mu^*-\mu^{k+1})\mathbf{p}^T-c\Delta_h\left(\mathbf{n}^*-\mathbf{n}^{k+1}\right)+\frac{1}{2}\frac{\partial\mu_0}{\partial n}(\xi_1^k)(\mathbf{n}^*-\mathbf{n}^k)^2 \\
&\quad=0.
\end{aligned}$$

Therefore, the relationship between errors at $k+1$ step and the k step can be expressed as

$$-c\Delta_h\left(\mathbf{n}^*-\mathbf{n}^{k+1}\right)-(\mu^*-\mu^{k+1})\mathbf{p}^T=-\frac{1}{2}\frac{\partial^2\mu_0}{\partial\mathbf{n}^2}(\xi_1^k)(\mathbf{n}^*-\mathbf{n}^k)^2. \tag{3.2.17}$$

From above equation, a second order convergence of the Newton iteration could be guaranteed with appropriate initial value.

3.2.3 Convex-splitting method

The convex-splitting based Newton iterative scheme

Borrowing the convex-splitting scheme for the time-dependent equation, we propose a convex-splitting method to solve the Euler-Lagrange equation (3.2.1a) and (3.2.1b) as follows,

$$-c\Delta_h \mathbf{n}^{k+1} = \mu^{k+1}\mathbf{p}^T - \mu_{01}(\mathbf{n}^{k+1}) + \mu_{02}(\mathbf{n}^k), \tag{3.2.18}$$

$$\sum_{i=1}^{M_t} n_i^{k+1} = \sum_{i=1}^{M_t} n_i^k = N^t. \tag{3.2.19}$$

To solve the above equations, the formula (3.2.18) is linearized by

$$\begin{aligned}-c\Delta_h \mathbf{n}^{k+1} &= \mu^{k+1}\mathbf{p}^T - \mu_{01}(\mathbf{n}^k) - \frac{\partial \mu_{01}}{\partial \mathbf{n}}(\mathbf{n}^k)(\mathbf{n}^{k+1} - \mathbf{n}^k) + \mu_{02}(\mathbf{n}^k) \\ &= \mu^{k+1}\mathbf{p}^T - \mu_0(\mathbf{n}^k) - \frac{\partial \mu_{01}}{\partial \mathbf{n}}(\mathbf{n}^k)(\mathbf{n}^{k+1} - \mathbf{n}^k). \end{aligned} \tag{3.2.20}$$

It can be reordered as

$$-c\Delta_h \mathbf{n}^{k+1} + \frac{\partial \mu_{01}}{\partial \mathbf{n}}(\mathbf{n}^k)\mathbf{n}^{k+1} = \mu^{k+1}\mathbf{p}^T - \mu_0(\mathbf{n}^k) + \frac{\partial \mu_{01}}{\partial \mathbf{n}}(\mathbf{n}^k)\mathbf{n}^k. \tag{3.2.21}$$

Energy decay property of the convex-splitting based Newton iterative scheme under the convergence condition

In this section, we will demonstrate the energy decay property of the convex-splitting based Newton iterative scheme (3.2.21) and (3.2.15). Taking the inner product of the equation (3.2.20) with $\mathbf{n}^{k+1} - \mathbf{n}^k$, then

$$\begin{aligned}\left\langle c\Delta_h \mathbf{n}^{k+1}, \mathbf{n}^{k+1} - \mathbf{n}^k \right\rangle &= -c\langle \nabla_h \mathbf{n}^{k+1} \cdot \nabla_h(\mathbf{n}^{k+1} - \mathbf{n}^k), 1\rangle \\ &= -\frac{c}{2}\left[\left\|\nabla_h \mathbf{n}^{k+1}\right\|^2 - \left\|\nabla_h \mathbf{n}^k\right\|^2 + \left\|\nabla_h\left(\mathbf{n}^{k+1} - \mathbf{n}^k\right)\right\|^2\right],\end{aligned}$$

According the following relations

$$f_{01}(n^k) = f_{01}(n^{k+1}) + \mu_{01}(n^{k+1})(n^k - n^{k+1}) + \frac{1}{2}\frac{\partial \mu_{01}}{\partial n}(\xi_1^k)(n^{k+1} - n^k)^2,$$

$$
f_{02}(n^{k+1}) = f_{02}(n^k) + \mu_{02}(n^k)(n^{k+1} - n^k) + \frac{1}{2}\frac{\partial \mu_{02}}{\partial n}(\xi_2^k)(n^{k+1} - n^k)^2,
$$

$$
\begin{aligned}
&f_0(n^{k+1}) - f_0(n^k) \\
&\quad = f_{01}(n^{k+1}) - f_{02}(n^{k+1}) - \big(f_{01}(n^k) - f_{02}(n^k)\big) \\
&\quad = \big(\mu_{01}(n^{k+1}) - \mu_{02}(n^k)\big)(n^{k+1} - n^k) - \frac{1}{2}\left(\frac{\partial \mu_{01}}{\partial n}(\xi_1^k) + \frac{\partial \mu_{02}}{\partial n}(\xi_2^k)\right)(n^{k+1} - n^k)^2 \\
&\quad = \Big[\mu_{01}(n^k) + \frac{\partial \mu_{01}}{\partial n}(n^k)(n^{k+1} - n^k) \\
&\qquad + \frac{1}{2}\frac{\partial^2 \mu_{01}}{\partial n^2}(\xi^k)(n^{k+1} - n^k)^2 - \mu_{02}(n^k)\Big](n^{k+1} - n^k) \\
&\qquad - \frac{1}{2}\left(\frac{\partial \mu_{01}}{\partial n}(\xi_1^k) + \frac{\partial \mu_{02}}{\partial n}(\xi_2^k)\right)(n^{k+1} - n^k)^2 \\
&\quad = \Big[\mu_0(n^k) + \frac{\partial \mu_{01}}{\partial n}(n^k)(n^{k+1} - n^k) + \frac{1}{2}\frac{\partial^2 \mu_{01}}{\partial n^2}(\xi^k)(n^{k+1} - n^k)^2\Big](n^{k+1} - n^k) \\
&\qquad - \frac{1}{2}\left(\frac{\partial \mu_{01}}{\partial n}(\xi_1^k) + \frac{\partial \mu_{02}}{\partial n}(\xi_2^k)\right)(n^{k+1} - n^k)^2,
\end{aligned}
$$

we have

$$
\begin{aligned}
&\left\langle \mu_0(\mathbf{n}^k) + \frac{\partial \mu_{01}}{\partial \mathbf{n}}(\mathbf{n}^k)(\mathbf{n}^{k+1} - \mathbf{n}^k), \mathbf{n}^{k+1} - \mathbf{n}^k \right\rangle \\
&\quad = \frac{1}{2}\left\langle \left(\frac{\partial \mu_{01}}{\partial \mathbf{n}}(\xi_1^k) + \frac{\partial \mu_{02}}{\partial \mathbf{n}}(\xi_2^k)\right)(\mathbf{n}^{k+1} - \mathbf{n}^k), \mathbf{n}^{k+1} - \mathbf{n}^k \right\rangle \\
&\qquad + \big\langle f_0(\mathbf{n}^{k+1}) - f_0(\mathbf{n}^k), 1 \big\rangle - \frac{1}{2}\left\langle \frac{\partial^2 \mu_{01}}{\partial \mathbf{n}^2}(\xi^k)(\mathbf{n}^{k+1} - \mathbf{n}^k)^3, 1 \right\rangle .
\end{aligned}
$$

