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Modeling studies and numerical analyses of coupled PDEs system in electrohydrodynamics

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MODELING STUDIES AND NUMERICAL ANALYSES OF COUPLED PDES SYSTEM IN ELECTROHYDRODYNAMICS

by

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ABSTRACT

MODELING STUDIES AND NUMERICAL ANALYSES OF COUPLED PDES SYSTEM IN ELECTROHYDRODYNAMICS

by

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Electrohydrodynamics (EHD) is the term used for the hydrodynamics coupled with electrostatics, whose governing equations consist of the electrostatic potential (Poisson) equation, the ionic concentration (Nernst-Planck) equations, and Navier-Stokes equations for an incompressible, viscous dielectric liquid. In this dissertation, we focus on a specific application of EHD - fuel cell dynamics - in the field of renewable and clean energy, study its traditional model and attempt to develop a new fuel cell model based on the traditional EHD model. Meanwhile, we develop a series of efficient and robust numerical methods for these models, and carry out their numerical analyses on the approximation accuracy. In particular, we analyze the error estimates of finite element method for a simplified 2D isothermal steady state two-phase transport model of Proton Exchange Membrane Fuel Cell (PEMFC) as well as its transient version. On the aspect of hydrodynamics arising in the fuel cell system, the fluid flow through the open channels and porous media at the same time, both Navier-Stokes equations and Darcys law are involved in the fluid domains, leading to a Navier-Stokes-Darcy coupling problem. In this dissertation, we study a one-continuum model approach, so-called Brinkman model, to overcome this problem in a more efficient way. To develop a new fuel cell model based on EHD theory, in addition to the two-phase transport model of fuel cells, we carry out numerical analyses for Poisson-Nernst-Planck (PNP) equations using both standard FEM and mixed FEM, which are the essential governing equations involved by EHD model. Finally, we are able to further extend the traditional fuel cell model to more general cases in view of EHD characteristics, and develop a new fuel cell model by appropriately combining PNP equations with the traditional fuel cell model. We conduct the error analysis for PNP-Brinkman system in this dissertation.

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I would like to thank my Ph.D. academic and dissertation advisor Dr. Pengtao Sun. Throughout the years of doing research with him, he has passed on to me the knowledge, the researching skills and methods and the important values of the academic world. He has given me advices, suggestions and guidance on countless occasions. He has always been kind and patient with me. Without the time and effort he put in, the completion of my dissertation would not have come this soon.

I would give all my love to my mom, Bin Gao, and my husband, Juan C. Mariscal. I thank them for supporting me emotionally, for understanding me through hard times, and for always being there for me whenever needed.

Ultimately, I would not have accomplished anything without my personal savior Jesus Christ, who has changed my life so fundamentally 7 years ago. His mercy and grace is beyond describable and His holiness is beyond my imagination. Though lacking of proving methods, I am proud of being a mathematician who believes His existence, surely as I believe the sun rises from the east and sets to the west.

"I am the Alpha and the Omega," says the Lord God, "who is, and who was, and who is to come, the Almighty." – Revelation 1:8.

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CHAPTER 1

INTRODUCTION

1.1 Introduction

In this dissertation, we are going to study a coupled system of partial differential equations (PDEs) which consists of multiple convection-diffusion-reaction equations, Stokes or Navier-Stokes or modified Navier-Stokes equations, and multiple Poisson equations together. Such coupled system of PDEs arises from many multiphysics problems, such as (1) fuel cell dynamics, in which the convection-diffusion-reaction equation is used to model the multiphase water, hydrogen and oxygen transports driven by the electrochemical kinetics model (Butler-Volmer equation), Navier-Stokes equations are used to model the clear fluid flow in gas channels, the Poisson-like Darcy equation is adopted to model the seepage flow in gas diffusion layers (porous media), and other Poisson equations are used to define the potential equations of proton and electron; (2) petroleum reservoir simulation, in which water, oil and gas present a multiphase transport phenomenon, and their saturations satisfy a convection-diffusion-reaction equation, the fluid velocity and pressure through the pores in the porous media are defined by Darcy's law and Darcy equation; (3) electrohydrodynamics (EHD), also known as electro-fluid-dynamics (EFD) or electrokinetics, is the study of the dynamics of electrically charged fluids, studying the motions of ionized particles or molecules and their interactions with electric fields and the surrounding fluid, where, the convection-diffusion-reaction equations, also particularly called Nernst-Planck equations, are used to model the ionic concentrations, the Poisson equation demonstrates the diffusive behavior of the electrostatic potential, and the fluid flow is modeled by Navier-Stokes equation, as always.

Taking into account the governing equations of the petroleum reservoir model, they basically contain most of the essential mathematical features of electrohydrodynamics except that the involved fluid flow is restricted as the seepage flow in the porous media, modeled by Darcy equation instead of Navier-Stokes equations. Additionally, there exists a large difference in the physical feature: its fluid flow does not carry on the electrically charged particles, which significantly differ the reservoir model from the electrohydrodynamics model. Comparing to the reservoir model, as a specific application of electrohydrodynamics in the field of electrochemistry through the combination of open gas channel and gas diffusion layers, fuel cell dynamics turns out to be more attractive because of its close relationship with the renewable and green energy technology in sciences and engineering, and its sophisticated model equations in mathematics which involve multiphysics, multiphase, multi-component, multi-domain with Navier-Stokes-Darcy coupling, and stackable structure, almost most of the challenging numerical difficulties are presented in fuel cell model.

In particular, proton exchange membrane fuel cells (PEMFC) have been the center of attention for over two decades as a possible candidate for next-generation energy conversion, being versatile, highly efficient and environmentally friendly. in the past three decades, research has accelerated in order to successfully deploy this promising technology in daily life particularly for terrestrial transportation to increase the overall energy conversion efficiency and reduce exhaust emissions of automobiles. Now the dream comes true soon. The Toyota Mirai, the world's first commercialized hydrogen fuel-cell sedan for the mass market was unveiled in 2014, and will go for the global sales during 2015. The Mirai features the Toyota Fuel Cell System, which combines fuel cell technology with hybrid technology. The system is more energy efficient than internal combustion engines, and offers excellent environmental performance without emitting CO_2 or other harmful substances during driving. in Japanese, "Mirai" means "future", and the Mirai is the future of motoring: It runs solely on hydrogen and its only emission is water. Expected later in 2015, the Mirai initially will be sold or leased just in California, where the infrastructure for hydrogen fueling exists.

Thus evidently, there is a huge and timely demand for an intensive research and development of fuel cell technologies. The research will be a multidisciplinary effort requiring expertise from many areas of science and engineering. Fuel cells draw energy through electrochemical reactions from, for example, hydrogen and oxygen and such electrochemical processes can be potentially modeled by mathematical equations derived from basic laws in physics and chemistry. With sophisticated mathematical model, advanced numerical techniques and high performance computing, computational and applied mathematicians can play a unique role and make a significant impact in the development of fuel cell technology. Fuel cell and automotive industries are presently placing their focus on fuel cell design and engineering for better performance, improved durability, cost reduction, and better cold-start characteristics. This new focus has led to an urgent need for powerful and efficient multiphysics simulation of hydrogen/air polymer electrolyte fuel cells.

In Chapter 3 of this dissertation, we will continue to carry out our research on the modeling and numerical studies for the multiphase transport model of PEM fuel cell, and more beyond, analyze the derived numerical methodologies and discretizations, eventually come up with the comprehensive numerical analyses including the theoretical proofs and the convergence error estimations. In addition, since fuel cells contain the open gas channels and diffusion layers (porous media) together through which the clear fluid couples with the seepage flow by contacting with each other across the interface in between, we adopt the modified (Navier-) Stokes equations, which is so-called Brinkman model, to describe such (Navier-) Stokes-Darcy coupling fluid dynamics existing in the fuel cell model, where, a no-slip interface condition is reasonably assumed on the surface of the solid portion of the interface between the clear fluid and the porous medium. In Chapter 3, we will also conduct a comprehensive modeling study and an asymptotic analysis between the Brinkman model and the corresponding Stokes-Darcy coupling model, further, a convergence error analysis of the mixed finite element method for Brinkman model.