$$
\begin{aligned}
&\frac{c}{2}\left[\left\|\nabla_h \mathbf{n}^{k+1}\right\|^2 - \left\|\nabla_h \mathbf{n}^k\right\|^2 + \left\|\nabla\left(\mathbf{n}^{k+1} - \mathbf{n}^k\right)\right\|^2\right] + \big\langle f_0(\mathbf{n}^{k+1}) - f_0(\mathbf{n}^k), 1 \big\rangle \\
&\quad = \mu^{k+1}\big\langle \mathbf{n}^{k+1} - \mathbf{n}^k, 1 \big\rangle + \frac{1}{2}\left\langle \left(\frac{\partial \mu_{01}}{\partial \mathbf{n}}(\xi_1^k) - \frac{\partial \mu_{02}}{\partial \mathbf{n}}(\xi_2^k)\right)(\mathbf{n}^{k+1} - \mathbf{n}^k), \mathbf{n}^{k+1} - \mathbf{n}^k \right\rangle \\
&\qquad + \frac{1}{2}\left\langle \frac{\partial^2 \mu_{01}}{\partial \mathbf{n}^2}(\xi^k)(\mathbf{n}^{k+1} - \mathbf{n}^k)^3, 1 \right\rangle \\
&\quad = -\frac{1}{2}\left\langle \left(\frac{\partial \mu_{01}}{\partial \mathbf{n}}(\xi_1^k) + \frac{\partial \mu_{02}}{\partial \mathbf{n}}(\xi_2^k)\right)(\mathbf{n}^{k+1} - \mathbf{n}^k), \mathbf{n}^{k+1} - \mathbf{n}^k \right\rangle
\end{aligned}
$$

$$+\frac{1}{2}\left\langle \frac{\partial^2 \mu_{01}}{\partial \mathbf{n}^2}(\xi^k)(\mathbf{n}^{k+1}-\mathbf{n}^k)^3, 1\right\rangle.$$

With suitable choice of the iterative initial data, the desirable convergent condition could guarantee

$$\left|\frac{\partial^2 \mu_{01}}{\partial \mathbf{n}^2}(\xi^k)(\mathbf{n}^{k+1}-\mathbf{n}^k)\right| < \frac{1}{2}\left[\frac{\partial \mu_{01}}{\partial \mathbf{n}}(\xi_1^k) + \frac{\partial \mu_{02}}{\partial \mathbf{n}}(\xi_2^k)\right].$$

Then

$$\begin{aligned}
&\frac{c}{2}\left[\left\|\nabla_h \mathbf{n}^{k+1}\right\|^2 - \left\|\nabla_h \mathbf{n}^k\right\|^2 + \left\|\nabla_h\left(\mathbf{n}^{k+1}-\mathbf{n}^k\right)\right\|^2\right] + \left\langle f_0(\mathbf{n}^{k+1}) - f_0(\mathbf{n}^k), 1\right\rangle \\
&\quad \le -\frac{1}{4}\left\langle \left(\frac{\partial \mu_{01}}{\partial \mathbf{n}}(\xi_1^k) + \frac{\partial \mu_{02}}{\partial \mathbf{n}}(\xi_2^k)\right)(\mathbf{n}^{k+1}-\mathbf{n}^k), \mathbf{n}^{k+1}-\mathbf{n}^k\right\rangle.
\end{aligned}$$

which is equivalent to the energy decay property

$$\mathbf{F}_h^{k+1} \le \mathbf{F}_h^k.$$

Convergence of this convex-splitting based Newton iterative scheme

In this section, we will show the convergence of the scheme (3.2.15) and (3.2.21). By expanding $F(\mathbf{n},\mu)$ at $(\mathbf{n}^k,\mu^k)$, we have

$$\begin{aligned}
F_1(\mathbf{n},\mu) =& -c\Delta_h \mathbf{n} - \mu \mathbf{p}^T + \mu_0(\mathbf{n}^k) + \frac{\partial \mu_0}{\partial n}(\mathbf{n}^k)(\mathbf{n}-\mathbf{n}^k) + \frac{\partial^2 \mu_0}{2\partial \mathbf{n}^2}(\eta^k)(\mathbf{n}-\mathbf{n}^k)^2 \\
=& -c\Delta_h \mathbf{n} - \mu \mathbf{p}^T + \mu_0(\mathbf{n}^k) + \frac{\partial \mu_{01}}{\partial \mathbf{n}}(\mathbf{n}^k)(\mathbf{n}-\mathbf{n}^k) \\
& -\frac{\partial \mu_{02}}{\partial \mathbf{n}}(\mathbf{n}^k)(\mathbf{n}-\mathbf{n}^k) + \frac{\partial^2 \mu_0}{2\partial \mathbf{n}^2}(\eta^k)(\mathbf{n}-\mathbf{n}^k)^2 \\
=& -c\Delta_h \mathbf{n} - \mu \mathbf{p}^T + \mu_0(\mathbf{n}^k) + \frac{\partial \mu_{01}}{\partial \mathbf{n}}(\mathbf{n}^k)(\mathbf{n}^{k+1}-\mathbf{n}^k) + \frac{\partial \mu_{01}}{\partial \mathbf{n}}(\mathbf{n}^k)(\mathbf{n}-\mathbf{n}^{k+1}) \\
& -\frac{\partial \mu_{02}}{\partial \mathbf{n}}(\mathbf{n}^k)(\mathbf{n}-\mathbf{n}^k) + \frac{\partial \mu_0^2}{2\partial \mathbf{n}^2}(\eta^k)(\mathbf{n}-\mathbf{n}^k)^2 \\
=& -\mu \mathbf{p}^T + \mu^{k+1}\mathbf{p}^T - c\Delta_h \mathbf{n} + c\Delta_h \mathbf{n}^{k+1} + \frac{\partial \mu_{01}}{\partial \mathbf{n}}(\mathbf{n}^k)(\mathbf{n}-\mathbf{n}^{k+1})
\end{aligned}$$

$$-\frac{\partial \mu_{02}}{\partial \mathbf{n}}(\mathbf{n}^k)(\mathbf{n}-\mathbf{n}^k)+\frac{\partial^2 \mu_0}{2\partial \mathbf{n}^2}(\eta^k)(\mathbf{n}-\mathbf{n}^k)^2.$$

For the exact solution $(\mathbf{n}^*, \mu^*)$, we have

$$\begin{aligned}
&F_1(\mathbf{n}^*, \mu^*) \\
&\quad = -(\mu^* - \mu^{k+1})\mathbf{p}^T - c\Delta_h\left(\mathbf{n}^* - \mathbf{n}^{k+1}\right) + \frac{\partial \mu_{01}}{\partial \mathbf{n}}(\mathbf{n}^k)(\mathbf{n}^* - \mathbf{n}^{k+1}) \\
&\qquad - \frac{\partial \mu_{02}}{\partial \mathbf{n}}(\mathbf{n}^k)(\mathbf{n}^* - \mathbf{n}^k) + \frac{\partial^2 \mu_0}{2\partial \mathbf{n}^2}(\eta^k)(\mathbf{n}^* - \mathbf{n}^k)^2 \\
&\quad = 0.
\end{aligned}$$

Therefore, the relationship between errors at $k+1$ step and the k step can be expressed as

$$\begin{aligned}
&-(\mu^* - \mu^{k+1})\mathbf{p}^T - c\Delta_h\left(\mathbf{n}^* - \mathbf{n}^{k+1}\right) + \frac{\partial \mu_{01}}{\partial \mathbf{n}}(\mathbf{n}^k)\left(\mathbf{n}^* - \mathbf{n}^{k+1}\right) \\
&\quad = \frac{\partial \mu_{02}}{\partial \mathbf{n}}(\mathbf{n}^k)(\mathbf{n}^* - \mathbf{n}^k) - \frac{\partial^2 \mu_0}{2\partial \mathbf{n}^2}(\eta^k)(\mathbf{n}^* - n^k)^2.
\end{aligned}$$

Reordering it, we can obtain

$$\begin{aligned}
&\left[-c\Delta_h + \frac{\partial \mu_{01}}{\partial \mathbf{n}}(\mathbf{n}^k)\right]\left(\mathbf{n}^* - \mathbf{n}^{k+1}\right) - (\mu^* - \mu^{k+1})\mathbf{p}^T \\
&\quad = \left[-\frac{\partial \mu_{02}}{\partial \mathbf{n}}(\mathbf{n}^k) + \frac{\partial^2 \mu_0}{2\partial \mathbf{n}^2}(\eta^k)(\mathbf{n}^* - \mathbf{n}^k)\right](\mathbf{n}^* - \mathbf{n}^k).
\end{aligned} \tag{3.2.22}$$

Combining (3.2.15) with (3.2.5), we have

$$\sum_{i=1}^{M_t}(n_i^* - n_i^{k+1}) = 0. \tag{3.2.23}$$

Let $-c\Delta_h = \mathbf{A}$, $\frac{\partial \mu_{01}}{\partial \mathbf{n}}(\mathbf{n}^k) = \mathbf{B}_k$, $-\frac{\partial \mu_{02}}{\partial \mathbf{n}}(\mathbf{n}^k) = \mathbf{C}_k$ and

$$\left[-\frac{\partial \mu_{02}}{\partial \mathbf{n}}(\mathbf{n}^k) + \frac{\partial^2 \mu_0}{2\partial \mathbf{n}^2}(\eta^k)(\mathbf{n}^* - \mathbf{n}^k)\right] = \hat{\mathbf{C}}_k,$$

then both $\mathbf{B}_k$ and $\mathbf{C}_k$ are diagonal positive definite matrices.

$$\mathbf{B}_k\left[\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I}\right]\left(\mathbf{n}^*-\mathbf{n}^{k+1}\right)+(\mu^*-\mu^{k+1})\mathbf{p}^T=\hat{\mathbf{C}}_k(\mathbf{n}^*-\mathbf{n}^k) \tag{3.2.24}$$

$$\begin{bmatrix} \mathbf{B}_k\left(\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I}\right) & \mathbf{p}^T \\ \mathbf{p} & 0 \end{bmatrix}\begin{bmatrix} \mathbf{n}^*-\mathbf{n}^{k+1} \\ \mu^*-\mu^{k+1} \end{bmatrix}=\begin{bmatrix} \hat{\mathbf{C}}_k & 0 \\ \mathbf{0} & 0 \end{bmatrix}\begin{bmatrix} \mathbf{n}^*-\mathbf{n}^k \\ \mu^*-\mu^k \end{bmatrix}$$

Multiplying both sides of above equation with reversible matrix $\begin{bmatrix} \mathbf{B}_k^{-1} & 0 \\ 0 & 1 \end{bmatrix}$, we have

$$\begin{bmatrix} \mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I} & \mathbf{B}_k^{-1}\mathbf{p}^T \\ \mathbf{p} & 0 \end{bmatrix}\begin{bmatrix} \mathbf{n}^*-\mathbf{n}^{k+1} \\ \mu^*-\mu^{k+1} \end{bmatrix}=\begin{bmatrix} \mathbf{B}_k^{-1}\hat{\mathbf{C}}_k & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} \mathbf{n}^*-\mathbf{n}^k \\ \mu^*-\mu^k \end{bmatrix} \tag{3.2.25}$$

Multiplying both sides of (3.2.25) with $\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ -\mathbf{p}(\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I})^{-1} & 1 \end{bmatrix}$, we can get

$$\begin{aligned}&\begin{bmatrix} \mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I} & \mathbf{B}_k^{-1}\mathbf{p}^T \\ 0 & -\mathbf{p}(\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I})^{-1}\mathbf{B}_k^{-1}\mathbf{p}^T \end{bmatrix}\begin{bmatrix} \mathbf{n}^*-\mathbf{n}^{k+1} \\ \mu-\mu^{k+1} \end{bmatrix}\\ &\quad=\begin{bmatrix} \mathbf{B}_k^{-1}\hat{\mathbf{C}}_k & 0 \\ -\mathbf{p}(\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I})^{-1}\mathbf{B}_k^{-1}\hat{\mathbf{C}}_k & 0 \end{bmatrix}\begin{bmatrix} \mathbf{n}^*-\mathbf{n}^k \\ \mu^*-\mu^k \end{bmatrix}\end{aligned} \tag{3.2.26}$$

Denoting $\mathbf{p}(\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I})^{-1}\mathbf{B}_k^{-1}\mathbf{p}^T =: \alpha$ and multiplying both sides of (3.2.26) with $\begin{bmatrix} \mathbf{I} & \alpha^{-1}\mathbf{B}_k^{-1}\mathbf{p}^T \\ \mathbf{0} & 1 \end{bmatrix}$, we can get

$$\begin{aligned}&\begin{bmatrix} \mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I} & 0 \\ 0 & -\alpha \end{bmatrix}\begin{bmatrix} \mathbf{n}^*-\mathbf{n}^{k+1} \\ \mu-\mu^{k+1} \end{bmatrix}\\ &\quad=\begin{bmatrix} \mathbf{B}_k^{-1}\hat{\mathbf{C}}_k-\alpha^{-1}\mathbf{B}_k^{-1}\mathbf{p}^T\mathbf{p}(\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I})^{-1}\mathbf{B}_k^{-1}\hat{\mathbf{C}}_k & 0 \\ -\mathbf{p}(\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I})^{-1}\mathbf{B}_k^{-1}\hat{\mathbf{C}}_k & 0 \end{bmatrix}\begin{bmatrix} \mathbf{n}^*-\mathbf{n}^k \\ \mu^*-\mu^k \end{bmatrix}\end{aligned} \tag{3.2.27}$$

$$\left(\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I}\right)(\mathbf{n}^*-\mathbf{n}^{k+1})=\left[\mathbf{I}-\alpha^{-1}\mathbf{B}_k^{-1}\mathbf{p}^T\mathbf{p}(\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I})^{-1}\right]\mathbf{B}_k^{-1}\hat{\mathbf{C}}_k(\mathbf{n}^*-\mathbf{n}^k)$$

Therefore,

$$\mathbf{n}^*-\mathbf{n}^{k+1}=\left(\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I}\right)^{-1}\left[\mathbf{I}-\alpha^{-1}\mathbf{B}_k^{-1}\mathbf{p}^T\mathbf{p}(\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I})^{-1}\right]\mathbf{B}_k^{-1}\hat{\mathbf{C}}_k(\mathbf{n}^*-\mathbf{n}^k) \tag{3.2.28}$$

The convergence will be proved by four steps. Firstly, we bring the restriction for the term $\hat{\mathbf{C}}_0(\mathbf{n}^0) = \frac{\partial \mu_{02}}{\partial \mathbf{n}}(\mathbf{n}^0) - \frac{\partial^2 \mu_0}{2\partial \mathbf{n}^2}(\eta^0)(\mathbf{n}^* - \mathbf{n}^0)$ by the term $\mathbf{C}_0(\mathbf{n}^0) = \frac{\partial \mu_{02}}{\partial \mathbf{n}}(\mathbf{n}^0)$. Then we will impose restriction on the term $\mathbf{B}_0^{-1}\mathbf{C}_0(\mathbf{n}^0) = \left(\frac{\partial \mu_{01}(\mathbf{n}^0)}{\partial \mathbf{n}}\right)^{-1} \frac{\partial \mu_{02}(\mathbf{n}^0)}{\partial n}$ when the initial data of the iteration $\mathbf{n}^0$ is close enough to the exact solution $\mathbf{n}^*$. After that, the upper bound for the infinity norm of the matrix $\left(\mathbf{B}_k^{-1}\mathbf{A} + \mathbf{I}\right)$ will be given. The bound of the matrix $\mathbf{I} - \alpha^{-1}\mathbf{B}_k^{-1}\mathbf{p}^T\mathbf{p}(\mathbf{B}_k^{-1}\mathbf{A} + \mathbf{I})^{-1}$ will be provided at last step. And finally, the convergence of this scheme will be detailedly formulated.