In summary, the fuel cell model basically involves the species transport (convection-diffusion-reaction) equations, fluid flow (Navier-Stokes-Darcy) equations, energy (heat convection-conduction) equation, and electrostatic potential (Poisson) equations, whose source terms are all characterized by a simplified electrochemical kinetics, so-called Butler-Volmer equation, based on the assumption of local equilibrium of the diffuse (polarization) layer. However, such equilibrium assumption for the diffuse charge distribution is not always held. When ions can be considered as point charges, without excluded volume, the structure of the electrolyte including the polarization layer that forms on the electrodes is described using the full, non-equilibrium Poisson-Nernst-Planck (PNP) model for the transport rates of all mobile ions through the electrolyte [Smith and White (1993)]. The PNP model completes the mathematical description without arbitrary assumptions such as local equilibrium or electro-neutrality of the electrolyte or for instance a prescribed, constant surface charge, and can be applied in such situations as thin electrolyte films (where diffusion layers overlap and/or the bulk electrical field is a significant portion of the field strength in the polarization layer), operation at large, super-limiting currents or large AC frequencies, which are all situations where the diffuse charge distribution loses its quasi-equilibrium structure, making the standard Butler-Volmer equation no longer fit.

The PNP model describes ion concentration and potential profiles both in the electrolyte bulk, as well as in the diffusion layers, all the way up to the reaction planes. The resulting PNP-fuel cell model can be generally used, for the equilibrium and non-equilibrium situation, as well as for steady-state and fully dynamic transport problems. Therefore, in Chapter 4 of this dissertation, we will design the appropriate numerical methodologies for PNP equations, as well as conduct their numerical analyses. Then in Chapter 5, we will develop a new fuel cell model that is distinguished form the traditional fuel cell model, in which the standard Butler-Volmer approach is replaced by solving the more general PNP equations. We will first carry out a numerical analysis for the combination of PNP equations and the modified Stokes (Brinkman) equations in Chapter 5, and leave the analysis for a more broader combination of other model equations, i.e., the species transports and energy equations, as the future work, which shall be analogous to the analyses carried out in Chapter

3 and 4.

1.2 Outline

This dissertation can be divided into four parts. In the first part, Chapter 2, we provide some useful preliminary results and introduce some notations used in the rest of dissertation.

The second part, Chapter 3, we mainly study the simplified traditional fuel cell model. Section 3.2 introduces a simplified 2D steady state two-phase transport model in the cathode GDL of PEMFC using Kirchhoff transformation, describes its finite element scheme, proves the approximation theorem and carries out the numerical experiment to verify the error estimate results proved in Section 3.2.4. Section 3.3 introduces a simplified 2D two-phase transport model in the cathode GDL of PEMFC using Kirchhoff transformation. The semi-discrete finite element scheme is presented and its error estimate is given in Section 3.3.3. A fully discrete finite element method with Crank-Nicolson scheme is designed and analyzed correspondingly in Section 3.3.4. Then, Section 3.4 studies the Brinkman model and its relationship with Darcy's law and Stokes equation with a parameter re-scaling technique. In Section 3.4.3, the asymptotic analyses are introduced between the Stokes system and Brinkman model and between the Darcy's law and Brinkman model. In Section 3.4.4 and Section 3.4.5, the mixed finite element schemes are described and the approximation theorems are proved for Brinkman model and Forchheimer model, respectively. In Section 3.4.6, the numerical experiment is carried out, in which a series of numerical convergence tests are given to verify the error estimate results proved in Section 3.4.4 and Section 3.4.5. Lastly, in Section 3.5, an innovation to the Butler-Volmer equations is introduced for the electrochemical kinetic model, leading to the Poisson-Nernst-Planck equation, which is going to be introduced in Chapter 4.

In the third part of this dissertation, Chapter 4, we put our focus on the Poisson-Nernst-Planck (PNP) equations. We study the a priori error estimates of the finite element approximation to a type of time-dependent PNP equations. We introduce the model problem and describe the semi- and full discretization of the problem using standard finite element method is Section 4.2.2 and 4.2.3. The main error estimates for semi-discretization and full dicretization are given in Section 4.2.4 and Section 4.2.5, respectively. Numerical experiments are reported in Section 4.2.6. Next, in Section 4.3, we propose the mixed finite element method to discretize the electrostatic potential equation in order to improve the convergence rate. Section 4.3.2 introduces the PNP system and its mixed weak forms, and the error analysis for the semi-discretization scheme with the mixed finite element method is given in Section 4.3.3. Section 4.3.4 conducts the full discretization scheme. Numerical experiments and validations are illustrated in Section 4.3.5.

The fourth part, Chapter 5, we introduce the new fuel cell model based on the results from Chapter 3 and Chapter 4, by deriving a new definition of transfer current density. Section 5.2 studies the a prior error estimate of the new time dependent PNP coupled with Brinkman model, where the semi-discritization of mixed finite element is used and the sub-optimal convergence order for velocity in L^2 norm and optimal convergence orders for all the other variables achieved.

CHAPTER 2

PRELIMINARIES AND NOTATIONS

We use the standard Lebesgue and Sobolev Spaces [Adams and Fournier (2003)]. Let $\Omega \subset \mathbb{R}^d$ be an open set, $m \in \mathbb{N}$, and $1 \leq p \leq \infty$. Let $L_p(\Omega)$ denote the linear space of measurable p^{th} power integrable function on Ω endowed with norm $\|\cdot\|_{L^p(\Omega)}$. The Sobolev space $W^{m,p}(\Omega)$ consists of functions $f \in L^p(\Omega)$ that have weak derivatives $D^\alpha f \in L^p(\Omega)$ up to m. For $1 \leq p < \infty$, the norm in $W^{m,p}(\Omega)$ is denoted by

$$\|u\|_{W^{m,p}} = \left(\int_\Omega \sum_{|\alpha| \leq m} |D^\alpha u|^p \, dx \right)^{\frac{1}{p}},$$

and for $p = \infty$,

$$\|u\|_{W^{m,\infty}} = \max_{|\alpha| \leq m} \|D^\alpha u\|_{L^\infty(\Omega)}.$$

We also use the standard notations for norms and seminorms associated with Sobolev spaces. In order to simplify the notation, we denote $W^{m,2}(\Omega)$ by $H^m(\Omega)$ and omit the index $p = 2$ and Ω whenever possible, that is, $\|u\|_{W^{m,2}} = \|u\|_{H^m}$. We also denote $W^{0,p}(\Omega)$ by $L^p(\Omega)$ and pomit the index $m = 0$ and Ω whenever possible, that is $\|u\|_{W^{0,p}} = \|u\|_{L^p}$. The notations $H_0^1(\Omega) = \{v \in H^1(\Omega) : v|_{\partial\Omega} = 0\}$ and the standard L^2 inner product $(\cdot, \cdot)$ are adopted.

Lemma 2.1 (Sobolev Embedding Theorem)**.** *Given an integer $j \geq 0$, we define the family of space $C_b^j(\Omega)$ by setting*

$$C_b^j(\Omega) = \{u \in C^j(\Omega) | \forall \alpha \in \mathbb{N}^d, |\alpha| \leq j, \exists K_\alpha, \|D^\alpha u\|_\infty \leq K_\alpha\}.$$

Given a Lipschitz open set Ω*, we have*

(1) If $d > mp$*, then* $W^{m,p}(\Omega) \hookrightarrow L^q(\Omega)$ *for every* $q \leq dp/(d-mp)$*.*

(2) If $d = mp$*, then* $W^{m,p}(\Omega) \hookrightarrow L^q(\Omega)$ *for every* $q < \infty$*. If* $p = 1$*, then* $W^{n,1}(\Omega) \hookrightarrow C_b(\Omega)$*.*

(3) If $mp > d$ *with* $d/p \notin \mathbb{N}$ *and if* j *satisfies* $(j-1)p < d < jp$*, then we have*

$$W^{m,p}(\Omega) \hookrightarrow C_b^{m-j,\lambda}(\Omega), \quad \forall \lambda \leq j - d/p.$$

If $d/p \in \mathbb{N}$ *and* $m \geq j = d/p + 1$*, then* $W^{m,p}(\Omega) \hookrightarrow C_b^{m-(d/p)-1,\lambda}(\Omega)$ *for every* $\lambda < 1$*.*

Lemma 2.2 (Poincaré inequality)**.** *Let* $\Omega \subset \mathbb{R}^d$ *be a bounded open set and* $1 \leq p < \infty$*. Then there exists* $M(p, \Omega)$ *such that for all* $u \in W_0^{1,p}(\Omega)$

$$\|u\|_{L^p(\Omega)} \leq M\|Du\|_{L^p(\Omega)}. \tag{2.1}$$

Lemma 2.3 (Hölder's inequality)**.** *Let* $1 \leq p \leq \infty$*, and* $1 \leq q \leq \infty$ *with* $1/p + 1/q = 1$*, then we have*

$$|(u, v)| = \|uv\|_{L^1(\Omega)} \leq \|u\|_{L^p(\Omega)}\|v\|_{L^q(\Omega)}. \tag{2.2}$$

When $p = q = 2$*, (2.2) gives a form of the Cauchy-Schwarz inequality.*

Lemma 2.4 (Young's inequality with ϵ)**.** *If* p *and* q *are positive real numbers such that* $1/p + 1/q = 1$*, then*

$$pq \leq \epsilon p^2 + \frac{1}{4\epsilon}q^2.$$

Lemma 2.5 (Grönwall's inequality)**.** *Let* J *denote an interval of the real line of the form* $[a, \infty)$ *or* $[a, b]$ *or* $[a, b)$ *with* $a < b$*. Let* α*,* β *and* u *be real-valued functions defined on* J*. Assume that* β *and* u *are continuous and that the negative part of* α *is integrable on every closed and bounded subinterval of* J*.*

(a) If β is non-negative and if u satisfies the integral inequality

$$u(t) \leq \alpha(t) + \int_a^t \beta(s)u(s)ds, \qquad \forall t \in J,$$

then

$$u(t) \leq \alpha(t) + \int_a^t \alpha(s)\beta(s) \exp\biggl(\int_s^t \beta(r)\,\mathrm{d}r\biggr)\mathrm{d}s, \qquad t \in J.$$

(b) If, in addition, the function α is non-decreasing, then

$$u(t) \leq \alpha(t) \exp\biggl(\int_a^t \beta(s)\,\mathrm{d}s\biggr), \qquad t \in J.$$

(c) Moreover, if β is the constant 1, then

$$u(t) \leq M\alpha(t), \qquad t \in J,$$

where M is a constant.

Lemma 2.6. *Let $\Omega \subset \mathbb{R}^d$ be a measurable set with the Lebesgue measure, $\forall u \in L^p$, $\forall v \in L^q$ and $\forall w \in L^2$,*

$$\int_\Omega |uvw|\, dx \leq \|u\|_{L^p}\|v\|_{L^q}\|w\|_{L^2},$$

where $\frac{1}{p} + \frac{1}{q} = \frac{1}{2}$, $p \geq 0$, $q > 0$.

Proof. By Hölder's inequality:

$$\begin{aligned}\int_\Omega |uvw|\, dx \leq \left(\int_\Omega u^2v^2 dx\right)^{1/2} \left(\int_\Omega w^2 dx\right)^{1/2} \\ \leq \left(\int_\Omega u^{2t} dx\right)^{1/2t} \left(\int_\Omega v^{2t'} dx\right)^{1/2t'} \left(\int_\Omega w^2 dx\right)^{1/2},\end{aligned}$$

where $\frac{1}{t} + \frac{1}{t'} = 1$. Now we let $p = 2t$ and $q = 2t'$, then $\frac{1}{p} + \frac{1}{q} = \frac{1}{2}$, and

$$\begin{aligned}\int_\Omega |uvw|\, dx \leq \left(\int_\Omega u^2v^2 dx\right)^{1/2} \\ \leq \left(\int_\Omega u^r dx\right)^{1/p} \left(\int_\Omega v^q dx\right)^{1/q} \left(\int_\Omega w^2 dx\right)^{1/2} \leq \|u\|_{L^p}\|v\|_{L^q}\|w\|_{L^2}.\end{aligned}$$

□

Lemma 2.7. *Under the same assumption given in Lemma 2.6, we have*

$$\|u\|_{L^3} \le \|u\|_{L^2}^{\frac{1}{2}} \|u\|_{H^1}^{\frac{1}{2}}. \tag{2.3}$$

Proof. By Lemma 2.6, we have

$$\|u\|_{L^3}^3 = \int_\Omega |u|^3 \, dx \le \|u\|_{L^2} \|u\|_{L^3} \|u\|_{L^6}. \tag{2.4}$$

Because for the dimension $d \le 3$, we have $H^1(\Omega) \hookrightarrow L^6(\Omega)$ by Rellich-Kondrachov theorem, then

$$\|u\|_{L^3}^2 \le \|u\|_{L^2} \|u\|_{L^6} \le \|u\|_{L^2} \|u\|_{H^1}. \tag{2.5}$$

Therefore (2.3) is obtained. □

The Poisson equation for vanishing Neumann conditions $g = 0$, that is

$$-\Delta u = f, \quad \text{in } \Omega, \quad \frac{\partial u}{\partial \boldsymbol{n}} = g, \quad \text{on } \partial\Omega, \tag{2.6}$$

is of special interest to our analysis and concerns the following regularity estimate for $1 < p < \infty$

$$\|u\|_{W^{2,p}} \le M \|f\|_{L^p}, \tag{2.7}$$

which is known to hold with necessary assumptions [Grisvard (1985)].

Lemma 2.8 (Lax-Milgram Theorem)**.** *Given a Hilbert space $(V, (\cdot,\cdot))$, if a bilinear form $a(\cdot,\cdot)$ is*

(a) continuous: if there exists positive constant $M_1 < \infty$ such that

$$|a(u, v)| \le M_1 \|u\|_V \|v\|_V, \qquad \forall u, v \in V$$

(b) coercive: on $U \subset V$, if there exists constant $M_2 > 0$ such that

$$a(v,v) \geq M_2 \|v\|_V^2, \qquad \forall v \in U$$

and a linear functional $F \in V'$ is continuous, then there exists a unique $u \in V$ such that

$$a(u,v) = F(v), \qquad \forall v \in V.$$

Lemma 2.9 (Ladyzhenskaya-Babuska-Brezzi (LBB) condition)**.** *Given Hilbert spaces $(U, (\cdot,\cdot))$ and $(V, (\cdot,\cdot))$, if a bilinear form $b(u,v)$ defined on $U \times V$ satisfies:*

$$\begin{aligned}
&(a) \qquad |b(u,v)| \leq M\|u\|_U \|v\|_V, && \forall u \in U, \forall v \in V,\\
&(b) \qquad \sup_{v \in V} \frac{b(u,v)}{\|v\|_V} \geq \beta \|u\|_U, && \forall u \in U,\\
&(c) \qquad \sup_{u \in U} |b(u,v)| > 0, && \forall v \neq 0,
\end{aligned}$$

where M, β are positive constants and also if $f \in V'$, there exists a unique $u^* \in U$, such that

$$b(u^*, v) = f(v), \quad \forall v \in V,$$

and

$$\|u^*\|_U \leq \frac{1}{\beta} \|f\|_{V'}.$$

Lemma 2.10 (Inverse estimate)**.** *Let $\{\mathcal{T}^h\}$, $0 < h \leq 1$, be a quasi-uniform family of subdivisions of a polyhedral domain $\Omega \subset \mathbb{R}^d$. Let $(K, \mathcal{P}, \mathcal{N})$ be a reference finite element such that $\mathcal{P} \subset W^{l,p}(K) \cap W^{m,q}(K)$ where $1 \leq p \leq \infty$, $1 \leq q \leq \infty$ and $0 \leq m \leq l$. For $T \in \mathcal{T}^h$, let $(T, \mathcal{P}_T, \mathcal{N}_T)$ be the affine-equivalent element, and $V^h = \{v : v$ is measurable and $v|_T \in \mathcal{P}_T$, $\forall T \in \mathcal{T}^h\}$. Then there exists $M = M(l,p,q,\rho)$*

such that

$$\left[\sum_{T\in\mathcal{T}^h}\|v\|^p_{W^{l,p(T)}}\right]^{\frac{1}{p}} \le Mh^{m-l+\min(0,\frac{d}{p}-\frac{d}{q})}\left[\sum_{T\in\mathcal{T}^h}\|v\|^q_{W^{m,q(T)}}\right]^{\frac{1}{q}}$$

for all $v \in V^h$. *When* $p = \infty$, $\left[\sum_{T\in\mathcal{T}^h}\|v\|^p_{W^{l,p(T)}}\right]^{\frac{1}{p}}$ *is interpreted as* $\max_{T\in\mathcal{T}^h}\|v\|_{W^{l,\infty}}$.

When $q = \infty$, $\left[\sum_{T\in\mathcal{T}^h}\|v\|^q_{W^{m,q(T)}}\right]^{\frac{1}{q}}$ *is interpreted as* $\max_{T\in\mathcal{T}^h}\|v\|_{W^{m,\infty}}$.