First step of proof

Restriction for $\hat{\mathbf{C}}_0 = -\frac{\partial \mu_{02}}{\partial \mathbf{n}}(\mathbf{n}^0) + \frac{\partial^2 \mu_0}{2\partial \mathbf{n}^2}(\eta^0)(\mathbf{n}^* - \mathbf{n}^0)$ by $\mathbf{C}_0 = \frac{\partial \mu_{02}}{\partial \mathbf{n}}(\mathbf{n}^0)$ with the condition $\left\|\mathbf{n}^* - \mathbf{n}^0\right\|_\infty < \varepsilon^*/2$.

From the expressions of $\frac{\partial \mu_{01}}{\partial n}$ and $\frac{\partial \mu_{02}}{\partial n}$, we can get

$$\frac{\partial^2 \mu_{01}}{\partial n^2} = \frac{\partial}{\partial n}\left[\frac{RT}{n\left(1-bn\right)^2}\right] = -\frac{RT\left[\left(1-bn\right)^2 - 2bn(1-bn)\right]}{n^2\left(1-bn\right)^4} = -\frac{RT(1-3bn)}{n^2\left(1-bn\right)^3}$$

$$\begin{aligned}\frac{\partial^2 \mu_{02}}{\partial n^2} &= \frac{\partial}{\partial n}\left[\frac{2a(T)\left(1+bn\right)}{\left(1+2bn-b^2n^2\right)^2}\right] \\ &= \frac{2a(T)\left[b\left(1+2bn-b^2n^2\right)^2 - 2\left(1+bn\right)\left(2b-2b^2n\right)\left(1+2bn-b^2n^2\right)\right]}{\left(1+2bn-b^2n^2\right)^4} \\ &= \frac{2a(T)b\left(-3+2bn+3b^2n^2\right)}{\left(1+2bn-b^2n^2\right)^3},\end{aligned}$$

$$\begin{aligned}\frac{\partial^2 \mu_0}{\partial n^2} &= \frac{\partial^2 \mu_{01}}{\partial n^2} - \frac{\partial^2 \mu_{02}(n)}{\partial n^2} \\ &= -\frac{RT(1-3bn)}{n^2\left(1-bn\right)^3} - \frac{2a(T)b\left(-3+2bn+3b^2n^2\right)}{\left(1+2bn-b^2n^2\right)^3}\end{aligned} \tag{3.2.29}$$

When

$$\frac{\partial^2 \mu_{02}}{\partial n^2} = \frac{2a(T)b\left(-3+2bn+3b^2n^2\right)}{\left(1+2bn-b^2n^2\right)^3} = 0,$$

$$n = \frac{\pm\sqrt{10}-1}{3b}.$$

Because $0 < n < 1/b$, $n = \dfrac{\sqrt{10}-1}{3b}$. At this time,

$$\frac{\partial \mu_{02}}{\partial n} = \frac{2a(T)\left(1+bn\right)}{\left(1+2bn-b^2n^2\right)^2} = \frac{\left(5\sqrt{10}+14\right)}{32}a(T) > 0.$$

Since

$$\frac{\partial^2 \mu_{02}}{\partial n^2} = \frac{2a(T)b\left(-3+2bn+3b^2n^2\right)}{\left(1+2bn-b^2n^2\right)^3} < 0$$

when $0 < n < \dfrac{\sqrt{10}-1}{3b}$, and

$$\frac{\partial^2 \mu_{02}}{\partial n^2} = \frac{2a(T)b\left(-3+2bn+3b^2n^2\right)}{\left(1+2bn-b^2n^2\right)^3} > 0$$

when $\dfrac{\sqrt{10}-1}{3b} < n < \dfrac{1}{b}$, $\dfrac{\partial \mu_{02}}{\partial n}$ gets its minimum at $n = \dfrac{\sqrt{10}-1}{3b}$, and

$$\min\left(\frac{\partial \mu_{02}}{\partial n}\right) = \frac{\left(5\sqrt{10}+14\right)}{32}a(T) > 0. \tag{3.2.30}$$

From (3.2.29), we know that $\dfrac{\partial^2 \mu_0}{\partial n^2}$ gets infinite value when

$$n^2\left(1-bn\right)^3 = 0 \iff n = 0 \quad or \quad n = 1/b$$

$$\left(1+2bn-b^2n^2\right)^3 = 0 \iff n = \frac{1\pm\sqrt{2}}{b}$$

Because $\dfrac{1 \pm \sqrt{2}}{b}$ are not in the adapted region of the solution $(0, 1/b)$, $\dfrac{\partial^2 \mu_{01}(n)}{\partial n^2}$ and $\dfrac{\partial^2 \mu_0(n)}{\partial n^2}$ get their infinite value only at the endpoint of the region $(0, 1/b)$, 0 and $1/b$. According to the continuous property of the function $\dfrac{\partial^2 \mu_0}{\partial n^2}$, $\dfrac{\partial^2 \mu_0}{\partial n^2}$ and the discrete property of n^*, we can put the following assertions:

1. Let $\varepsilon^* = \min\{|bn_i^* - 1|, |bn_i^*|, i = 1, 2, ..., M_t\}$, where M_t is the number of the elements of the vector n^*, then $\varepsilon^* \in (0, 1)$ and for any $i = 1, 2, ..., M_t$, $bn_i^* \in [\varepsilon^*, 1/b - \varepsilon^*]$;

2. There is a $\bar{M} > 0$ which satisfies that: for any $bn_i \in [\varepsilon^*/3, 1-\varepsilon^*/3]$, $\dfrac{\partial^2 \mu_{01}(n_i)}{\partial n^2} \leq \bar{M}$, $\dfrac{\partial^2 \mu_0(n_i)}{\partial n^2} \leq \bar{M}$;

3. For any $\epsilon > 0$, if we choose

$$\varepsilon_0 = \min\left\{\frac{2\varepsilon^*}{3}, 2b\epsilon \min\left(\frac{\partial \mu_{02}(n)}{\partial n}\right)/\bar{M} = b\epsilon \frac{\left(5\sqrt{10} + 14\right)}{16\bar{M}} a(T)\right\},$$

then if $|bn^0 - bn^*| < \varepsilon_0$, then

(a)

$$\min\left\{\left(\frac{\partial \mu_{01}}{\partial n}\right)^{-1} : i = 1, 2, ..., M_t\right\}(n_i^0)$$
$$\geq \left[\frac{\partial \mu_{01}}{\partial n}\left(bn = 1 - \frac{\varepsilon^*}{3}\right)\right]^{-1} = \frac{\left(\frac{\varepsilon^*}{3}\right)^2 \left(1 - \frac{\varepsilon^*}{3}\right)}{bRT};$$

(b) for any η^0 between n^* and n^0,

$$\left\|\frac{\partial^2 \mu_0}{2\partial n^2}(\eta^0)(n^* - n^0)\right\| < \epsilon \min\left(\frac{\partial \mu_{02}(n)}{\partial n}\right) = \epsilon \frac{\left(5\sqrt{10} + 14\right)}{32} a(T)$$

hence,

$$\left\| \frac{\partial \mu_{02}}{\partial n}(n^0) - \frac{\partial^2 \mu_0}{2\partial n^2}(\eta^0)(n^* - n^0) \right\| < (1+\epsilon) \left\| \frac{\partial \mu_{02}(n)}{\partial n}\left(n^0\right) \right\|.$$

The second step of proof

Maximum of the norm of the matrix $\left(\frac{\partial \mu_{01}(n)}{\partial n}\right)^{-1} \frac{\partial \mu_{02}(n)}{\partial n}$.