CHAPTER 3

TRADITIONAL FUEL CELL MODEL

3.1 Introduction to proton exchange membrane fuel cells

Proton exchange membrane fuel cells (PEMFCs), owing to their high energy efficiency, low emission, and low noise, are widely considered as the most promising alternative power source in the twenty first century for automotive, portable, and stationary applications. Since PEMFCs simultaneously involve electrochemical reactions, current distribution, two-phase flow transport and heat transfer, an extensive mathematical modeling of multi-physics system combined with the advanced numerical techniques shall make a significant impact in gaining a fundamental understanding of the interacting electrochemical and transport phenomena and providing a computer-aided tool for the design and optimization of PEMFCs.

Figure 3.1 and Figure 3.2 schematically show a single PEMFC in 2D and 3D, respectively. A typical PEMFC consists of several distinct components [Wang (2004)]: the membrane electrode assembly (MEA) comprised of a proton conducting electrolyte membrane sandwiched between two catalyst layers (CL), the porous gas diffusion layers (GDL), and the bipolar plates with embedded gas channels. In the anode CL, the hydrogen oxidation reaction (HOR) splits the hydrogen into electrons, which are transmitted via the external circuit, and protons, which migrate through the membrane and participate in the oxygen reduction reaction (ORR) in the cathode

CL to recombine with oxygen and produce water and waste heat.

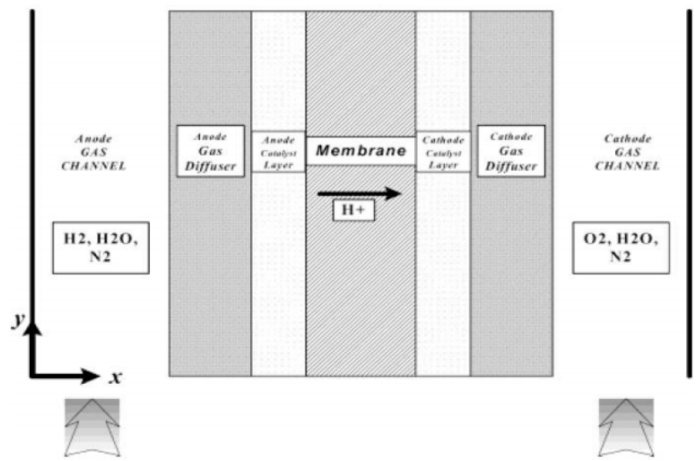

Figure 3.1. A schematic 2D PEMFC [Wang (2004)]

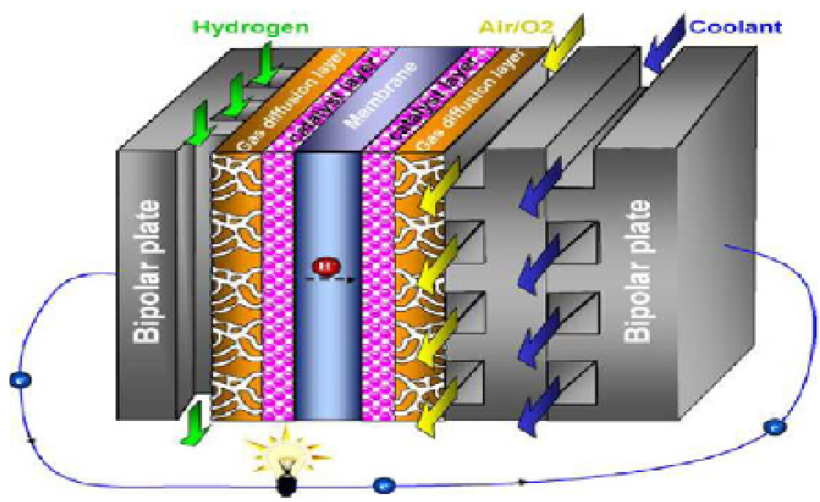

Figure 3.2. A schematic 3D PEMFC

In the past two decades, the multiphase mixture (M^2) model [Wang (2004); Wang and Cheng (1997, 1996); Wang et al. (2001); Pasaogullari et al. (2007); Pasaogullari and Wang (2004); Wang et al. (1999); Liu and Wang (2007a,b)] has been widely used for modeling PEMFCs due to its following features: (1) mathematically exactly equivalent to separate multiphase flow model; (2) based on mixture variables only and thus involve much fewer PDEs; (3) replace some PDEs with algebraic equations (for instance, the relationship between the phase velocity and mixture velocity) that can be calculated in a post-processing fashion; (4) resemble the single-phase transport theory; (5) a single-domain fixed grid formulation, eliminating the need for interface tracking; (6) computationally efficient and require less data storage. The most significant ability of M^2 model behaves at capturing the most common scenario encountered in fuel cells, that is, a two-phase zone coexisting with a single-phase region with an irregular front in between. During transient operation, this phase front would evolve not only spatially but also temporally.

A multiphysics, two-phase PEMFC model consists the following governing equations: [Sun (2011)]

(1) General species transport equations, in channel and porous media, respectively, for $J = H_2O$, H_2 and O_2,

$$-\nabla \cdot (D_g^J \nabla C^J) + \nabla \cdot (\boldsymbol{u} C^J) = 0, \tag{3.1}$$

$$-\nabla \cdot (D_g^J \nabla C^J) + \nabla \cdot (\gamma_c \boldsymbol{u} C^J) - G_J = S_J(j) + \nabla \cdot (\tfrac{C^J}{\rho_g} \Gamma \nabla C^J), \tag{3.2}$$

where j is the volumetric transfer current density of the reaction given by the modified Butler-Volmer equation in the anode and cathode derived from the following general Butler-Volmer equation

$$j = ai_0(\exp(\frac{\alpha_a F}{RT}(\Phi_s - \Phi_e - U_0)) - \exp(\frac{\alpha_c F}{RT}(\Phi_s - \Phi_e - U_0))). \tag{3.3}$$

(2) Fluid flow equation

$$\frac{1}{\epsilon^2}\nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}^T) = \nabla \cdot (\mu \nabla \boldsymbol{u}) - \nabla p - \frac{\mu}{K}\boldsymbol{u}, \tag{3.4}$$

$$\nabla \cdot (\rho \boldsymbol{u}) = S_m(j). \tag{3.5}$$

(3) Energy equation

$$\nabla \cdot (K\nabla T) + \nabla \cdot (\gamma_T \rho c_p \boldsymbol{u} T) = S_T(j). \tag{3.6}$$

(4) Electrostatic potential equations for proton transport and electron transport, respectivley,

$$\nabla \cdot (\kappa^{eff} \nabla \Phi_e) = S_{\Phi_e}(j), \tag{3.7}$$

$$\nabla \cdot (\sigma_s^{eff} \nabla \Phi_s) = S_{\Phi_s}(j). \tag{3.8}$$

All the parameter values and relations in (3.1)-(3.8) are given in [Sun (2011)].

Considering water is the only species which bears two-phase characteristics, and water management is one of the most crucial parts in fuel cell dynamics, we will intensively study the finite element approximation of the coupled water concentration equation and fluid flow equations and its convergence error analysis in the remaining sections of Chapter 3. The numerical analyses of other governing equations shall be analogous to or less complicated than this one, and thus excluded in this dissertation.

3.2 Finite element approximation analysis for a steady state two-phase transport model of proton exchange membrane fuel cell

3.2.1 Introduction

Water management is critical to achieving high performance of proton exchange membrane fuel cells (PEMFC), and is a significant technical challenge. Despite significant progress in recent years in enhancing the overall cell performance, a major limitation arises from the two-phase transport. This is primarily owing to the blockage of the open pore paths due to liquid water generated in the cathode gas diffusion layer due to the electrochemical reaction of H^+/O_2. If the water generated is not removed from the cathode at a sufficient rate, it may hinder oxygen transport from the gas channels to the active reaction sites in the catalyst layers. Thus, a relatively dry air at the cathode inlet is sometimes helpful to remove excessive water [Sun et al. (2009a)]. At the mean time, the polymer electrolyte membrane requires sufficient water to exhibit a high ionic conductivity. During fuel cell operation, water molecules migrate through the membrane under electro-osmotic drag, hydraulic permeation, and molecular diffusion, making it difficult to retain a high water content within the membrane. Generally, humidification is applied to the inlet gases of the anode and/or cathode in order to keep the membrane hydrated. Gas diffusion layer thus plays a crucial role in the overall water management, which requires a delicate balance between reactant transport from the gas channels and water removal from the electrochemically active sites [Wang (2004)]. This is referred as balancing membrane hydration with flooding avoidance.