Let $u = \frac{\frac{\partial \mu_{02}(n)}{\partial n}}{\frac{\partial \mu_{01}(n)}{\partial n}} = \left(\frac{2a(T)n\,(1+bn)\,(1-bn)^2}{RT\,(1+2bn-b^2n^2)^2}\right)$, then

$$\begin{aligned}
\frac{\partial u}{\partial n} =& \frac{\partial \left(\frac{2a(T)n(1+bn)(1-bn)^2}{RT(1+2bn-b^2n^2)^2}\right)}{\partial n} \\
=& \frac{2a(T)}{RT}\left[\frac{(1+bn)\,(1-bn)^2 + bn\,(1-bn)^2 - 2bn(1-b^2n^2)}{(1+2bn-b^2n^2)^2}\right. \\
&\left. - \frac{n\,(1+bn)\,(1-bn)^2\,2\,(2b-2b^2n)}{(1+2bn-b^2n^2)^3}\right] \\
=& \frac{2a(T)}{RT}\left[\frac{1-3bn-b^2n^2+3b^3n^3+bn-2b^2n^2+b^3n^3}{(1+2bn-b^2n^2)^2}\right. \\
&\left. - \frac{4bn\,(1-2bn+b^2n^2-b^2n^2+2b^3n^3-b^4n^4)}{(1+2bn-b^2n^2)^3}\right] \\
=& \frac{2a(T)\,(1+3b^4n^4-4bn)}{RT\,(1+2bn-b^2n^2)^3} \\
=& \frac{-2a(T)\,(1-bn)\,(3b^3n^3+3b^2n^2+3bn-1)}{RT\,(1+2bn-b^2n^2)^3}
\end{aligned} \tag{3.2.31}$$

Because $0 < bn < 1$, $1 - bn \neq 0$, when $\frac{\partial u}{\partial n} = 0$,

$$3b^3n^3 + 3b^2n^2 + 3bn - 1 = 0. \tag{3.2.32}$$

Now we use Shengjin's Formulas to solve this cubic equation. Here, $\bar{a} = 3b^3$, $\bar{b} = 3b^2$, $\bar{c} = 3b$, $\bar{d} = -1$ for the original cubic equation $\bar{a}n^3 + \bar{b}n^2 + \bar{c}n + \bar{d} = 0$.

$$\begin{aligned}
A &= \bar{b}^2 - 3\bar{a}\bar{c} = 9b^4 - 27b^4 = -18b^4, \\
B &= \bar{b}\bar{c} - 3\bar{a}\bar{d} = 9b^3 + 27b^3 = 36b^3, \\
C &= \bar{c}^2 - 3\bar{b}\bar{d} = 9b^2 + 9b^2 = 18b^2, \\
\triangle &= B^2 - 4AC = (36b^3)^2 + 4 * 18b^4 * 18b^2 = 2 * (36b^3)^2 > 0.
\end{aligned}$$

So the cubic equation has only one real solution.

$$\begin{aligned}
Y1, Y2 &= A\bar{b} + 3\bar{a}\left[-B \pm (B^2 - 4AC)^{1/2}\right]/2 \\
&= -18b^4 * 3b^2 + 3 * 3b^3\left[-36b^3 \pm \left(2 * (36b^3)^2\right)^{1/2}\right]/2 \\
&= -54b^6 + 9b^6 * \left(-18 \pm 18\sqrt{2}\right) \\
&= -54b^6\left(1 + 3 \mp 3\sqrt{2}\right) = -54b^6\left(4 \mp 3\sqrt{2}\right) \\
(Y1)^{1/3} &= -3\sqrt[3]{2}b^2(4 - 3\sqrt{2})^{1/3} = 3b^2 * 0.7858, \\
(Y2)^{1/3} &= -3\sqrt[3]{2}b^2(4 + 3\sqrt{2})^{1/3} = -3b^2 * 2.5451, \\
&= \frac{[-3b^2 - 3b^2 * 0.7858 + 3b^2 * 2.5451]}{3 * 3b^3} \\
&= \frac{[-1 - 0.7858 + 2.5451]}{3b} = \frac{0.7593}{3b} = \frac{0.2531}{b}.
\end{aligned}$$

Therefore, $u = \dfrac{\frac{\partial \mu_{02}(n)}{\partial n}}{\frac{\partial \mu_{01}(n)}{\partial n}}$ gets its maximum value when $n = \dfrac{0.2531}{b}$. At this time,

$$u_{max} = \frac{2a(T)\frac{0.2531}{b}(1 + 0.2531)(1 - 0.2531)^2}{RT(1 + 2 * 0.2531 - 0.2531^2)^2} = \frac{0.1701a(T)}{RTb}$$

According the expressions of $a(T)$ and $b(T)$, we have

$$u_{max} = \frac{0.354a(T)}{RTb} = \frac{0.1701 * \left(0.45724\frac{R^2T_c^2}{P_c}\left(1 + m\left(1 - \sqrt{\frac{T}{T_c}}\right)\right)^2\right)}{RT\left(0.07780\frac{RT_c}{P_c}\right)}$$

$$=\frac{T_c}{T}\left(1+m\left(1-\sqrt{\frac{T}{T_c}}\right)\right)^2.$$

For any $\delta > 0$, if

$$\frac{T_c}{T}\left(1+m\left(1-\sqrt{\frac{T}{T_c}}\right)\right)^2 < \delta, \tag{3.2.33}$$

or

$$T_r = \frac{T}{T_c} > \left(\frac{m+1}{m+\sqrt{\delta}}\right)^2, \quad \text{when} \quad 0 < m \leq \sqrt{\delta}, \tag{3.2.34}$$

$$\left(\frac{m+1}{m+\sqrt{\delta}}\right)^2 < T_r = \frac{T}{T_c} < \left(\frac{m+1}{m-\sqrt{\delta}}\right)^2, \quad \text{when} \quad m > \sqrt{\delta}, \tag{3.2.35}$$

then

$$\left\|\mathbf{B}^{-1}\mathbf{C}_k\right\| < \delta \tag{3.2.36}$$

can be satisfied for any iterative step.

The third step for the proof of convergence

Upper bound for $\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I}$. Because $\mathbf{B}_k$ is a positive definite diagonal matrix, $\mathbf{A}$ is diagonally-dominant positive definite M-matrix, $\mathbf{B}_k^{-1}\mathbf{A}$ is also diagonally-dominant positive definite, $\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I}$ is diagonal strictly dominant positive definite. In this passage, we apply the following definitions and results provided by [102] to obtain the upper bound for $\left\|\left(\mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I}\right)^{-1}\right\|_\infty$. Let

$$\mathbf{G}_k = \mathbf{B}_k^{-1}\mathbf{A}+\mathbf{I},$$

then $\mathbf{G}_k = (g_{ij})$ is an $M_t \times M_t$ strictly diagonally dominant M-matrix. From the reference paper [102], we have

$$\left\|\left(-c\Delta_h + \frac{\partial\mu_{01}}{\partial n}(n^0)\right)^{-1}\frac{\partial\mu_{01}}{\partial n}(n^0)\right\|_\infty$$

$$= \left\|\mathbf{G}_k^{-1}\right\|_\infty \leq \max_{i=1}^{M_t} \left\{ \frac{1}{|\mathbf{G}_{k_{ii}}| - \sum_{j=1,2,\ldots,N,j\neq i} |\mathbf{G}_{ij}|} \right\} \leq 1.$$