Since there are two important and also conflicting needs in PEMFCs: to hydrate the polymer electrolyte and to avoid flooding in porous electrodes and GDL for reactant/product transport, in order to focus on the most important issue in PEMFCs – water management, only the water transport phenomenon, together with its two-phase transport modeling and its finite element approximation analysis are considered in this dissertation. The numerical analysis method carried out in this dissertation can be equivalently applied to other species transport equations occurring in FEMFCs.

For water concentration equation, in order to present a unified model that encompasses both the single- and two-phase regimes, and to ensure a smooth transition between the two, a discontinuous and degenerate function is introduced [Wang et al. (2001)] as diffusivity of the transport equation in terms of water concentration. In gaseous water region, the water concentration is below a fixed value called saturated water concentration ($16mol/m^3$ at 80^oC), coinciding with nonzero constant diffusivity. Once water concentration exceeds this fixed value, excess gaseous water is generated and condensed to liquid water. Correspondingly, water diffusivity suddenly jumps down to zero at this point and then slowly grows up to a smooth function with respect to liquid water concentration (a third degree polynomial in terms of liquid saturation). Thus a degenerate and discontinuous water transport equation is formed.

Comparing to the plentiful of literature on modeling and experimental study of fuel cells, less work is contributed to the efficient numerical methodology of two-phase transport PEMFC model. P. Sun et al [Sun (2011); Sun et al. (2008, 2009a,b, 2012)] lead the field in numerical studies for PEMFC due to the cutting edge work on the efficient numerical techniques for the multiphase mixture (M^2) model of PEMFC, where, finite element method is adopted to discretize the governing equations of PEMFC model, and Kirchhoff transformation [Arbogast et al. (1996); Eyres et al. (1966); Rose (1983); Sun et al. (2008, 2009b)] is employed to specifically handle the derived discontinuous and degenerate water diffusivity arising in the two-phase water transport model of PEMFC with the intention to accelerate the nonlinear iteration and obtain an accurate solution. However, the error estimates of finite element method with Kirchhoff transformation have not been discussed yet for either steady state or transient PEMFC model in these papers. The goal of this section is to accurately analyze the error estimates of finite element approximation for a simplified steady state two-phase transport model in the cathode gas diffusion layer (GDL) of PEMFC. We obtain the optimal error estimate in H^1 norm and the sub-optimal error estimate in L^2 norm for the present finite element approximation scheme. Numerical experiments are carried out as well to demonstrate the consistency between the numerical convergence rate and the theoretical result.

The rest of this section is organized as follows. A simplified 2D steady state two-phase transport model in the cathode GDL of PEMFC is studied in Section 3.2.2. Then, in Section 3.2.3, Kirchhoff transformation is introduced to describe the reformulated water concentration equation, and its efficiency is demonstrated on dealing with the discontinuous and degenerate water diffusivity. In Section 3.2.4, the finite element scheme is described and its approximation theorem is proved. In Section 3.2.5, the numerical experiment is carried out, in which a series of numerical convergence tests are given to verify the error estimate results proved in Section 3.2.4.

3.2.2 A simplified two-phase transport model in the cathode GDL of PEMFC

In this section, the governing equations for a simplified steady state two-phase transport problem in the cathode GDL of PEMFC, together with the computational domain and boundary conditions are described.

GDL is the major component in PEMFC that contains both liquid water and gaseous water vapor. As mentioned in Section 3.2.1, water management is the most important and challenging work in PEMFC model. Therefore, in this section, attention is put on only the water species in GDL instead of all species spreading everywhere. To define a simplified steady state isothermal two-phase transport model in the cathode GDL based on the multiphase mixture (M^2) [Wang and Cheng (1996)] model, we only need to address a pressure equation using Darcy's law, and a water concentration equation in which Darcy's velocity is used. The two-phase transport model is defined as follows with respect to water's molar concentration C and pressure p [Sun et al. (2009b); Wang and Cheng (1996)], where all the physical parameters and coefficients are defined in Table 3.1 and Table 3.2:

$$-\nabla \cdot (D(C)\nabla C) + \nabla \cdot (\gamma_c \boldsymbol{u} C) = 0, \tag{3.9}$$

$$\nabla \cdot \left(\frac{K}{\epsilon_0 \nu(C)} \nabla p \right) = 0, \tag{3.10}$$

here the Darcy's velocity $\boldsymbol{u}$ is defined as $\boldsymbol{u} = -\frac{K}{\epsilon_0 \rho \nu} \nabla p$, and (3.10) is introduced assuming the incompressibility condition $\nabla \cdot (\rho \boldsymbol{u}) = 0$. The diffusivity $D(C)$ in GDL is defined as

$$D(C) = \begin{cases} D_g f(\epsilon_0), & \text{if } C \le C_{sat}, \\ \left(\frac{1}{M_w} - \frac{C_{sat}}{\rho_g}\right) \Gamma_{capdiff}, & \text{if } C > C_{sat}, \end{cases}$$

where D_g is the effective water vapor diffusivity given as a constant for isothermal model. $f(\epsilon_0) = \epsilon_0^{1.5}$ and ϵ_0 is the porosity of GDL.

$$\Gamma_{capdiff} = \frac{M_w}{\rho_l - C_{sat} M_w} \frac{\lambda_l \lambda_g}{\nu} \sigma \cos\theta_c (\epsilon_0 K)^{\frac{1}{2}} \frac{dJ(s)}{ds},$$

is the capillary diffusion coefficient, as shown in Figure 3.3 for $C > C_{sat}$. γ_c is the

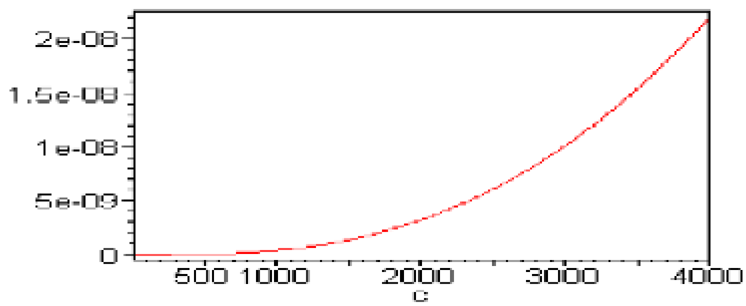

Figure 3.3. $\Gamma_{capdiff}$ in two-phase region

advection correction factor, given as

$$\gamma_c = \begin{cases} 1, & \text{if } C \le C_{sat}, \\ \frac{\rho}{C}\left(\frac{\lambda_l}{M_w} + \frac{\lambda_g}{\rho_g} C_{sat}\right), & \text{if } C > C_{sat}, \end{cases}$$

where λ_g and λ_l are the relative mobilities of water of liquid and gaseous phases, and ρ_g and ρ_l are the water density of liquid and gaseous phases, C_{sat} is the saturated water concentration which is a constant in this isothermal case. $J(s)$ is the Leverett function defined as

$$J(s) = \begin{cases} 1.417(1-s) - 2.120(1-s)^2 + 1.263(1-s)^3, & \text{if } \theta_c < 90°, \\ 1.417s - 2.120s^2 + 1.263s^3, & \text{if } \theta_c > 90°, \end{cases}$$

here $s \in [0, 1]$ denotes the liquid saturation, which has coequality with water concentration, shown as

$$s = \frac{C - C_{sat}}{\frac{\rho_l}{M_w} - C_{sat}}.$$

It is not difficult to see $\Gamma_{capdiff} \to 0$ when $C \to C_{sat}$, therefore $D(C)$ nearly degenerates at C_{sat}, as shown in Figure3.4.