The fourth step to prove the convergence

Suppose we can get

$$\left\|\mathbf{I} - \alpha^{-1}\mathbf{B}_k^{-1}\mathbf{p}^T\mathbf{p}(\mathbf{B}_k^{-1}\mathbf{A} + \mathbf{I})^{-1}\right\| < 2$$

Derivation of the convergence

In this subsection, we give the conclusion of all the above theoretical results. Let $\mathbf{C}_k = \dfrac{\partial\mu_{02}}{\partial n}(n^0)$, then

$$\begin{aligned}
&\left\| \left(-c\Delta_h + \frac{\partial\mu_{01}}{\partial n}(n^0) \right)^{-1} \frac{\partial\mu_{02}}{\partial n}(n^0) \right\|_\infty \\
&= \left\| (\mathbf{A} + \mathbf{B}_k)^{-1} \mathbf{C}_k \right\|_\infty \\
&= \left\| (\mathbf{A} + \mathbf{B}_k)^{-1} \mathbf{B}_k \mathbf{B}^{-1} \mathbf{C}_k \right\|_\infty \\
&\leq \left\| (\mathbf{A} + \mathbf{B}_k)^{-1} \mathbf{B}_k \right\|_\infty \left\| \mathbf{B}^{-1} \mathbf{C}_k \right\|_\infty \\
&\leq \left\| \mathbf{B}^{-1} \mathbf{C}_k \right\|_\infty
\end{aligned} \tag{3.2.37}$$

From the second subsubsection of this part, for any $0 < \delta < 1$, if

$$\frac{T_c}{T}\left(1 + m\left(1 - \sqrt{\frac{T}{T_c}}\right)\right)^2 < \delta, \quad \left\|\mathbf{B}^{-1}\mathbf{C}_k\right\|_\infty \leq \delta,$$

then

$$\begin{aligned}
\left\|n^* - n^1\right\|_\infty &\leq 2\left(1 + \epsilon\right) \left\| \left(-c\Delta_h + \frac{\partial\mu_{01}}{\partial n}(n^0) \right)^{-1} \frac{\partial\mu_{02}}{\partial n}(n^0) \right\|_\infty \left\|n^* - n^0\right\|_\infty \\
&\leq 2\delta\left(1 + \epsilon\right) \left\|n^* - n^0\right\|_\infty
\end{aligned} \tag{3.2.38}$$

$$\left\|n^* - n^2\right\|_\infty \leq 2 \left\| \left(c\Delta_h - \frac{\partial\mu_{01}}{\partial n}(n^1) \right)^{-1} (1 + \epsilon) \frac{\partial\mu_{02}}{\partial n}(n^1) \right\|_\infty \left\|n^* - n^1\right\|_\infty$$

$$= 2\,(1+\epsilon)\left\|\left(-c\Delta_h + \frac{\partial\mu_{01}}{\partial n}(n^1)\right)^{-1}\frac{\partial\mu_{02}}{\partial n}(n^1)\right\|_\infty \left\|n^* - n^1\right\|_\infty \quad (3.2.39)$$

If $\left\|n^0 - n^*\right\| < \varepsilon_0$ and $\delta\,(1+\epsilon) \leq 1$,

$$\left\|n^* - n^1\right\| \leq \left\|n^* - n^0\right\|_\infty < \varepsilon_0$$

then

$$\left\|\frac{\partial^2\mu_0}{2\partial n^2}(\eta^1)(n^* - n^1)\right\| < \epsilon \min\left(\frac{\partial\mu_{02}(n)}{\partial n}\right) = \epsilon\frac{\left(5\sqrt{10}+14\right)}{32}a(T),$$

$$\left\|\frac{\partial\mu_{02}}{\partial n}(n^1) - \frac{\partial^2\mu_0}{2\partial n^2}(\eta^1)(n^* - n^1)\right\| < (1+\epsilon)\left\|\frac{\partial\mu_{02}(n)}{\partial n}\left(n^0\right)\right\|.$$

From (3.2.38), we have

$$\left\|\left(c\Delta_h - \frac{\partial\mu_{01}}{\partial n}(n^1)\right)^{-1}\frac{\partial\mu_{02}}{\partial n}(n^1)\right\|_\infty \leq \delta,$$

Therefore,

$$\begin{aligned}\left\|n^* - n^2\right\| &\leq 2\,(1+\epsilon)\left\|\left(c\Delta_h - \frac{\partial\mu_{01}}{\partial n}(n^1)\right)^{-1}\frac{\partial\mu_{02}}{\partial n}(n^1)\right\|_\infty \left\|n - n^1\right\|_\infty \\ &\leq 2\,(1+\epsilon)\,\delta\left\|n^* - n^1\right\|_\infty \\ &\leq 2\left\|n^* - n^1\right\|_\infty \leq \left\|n^* - n^0\right\|_\infty\end{aligned}$$

If we assume that

$$\left\|n^* - n^l\right\| | \leq \delta\,(1+\epsilon)\left\|n^* - n^{l-1}\right\|_\infty \leq \left\|n^* - n^0\right\|_\infty$$

for $l = 1, 2, ..., k$, under the condition $\delta \leq \dfrac{1}{\epsilon+1}$, then

$$\left\|n^* - n^{k+1}\right\|_\infty$$

$$\leq 2\left\|\left(-c\Delta_h+\frac{\partial\mu_{01}}{\partial n}(n^k)\right)^{-1}\left[\frac{\partial\mu_{02}}{\partial n}(n^k)-\frac{\partial^2\mu_0}{2\partial n^2}(\eta^k)\left(n^*-n^k\right)\right]\right\|_\infty\left\|n^*-n^k\right\|_\infty$$

$$\leq 2\left(1+\epsilon\right)\left\|\left(-c\Delta_h+\frac{\partial\mu_{01}}{\partial n}(n^k)\right)^{-1}\frac{\partial\mu_{02}}{\partial n}(n^k)\right\|_\infty\left\|n^*-n^k\right\|_\infty$$

$$\leq 2\left(1+\epsilon\right)\delta\left\|n^*-n^k\right\|_\infty$$

$$\leq 2\left(1+\epsilon\right)^{k+1}\delta^{k+1}\left\|n^*-n^0\right\|_\infty$$

$$\leq 2\left\|n^*-n^k\right\|_\infty\leq\left\|n^*-n^0\right\|_\infty$$

In conclusion, for any $\epsilon>0$, if we choose n^0 satisfies $\|n^0-n^*\|_\infty<\varepsilon_0$, where

$$\varepsilon_0=\min\left\{\frac{\varepsilon^*}{4},2\epsilon\min\left(\frac{\partial\mu_{02}(n)}{\partial n}/M_t\right)=\epsilon\frac{\left(5\sqrt{10}+14\right)}{16M}a(T)\right\},\tag{3.2.40}$$

$$\varepsilon^*=\min\left\{\left|n_i^*-\frac{1}{b}\right|,|n_i^*|\,,i=1,2,...,M_t\right\},$$

then for the substance which satisfies

$$\left\|\left(\frac{\partial\mu_{01}}{\partial n}(n^0)\right)^{-1}\left(\frac{\partial\mu_{02}}{\partial n}(n^0)\right)\right\|_\infty<\delta=\frac{1}{2(1+\epsilon)},\tag{3.2.41}$$

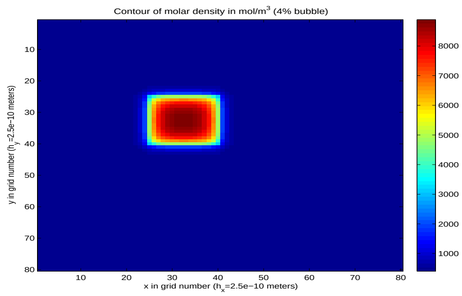
the convex-splitting based Newton iterative scheme (3.2.21) and (3.2.15) is convergent. □

3.3 Numerical Examples

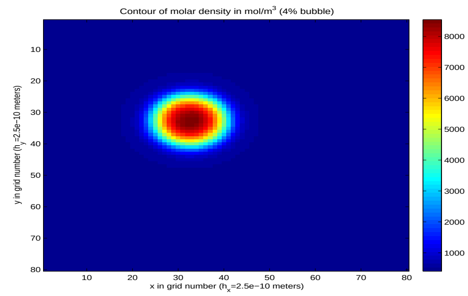
In this section, we will provide examples to show the free energy evolution properties of the original Newton iteration (3.2.14)-(3.2.15) and the convex-splitting based Newton iterative scheme (3.2.18)-(3.2.19). The mass conservation of the original Euler-Lagrange equation is guaranteed by introducing the mass conservation restriction using the auxiliary Lagrangian multiplier, which is also viewed as an unknown variable. We also use isobutane (nC_4) at the temperature of 350K for our numerical experimentations. The considered domain is $\Omega = [0, L_x] \times [0, L_y]$, where both L_x and L_y equal $2.0e-8$ meters with mesh width $h_x = h_y = 2.5e-10$ meters. The tolerance of the relative error between two contiguous iterative step of both methods are set to be 10^{-8}. Fig. 3.1 and Fig. 3.2 depict results obtained from the original Newton iteration and the convex splitting method, showing that, these two methods provides similar molar density evolution history and final state. Both of them provide clear descriptions that the shape of the liquid bubble becomes rounded, and has a circular final state with a visible gas-liquid interface. However, Fig. 3.1 (g) reveals that there are energy jumps during Newton iterations, which does not coincide with the physical principle. Comparatively, the recent energy evolution trend of the convex-splitting method showed in Fig. 3.2 (g) is satisfied by all the other short time continuous iterative steps. This certifies the energy stability of the convex-splitting method.

3.4 Chapter summary

In conclusion, the Euler-Lagrange equation for the single-component, two-phase substance is solved by a convex-splitting method. We applied its unconditional energy stability to obtain a physically appropriate iteration. Numerical results demonstrate this energy decay property clearly. The energy stability of this method could be guaranteed theoretically based on the convergence condition. However, the convergence of this method is really hard to obtain due to the high nonlinearity of the involved functions and the difficulty to satisfy the requirement of the application background. Our future work will still concern on this meaningful task based on the previous achievements [11, 55, 64, 65, 57, 76, 77, 102].



(a)



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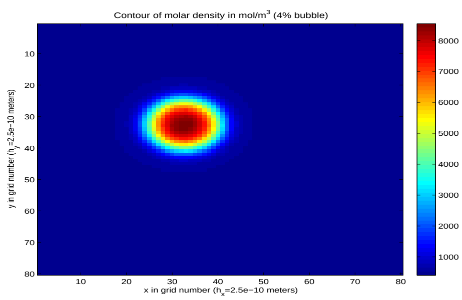

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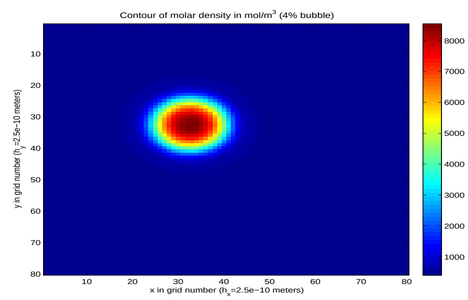

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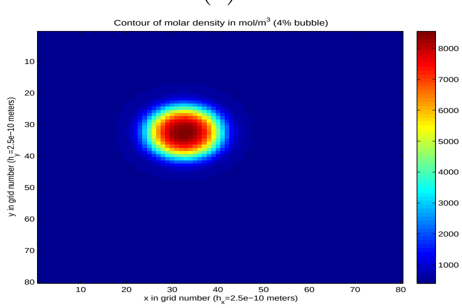

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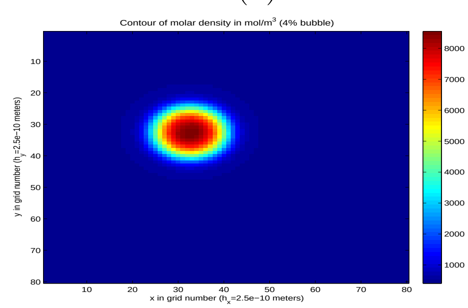
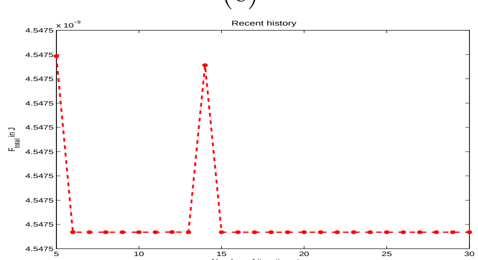
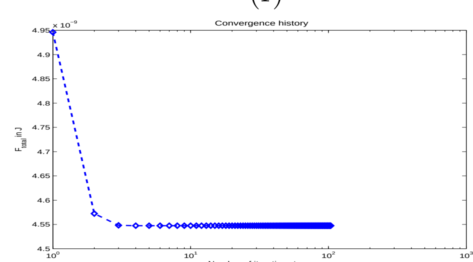


(f)



(g)



(l)

Figure 3.1: The results given by Newton iterative method. The molar density of the pure component at (a): initial time, (b): the 15th iterative step, (c): the 30th iterative step, (d): the 60th iterative step, (e): the 90th iterative step, (f): the final state at 104 iterative step; (g): the total Helmoholtz free energy decay history from the 5th to the 30th iterative step, (h): the whole total Helmoholtz free energy decay history.