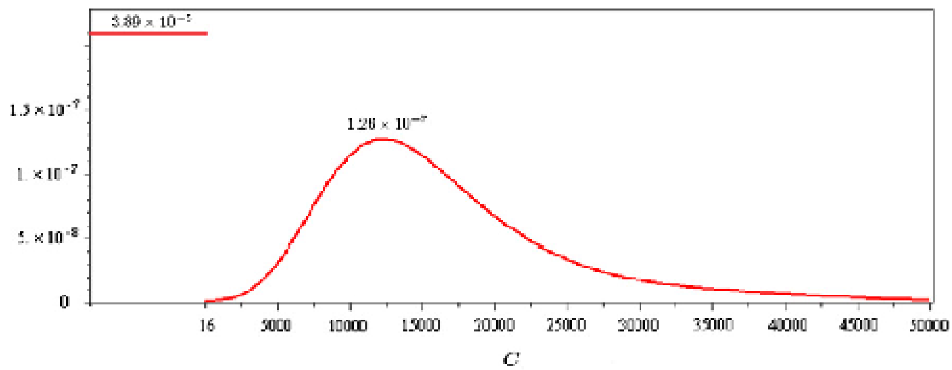

Figure 3.4. Water Diffusivity $D(C)$ in GDL

For the sake of simplifying notations, we introduce a new advection correction factor $\bar{\gamma}_c = -\frac{K\gamma_c}{\epsilon_0 \rho \nu}$, then the governing equations (3.9) and (3.10) can be written as

$$-\nabla \cdot (D(C)\nabla C) + \nabla \cdot (\bar{\gamma}_c \nabla p C) = 0, \tag{3.11}$$

$$\nabla \cdot \left(\frac{K}{\epsilon_0 \nu(C)} \nabla p \right) = 0. \tag{3.12}$$

The governing equations (3.11) and (3.12) take place in the cathode GDL of PEMFC, as shown in Figure 3.5. The x-axis represents the flow direction and the y-axis points in the through-plane direction. The dimension sizes of this computational domain are marked in Figure 3.5 as well. $\frac{\partial C}{\partial n} = 0$ and $\frac{\partial p}{\partial n} = 0$ on the left and right walls, $(\partial\Omega)_2$ and $(\partial\Omega)_3$. On the bottom wall connecting with gas channel, $(\partial\Omega)_1$, C is given as

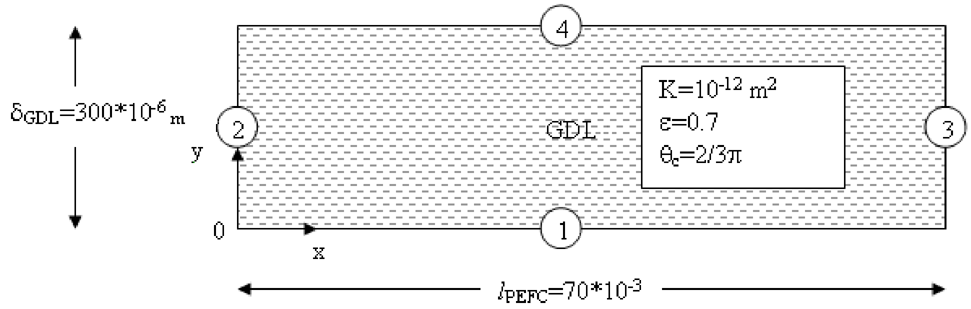

Figure 3.5. Computational Domain

constant C_b and $p(x) = p_1 - (p_1 - p_2)\frac{x}{l_{\text{PEMFC}}}$. On the top wall connecting with catalyst layer, $(\partial\Omega)_4$, $\frac{\partial p}{\partial n} = 0$, and, to simulate the electrochemical reaction effect occurring in the catalyst layer, the nonhomogeneous Neumann boundary condition is assigned to water concentration C here: $D(C)\nabla C \cdot \boldsymbol{n} - (\bar{\gamma}_c \nabla p C) \cdot \boldsymbol{n} = \frac{I(x)}{2F}$, where F is the Faraday constant and $I(x)$ the volumetric transfer current density of reaction [Sun et al. (2009b)], given as $I(x) = \left(I_1 - (I_1 - I_2)\frac{x}{l_{\text{PEMFC}}}\right)$. Here p_1, p_2, I_1 and I_2 are the prescribed constants given in Table 3.2. In fact, $I(x)$ is the linear reduction of Butler-Volmer equation, indicating that the transfer current density linearly decreases from the inlet to the outlet.

Density	$\rho = \rho_l s + \rho_g(1-s)$
Molar concentration	$C = C_l s + C_g(1-s)$
Kinematic viscosity	$\nu = \left(\frac{k_{rl}}{\nu_l} + \frac{k_{rg}}{\nu_g}\right)^{-1}$
Relative mobilities	$\lambda_l(s) = \frac{k_{rl}/\nu_l}{k_{rl}/\nu_l + k_{rg}/\nu_g}$, $\lambda_g(s) = 1 - \lambda_l(s)$
Relative permeabilities	$k_{rl} = s^3$, $k_{rg} = (1-s)^3$

Table 3.1. Parameters and their physical relations [Wang (2004)]

Parameter	Symbol	Value
Contact angle between two phases	θ_c	$\frac{2}{3}\pi$
Current density at the left end	I_1	$20000\ [A/m^2]$
Current density at the right end	I_2	$10000\ [A/m^2]$
Effective water vapor diffusivity	D_g	$2.6 \times 10^{-5}\ [m^2/s]$
Faraday constant	F	$96487\ [A \cdot s/mol]$
GDL length	l_{GDL}	$7 \times 10^{-2}\ [m]$
GDL thickness	δ_{GDL}	$3 \times 10^{-4}\ [m]$
Kinematic liquid water viscosity	ν_l	$3.533 \times 10^{-7}\ [m^2/s]$
Kinematic vapor viscosity	ν_g	$3.59 \times 10^{-5}\ [m^2/s]$
Liquid water density	ρ_l	$971.8\ [kg/m^3]$
Permeability of GDL	K	$8.69 \times 10^{-12}\ [m^2]$
Porosity of GDL	ϵ_0	0.3
Pressure at the left end	p_1	$101325\ [pa]$
Pressure at the right end	p_2	$10100\ [pa]$
Saturated water concentration	C_{sat}	$C_{sat} = 16.11\ [mol/m^3]$ (for $80°C$)
Surface tension	σ	$0.0625\ [kg/s^2]$
Vapor density	ρ_g	$0.882\ [kg/m^3]$
Water molecular mass	M_w	$0.018\ [kg/mol]$

Table 3.2. Parameters values

3.2.3 Reformulation of water equation by Kirchhoff transformation

As discussed in Section 3.2.2, $D(C)$ is nearly degenerate and also discontinuous at C_{sat}, which causes an oscillatory and instable nonlinear iteration in the numerical simulation. In order to resolve such computational difficulties, we introduce the so-called Kirchhoff transformation [Sun et al. (2009b)] as

$$W(C) = \int_0^C D(w)dw. \tag{3.13}$$

Thus

$$W(C) = \begin{cases} D_g f(\epsilon_0)C, & \text{if } C \leq C_{sat}, \\ D_g f(\epsilon_0)C_{sat} + \int_{C_{sat}}^{C} \left(\frac{C_{sat}}{\rho_g} - \frac{1}{M_w}\right) \Gamma_{capdiff}(w)dw, & \text{if } C > C_{sat}. \end{cases} \tag{3.14}$$

Furthermore, since $\Delta W(C) = \nabla \cdot (D(C)\nabla C)$,

$$\Delta W(C) = \begin{cases} \nabla \cdot (D_g f(\epsilon_0) \nabla C), & \text{if } C \le C_{sat}, \\ \nabla \cdot \left(\left(\frac{C_{sat}}{\rho_g} - \frac{1}{M_w} \right) \Gamma_{capdiff} \nabla C \right), & \text{if } C > C_{sat}. \end{cases}$$

Therefore, we are able to reformulate the water concentration equation (3.11) with Kirchhoff transformation as follows

$$-\Delta W = -\nabla \cdot (\bar{\gamma}_c \nabla p C) \qquad \text{in } \Omega, \tag{3.15}$$

$$W = \int_0^{C_b} D(w) dw \qquad \text{on } (\partial\Omega)_1, \tag{3.16}$$

$$\frac{\partial W}{\partial n} = 0 \qquad \text{on } (\partial\Omega)_2, (\partial\Omega)_3, \tag{3.17}$$

$$\nabla W \cdot \boldsymbol{n} - \bar{\gamma}_c \nabla p C(W) \cdot \boldsymbol{n} = \frac{I(x)}{2F} \qquad \text{on } (\partial\Omega)_4. \tag{3.18}$$

It may be improper if one insists on applying Kirchhoff transformation to $\nabla \cdot (\bar{\gamma}_c \nabla p C)$, because a new convection term that explicitly depends on W will thus be obtained as

$$\nabla \cdot (\bar{\gamma}_c \nabla p C) = \bar{\gamma}_c \nabla p \cdot \nabla C + \nabla \cdot (\bar{\gamma}_c \nabla p) C = \bar{\gamma}_c \nabla p \cdot \frac{\nabla W}{D(C)} + \nabla \cdot (\bar{\gamma}_c \nabla p) C,$$

then the corresponding reformulated water concentration equation becomes

$$-\Delta W + \bar{\gamma}_c \nabla p \cdot \frac{\nabla W}{D(C)} = -\nabla \cdot (\bar{\gamma}_c \nabla p) C(W), \tag{3.19}$$

where, a huge convection term may be produced when the water concentration C is close to the degenerate point C_{sat}. Therefore, for the interest of numerical stability, it is better to avoid applying Kirchhoff transformation to the convection term in (3.15), and leave it to the right hand side as an equivalent force term in order to achieve a stable numerical iteration.

In order to extend the error estimates of finite element method, which will be given in Section 3.2.4, to a more general case, the reformulated water concentration equation (3.19) can be further generalized to the following form of convection-diffusion-reaction equation

$$-\Delta W + \boldsymbol{b}(C, \nabla p) \cdot \nabla W = f(C, \nabla p, \Delta p), \tag{3.20}$$

where

$$\boldsymbol{b}(C, \nabla p) = \frac{\bar{\gamma}_c \nabla p}{D(C)},\ f(C, \nabla p, \Delta p) = -\nabla \cdot (\bar{\gamma}_c \nabla p)\, C.$$

Obviously, (3.15) and (3.19) are just special cases of (3.20). Without loss of generality, in what follows, we will carry out the error estimates of finite element method for (3.20) instead of (3.15) or (3.19).

We also define that $g(C) = \frac{K}{\epsilon_0 \nu(C)}$. We assume that all the necessary coefficient functions and their proper derivatives are Lipschitz continuous and bounded, satisfying the following conditions for $C \geq 0$,

$$\begin{aligned} 0 < d \leq D(C) \leq D, |\gamma(C)| < \Gamma, 0 < g_0 \leq g(C), \tfrac{\partial g(C)}{\partial C} \leq G_c \\ b < |\boldsymbol{b}(C, \phi)| < B, b_q < \left| \tfrac{\partial \boldsymbol{b}(C,\phi)}{\partial \phi} \right| < B_q, \\ f < |f(C, \phi, \psi)| < F, f_c < \left| \tfrac{\partial f(C,\phi,\psi)}{\partial C} \right| < F_c, f_{cc} < \left| \tfrac{\partial^2 f(C,\phi,\psi)}{\partial C^2} \right| < F_{cc}. \end{aligned} \tag{3.21}$$

However, since $D(C)$ is discontinuous at C_{sat}, $\boldsymbol{b}(C, \phi)$ is also discontinuous at C_{sat}, in other words, it is piecewise continuous function on either side of C_{sat}. Therefore the following conditions are to be satisfied when C is on either side of C_{sat} as follows,

$$b_c < \left| \frac{\partial \boldsymbol{b}(C,\phi)}{\partial C} \right| < B_c, b_{cc} < \left| \frac{\partial^2 \boldsymbol{b}(C,\phi)}{\partial C^2} \right| < B_{cc}. \tag{3.22}$$

In order to simplify notation, in what follows, we denote $\boldsymbol{b}(C, \nabla p)$, $f(C, \nabla p, \Delta p)$, and $g(C)$ as $\boldsymbol{b}$, f and g, respectively, and use the notations $\partial_c \boldsymbol{b}$, $\partial_q \boldsymbol{b}$, $\partial_c^2 \boldsymbol{b}$, $\partial_c f$ and $\partial_c^2 f$ instead of $\frac{\partial \boldsymbol{b}(C,\phi)}{\partial C}$, $\frac{\partial \boldsymbol{b}(C,\phi)}{\partial \phi}$, $\frac{\partial^2 \boldsymbol{b}(C,\phi)}{\partial C^2}$, $\frac{\partial f(C,\phi,\psi)}{\partial C}$ and $\frac{\partial^2 f(C,\phi,\psi)}{\partial C^2}$, respectively.

Further, using (3.10), it is not difficult to get

$$\begin{aligned} -\nabla \cdot \boldsymbol{b} &= -\nabla \cdot \frac{\bar{\gamma}_c \nabla p}{D(C)} = \nabla \cdot \frac{K \gamma_c \nabla p}{\epsilon_0 \rho \nu D(C)} \\ &= \frac{K \nabla p}{\epsilon_0 \rho \nu} \cdot \nabla \left(\frac{\gamma_c}{D(C)} \right) = -\boldsymbol{u} \cdot \nabla \left(\frac{\gamma_c}{D(C)} \right). \end{aligned}$$

Then by the definition of γ_c and $D(C)$, we know $-\nabla \cdot \boldsymbol{b} = 0$ if $C \leq C_{sat}$. Meanwhile, if $C > C_{sat}$,

$$\nabla \left(\frac{\gamma_c}{D(C)} \right) = \frac{\nabla \gamma_c}{D(C)} - \frac{\gamma_c \nabla D(C)}{D^2(C)}. \tag{3.23}$$

Since $D(C)$ is an increasing function with respect to C when $C < 10000$ $[mol/m^2]$ and γ_c is a decreasing function with respect to C, then we can conclude that (3.23) should become a negative function multiplied by ∇C. Therefore we have

$$-\nabla \cdot \boldsymbol{b} \geq 0, \tag{3.24}$$

assuming $C < 10000$ $[mol/m^2]$, which is practically true in FEMFCs, and $\boldsymbol{u} \cdot \nabla C > 0$. However, since in practice we adopt (3.15) for the reformulated water transport equation which is much more stable than (3.19), we will not actually need the condition (3.24). So (3.24) is a weak and less important condition for our actual need.

According to the definition of Kirchhoff transformation in (3.14), the expression for C is not explicit. For the case of $C \leq C_{sat}$, since the Kirchhoff transformation is just linear, it is easy to calculate C directly from W using

$$C = (D_g f(\epsilon_0))^{-1} W. \tag{3.25}$$

However, if $C > C_{sat}$, it is necessary to adopt Newton's method to find a proper solution C, given by the following iterative scheme [Sun et al. (2009b)]($k = 0, 1, 2, \ldots$):

$$C_{k+1} = C_k + \frac{W_{k+1} - D_g f(\epsilon_0) C_{sat} - \int_{C_{sat}}^{C_k} D(w)dw}{D(C_k)}. \tag{3.26}$$

Due to the locally quadratic convergence rate of Newton's method, (3.26) may only take a few steps to approach a reasonable solution C.

3.2.4 Finite element discrete scheme and its error estimate

First of all, we assume the following regularity properties hold for W and p in the semi-discretization analysis:

$$C \in H^{k+1} \cap W^{1,\infty}(\Omega) \text{ and } p \in W^{k+1,\infty}(\Omega). \tag{3.27}$$

We define spaces

$$H_w = \left\{ W \in H^{k+1}(\Omega); W|_{(\partial\Omega)_1} = \int_0^{C_b} D(w)dw \right\},$$

$$H_p = \left\{ p \in H^{k+1}(\Omega); p|_{(\partial\Omega)_1} = p_1 - (p_1 - p_2)\frac{x}{l_{\text{PEMFC}}} \right\}$$

and their corresponding finite element spaces

$$H_w^0 = \left\{ W \in H_w; W|_{(\partial\Omega)_1} = 0 \right\},$$

$$H_p^0 = \left\{ p \in H_p; p|_{(\partial\Omega)_1} = 0 \right\}.$$

To apply standard finite element method to the general reformulated water equation (3.20), we first define the weak form of (3.20) and (3.10) as: find $(W, p) \in H_w \times H_p$, such that for any $(v, q) \in H_w^0 \times H_p^0$:

$$(\nabla W, \nabla v) + (\boldsymbol{b} \cdot \nabla W, v) = (f, v) + \int_{(\partial\Omega)_4} \frac{I(x)}{2F} v ds, \tag{3.28}$$

$$(g\nabla p, \nabla q) = 0. \tag{3.29}$$

Define the piecewise linear polynomial finite element spaces, $S_h \subset H_w$, $T_h \subset H_p$, $S_h^0 \subset H_w^0$ and $T_h^0 \subset H_p^0$. Then the discretization of (3.20) and (3.10) is given as: find $(W_h, p_h) \in S_h \times T_h$ such that for any $(v_h, q_h) \in S_h^0 \times T_h^0$,

$$(\nabla W_h, \nabla v_h) + (\boldsymbol{b_h} \cdot \nabla W_h, v_h) = (f_h, v_h) + \int_{(\partial\Omega)_4} \frac{I(x)}{2F} v_h ds, \tag{3.30}$$

$$(g_h \nabla p_h, \nabla q_h) = 0, \tag{3.31}$$

where g_h, $\boldsymbol{b_h}$ and f_h represents $g(C_h)$, $\boldsymbol{b}(C_h, \nabla p_h)$ and $f(C_h, \nabla p_h, \Delta p_h)$, respectively.