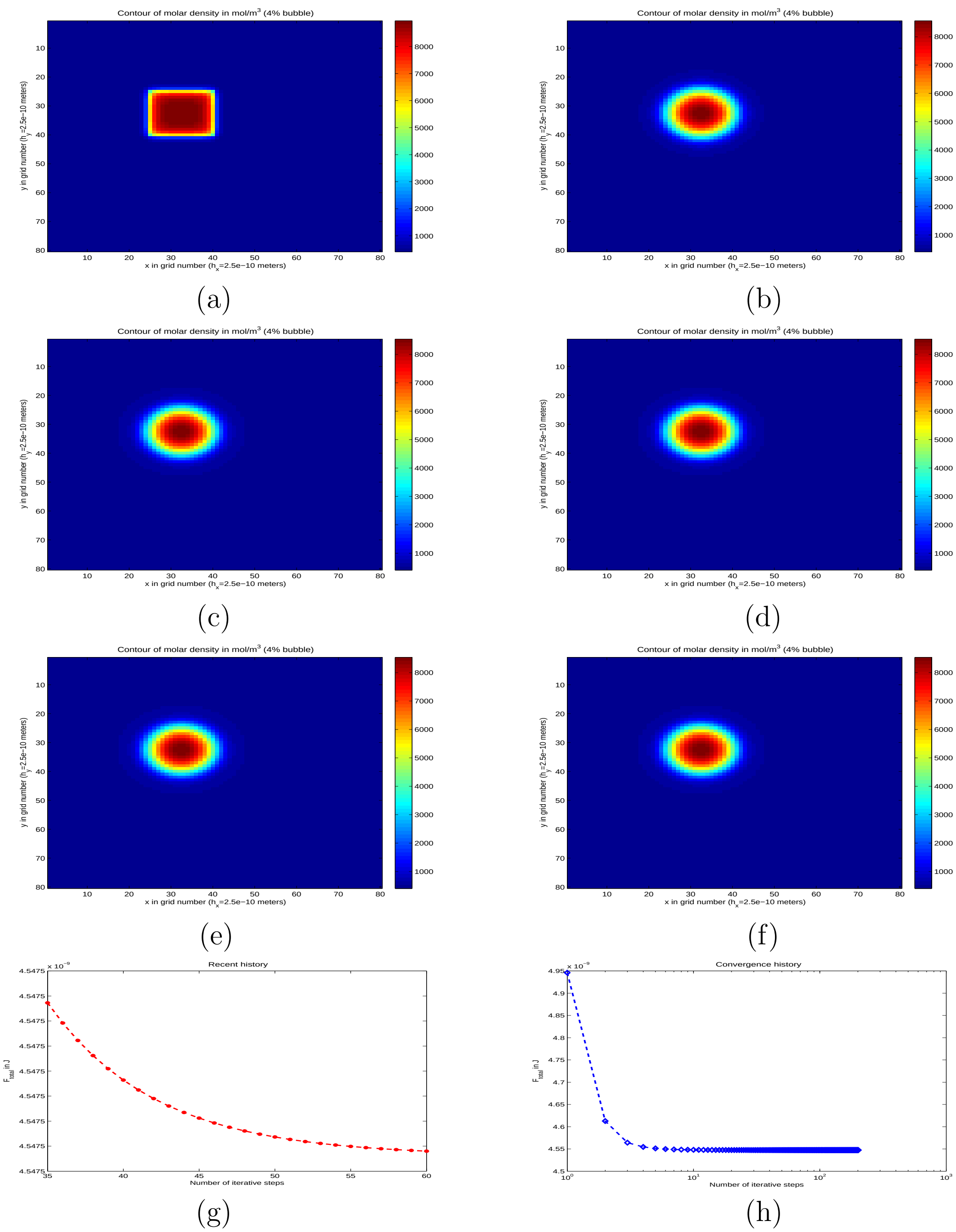


Figure 3.2: The results given by the convex-splitting based Newton iterative scheme. The molar density of the pure component at (a): initial time, (b): the 30th iterative step, (c): the 60th iterative step, (d): the 90th iterative step, (e): the 150th iterative step, (f): the 202th iterative step; (g): the total Helmoholtz free energy decay history from the 35th to the 60th step, (h): the whole total Helmoholtz free energy decay history.

Chapter 4

Conclusions and Future Work

In this chapter, we would like to finish this thesis with some concluding remarks and outline of possible future work.

4.1 Concluding Remarks

In this dissertation, we have investigated a diffusive interface model with Peng-Robinson EOS for oil-gas systems involved in oil-exploitation engineering. Although voluminous achievements have been made based on the phase field model, the research work for the partial differential equations derived from a realistic equation of state for practical industrial materials is relatively few. The application of Peng-Robinson EOS for derivation of the mathematical differential equations to describe the flowing process and the steady state of special substances is really recent [58, 59, 60, 85]. The high nonlinear property of these equations, which arises from the free energy given by the equation of state, poses great obstacles to solve them theoretically or numerically.

Our work concentrates on efficient numerical methods for these equations. This thesis concerns numerical simulations of the single-component, two-phase fluids in two dimensional space. The fourth-order parabolic equation and the Euler-Lagrange equation are our main focus of study.

For the fourth-order parabolic equation of pure substance, we have applied a first-order convex-splitting scheme, the Crank-Nicolson scheme and a second order linearization scheme to solve it. Their mass conservation, unconditional energy stability, unique solvability and L^{∞} convergence are proved systematically. The high nonlinearity of the original homogeneous free energy density brings great requirement of these numerical schemes to satisfy the convergence condition. This barrier was overcome by applying the idea proposed by Li et al.[63] in 2012 from a theoretical standpoint. The approach used in our work is able to shed light on ways of overcoming similar difficulty involved in the derivation of the convergence of a numerical scheme for other phase field models. In addition, this nonlinear property and the unboundness of the homogeneous free energy density pose obstacles to approach the steady state for the numerical schemes of the investigated equation. The temporal step was required to be set sufficiently small to reach to final state. This complexity of the free energy functional arising from the real cubic Peng-Robinson equation of state does not exist for the classical quartic Ginzburg-Landau free energy functional, and involves more difficulties than the double-well free energy functional with logarithmic terms. Therefore, the numerical schemes proposed for the fourth-order parabolic equation investigated in our work could be applied to the same kind equations based on the double-well potential. Moreover, numerical results have demonstrated the reasonability of the theoretical demands and shown great agreement with previous published results.

The discrete Euler-Lagrange equation is studied by Picard iteration, Newton iteration and a convex-splitting based Newton iterative method. The first order convergence of Picard iteration could not be satisfied due to the unboundedness of the substance's homogeneous chemical potential and its first order derivative with respect to variable $n(\mathbf{x})$. The numerical test of this method failed to provide an acceptable equilibrium state of the one-component, two-phase fluids. The second order convergent Newton iteration can provide reasonable solution to the discrete Euler-Lagrange equation if appropriate initial data is given. However, the total discrete energy evolution trend was not always decreasing, which does not coincide with the physical principle. The convex-splitting based Newton iterative method is firstly used to the time-independent equation to guarantee its energy stability at every iterative step without loss of the the symmetry and positive-definite property of the matrix of coefficients. This kind of energy stability is also verified by numerical experiments. The derivation of the convergence of this iterative method is hindered by nontrival barriers. However, it is still meaningful to overcome these difficulties for guidance of application of this method.

4.2 Future work

As mentioned above, this dissertation is just a starting work for mathematical models based on Peng-Robinson EOS on real oil-exploitation practice. Future work based on these achievements could be conducted from following perspectives as discussed below.

Firstly, the Euler-Lagrange equations of the single or more components need to be analyzed from both theoretical and numerical aspects. Theoretically, one can not ignore its solvability and the properties of its potential solution. Numerically, more iterative methods could be proposed and analyzed in detail. The requirements from the chemical or physical properties of different substances for the iteration may be presented for practical application. The convergence analysis of the convex-splitting scheme for the pure substance is still worth of further investigation.

Next, the solution of the proposed parabolic equation, both second-order and fourth-order for one or more substances, are potential candidates to be approached by theoretical and numerical methods. On the one hand, further theoretical analyses of their solutions are not only essential to obtain their analytic solutions, but also important to provide significant guidance to devise numerical schemes. Ingenious ideas investigated for analysis of the Cahn-Hilliard equation [15, 29, 44, 90], phase-field crystal model [33, 42, 43, 81, 84] would be of great help on this aspect. On the other hand, previous studied numerical methods for phase field equations could be tentatively used, such as different linearization techniques [45, 63, 86, 96], stabilized schemes [52, 68, 113], higher order numerical approaches [62, 86, 92, 112], spectral method [22, 68] or finite element method [25] with high order [40] or more complicated domains with different initial or boundary conditions. Moreover, both spatial and temporal adaptive strategies [27, 88, 108, 111, 117, 118] could be applied. Furthermore, it is not an easy task to extend numerical schemes developed in this work for single-component fluids to multi-component case due to cross-product terms of the parameters and molar density for different components involved in their molar density equations. A rigid convex-splitting analysis will be studied in our future work to overcome this difficulty.

Finally, practical flowing process could be simulated by combination of the previous dynamic equations of this diffusive model with the equations on flow field. This work may involve many non trivial tasks, such as improvement of the existing models derived from the thermodynamic framework [12, 26, 48, 71, 72, 73, 74, 75, 78, 103], devising appropriate numerical methods to solve these equations in two or three dimensional spaces based on the references of [5, 47, 46, 49, 106, 109, 115].

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