Lemma 3.1. *Let W be the solution of (3.28) and W_h be the solution of (3.30). Suppose W and C satisfy the relation (3.14), C_h is obtained from the Kirchhoff inverse transformation (3.25) and (3.26), then we have following error estimates*

$$d\|C\|_{H^{k+1}} \leq \|W\|_{H^{k+1}} \leq D\|C\|_{H^{k+1}}, \tag{3.32}$$

Proof. Since $W = \int_0^C D(w)dw$, by taking derivatives with respect to space, one has $\nabla W = D(C)\nabla C$. Because $d \leq D(C) \leq D$, and only weak derivatives are needed, (3.32) can be obtained easily. □

Let $\tilde{p} \in S_h$ be the H^1 projection of p that satisfies

$$(g\nabla(p-\tilde{p}), \nabla q_h) = 0, \ \forall q_h \in T_h^0. \tag{3.33}$$

We first recall the standard error estimates of the above H^1 projection in various norms [Ciarlet (1978); Wheeler (1973)], as shown in the following lemma.

Lemma 3.2. *Let p be the solution of (3.29), and p_h be the solution of (3.31). Let $\tilde{p}$ be defined in (3.33), then we have the following error estimates:*

$$\|p-\tilde{p}\|_{L^2} + h\|\nabla\left(p-\tilde{p}\right)\|_{L^2} \le Mh^{k+1}\|p\|_{H^{k+1}}, \tag{3.34}$$

and

$$\|\nabla(p-\tilde{p})\|_{L^\infty} \le Mh^k\|p\|_{W^{k+1,\infty}}. \tag{3.35}$$

From (3.35) and (3.27), we can conclude that $\|\nabla\tilde{p}\|_{L^\infty}$ is bounded.

In the following lemma, we prove the error estimates of $\tilde{p} - p_h$.

Lemma 3.3. *Let (W, p) be the solution of (3.28)-(3.29), and (W_h, p_h) be the solution of (3.30)-(3.31). Suppose W and C satisfy the relation (3.14) and $\tilde{p}$ is defined in (3.33), then we have the following error estimates:*

$$\|\tilde{p}-p_h\|_{L^2} + \|\nabla\left(\tilde{p}-p_h\right)\|_{L^2} \le M\|C-C_h\|_{L^2}, \tag{3.36}$$

Proof. Subtract (3.31) from (3.29), use (3.33), and let $q_h = \tilde{p} - p_h$,

$$(g\nabla\tilde{p} - g_h\nabla p_h, \nabla(\tilde{p}-p_h)) = 0,$$

that is

$$((g-g_h)\nabla\tilde{p}, \nabla(\tilde{p}-p_h)) + (g_h\nabla(\tilde{p}-p_h), \nabla(\tilde{p}-p_h)) = 0.$$

Since

$$\|g(C) - g(C_h)\|_{L^2} \leq G_c \|C - C_h\|_{L^2},$$

and (3.21), we get that

$$g_0 \|\nabla(\tilde{p} - p_h)\|_{L^2}^2 \leq M \|\nabla \tilde{p}\|_{L^\infty} \|C - C_h\|_{L^2} \|\nabla(\tilde{p} - p_h)\|_{L^2}.$$

Since $\|\tilde{p}\|_{L^\infty}$ is bounded, we have

$$\|\nabla \left(\tilde{p} - p_h\right)\|_{L^2} \leq M \|C - C_h\|_{L^2}.$$

By the commonly used Aubin-Nitsche duality argument for the error estimate in L^2 norm for the nonlinear elliptic equation [Douglas and Dupont (1975); Liu et al. (1996); Hlavacek et al. (1994); Harrell and Layton (24); Abdulle and Vilmart (2012)], we can get that

$$\|\tilde{p} - p_h\|_{L^2} \leq Mh \|\nabla \left(\tilde{p} - p_h\right)\|_{L^2} + M \|C - C_h\|_{L^2}.$$

Thus we get (3.36). □

By (3.34) and (3.36), we can easily get the error estimates of $p - p_h$ in L^2 and H^1 norms, as shown in the following lemma.

Lemma 3.4. *Let (W, p) be the solution of (3.28)-(3.29), and (W_h, p_h) be the solution of (3.30)-(3.31). Suppose W and C satisfy the relation (3.14) and $\tilde{p}$ is defined in (3.33), then we have the following error estimates:*

$$\|p - p_h\|_{L^2} \leq Mh^{k+1} \|p\|_{H^{k+1}} + M \|C - C_h\|_{L^2}, \tag{3.37}$$

and

$$\|\nabla(p - p_h)\|_{L^2} \leq Mh^k \|p\|_{H^{k+1}} + M \|C - C_h\|_{L^2}. \tag{3.38}$$

Now we define a H^1 projection operator $P_h : H_w \mapsto S_h$, and let $\tilde{W} = P_h W \in S_h$ satisfy

$$(\nabla(W - \tilde{W}), \nabla v_h) + (\boldsymbol{b} \cdot \nabla(W - \tilde{W}), v_h) = 0,\ \forall v_h \in S_h, \tag{3.39}$$

and prove its convergence property in the following lemma.

Lemma 3.5. *Let W be the solution of (3.28) and W_h be the solution of (3.30). Suppose W and C satisfy the relation (3.14) and $\tilde{W}$ is the projection defined in (3.39), then we have following error estimate,*

$$\|W - \tilde{W}\|_{L^2} + h\|W - \tilde{W}\|_{H^1} \leq M h^{k+1} \|C\|_{H^{k+1}}. \tag{3.40}$$

Proof. Let $\Pi_h W \in S_h$ be the interpolation of W, since $\Pi_h W - \tilde{W} \in S_h$, by (3.39),

$$\begin{aligned}
&(\nabla(W - \tilde{W}), \nabla(W - \tilde{W})) + (\boldsymbol{b} \cdot \nabla(W - \tilde{W}), W - \tilde{W}) \\
&\qquad = (\nabla(W - \tilde{W}), \nabla(W - \Pi_h W)) + (\boldsymbol{b} \cdot \nabla(W - \tilde{W}), W - \Pi_h W).
\end{aligned}$$

Since

$$(\boldsymbol{b} \cdot \nabla(W - \tilde{W}), W - \tilde{W}) = (\boldsymbol{b}, \frac{1}{2}\nabla(W - \tilde{W})^2) = -\frac{1}{2}(\nabla \cdot \boldsymbol{b}, (W - \tilde{W})^2),$$

where $-\nabla \cdot \boldsymbol{b} \geq 0$ by (3.24), then together with the bounds given in (3.21), we have

$$\begin{aligned}
&b\|\nabla(W - \tilde{W})\|_{L^2}^2 \\
&\qquad \leq \|\nabla(W - \tilde{W})\|_{L^2}\|\nabla(W - \Pi_h W)\|_{L^2} + B\|\nabla(W - \tilde{W})\|_{L^2}\|W - \Pi_h W\|_{L^2}
\end{aligned}$$

thus

$$b\|\nabla(W - \tilde{W})\|_{L^2} \leq \|\nabla(W - \Pi_h W)\|_{L^2} + B\|W - \Pi_h W\|_{L^2}.$$

This implies

$$\|W-\tilde{W}\|_{H^1} \le M \inf_{\Pi_h W \in S_h} \|W-\Pi_h W\|_{H^1} \le Mh^k\|W\|_{H^{k+1}} \le Mh^k\|C\|_{H^{k+1}}.$$

Now we move our focus to the L^2 error estimate of $W-\tilde{W}$. We define $w \in H^2(\Omega)\cap H_0^1(\Omega)$ to satisfy the adjoint problem of (3.39) as follows,

$$\begin{cases} -\Delta w - \nabla\cdot(\boldsymbol{b}w) = W-\tilde{W}, & \text{in } \Omega, \\ w = 0, & \text{on } \partial\Omega. \end{cases}$$

Then by (3.39) we have

$$\begin{aligned} \|W-\tilde{W}\|_{L^2}^2 &= -\Big(W-\tilde{W}, \Delta w\Big) - \Big(W-\tilde{W}, \nabla\cdot(\boldsymbol{b}w)\Big) \\ &= \Big(\nabla(W-\tilde{W}), \nabla\left(w-\Pi_h w\right)\Big) + \Big(\nabla(W-\tilde{W}), \boldsymbol{b}\left(w-\Pi_h w\right)\Big) \\ &\le M\|W-\tilde{W}\|_{H^1}\|w-\Pi_h w\|_{H^1}, \end{aligned}$$

where $\Pi_h w$ is the interpolation of w. Since $\|w-\Pi_h w\|_{H^1} \le Mh\|w\|_{H^2}$ and $\|w\|_{H^2} \le \|W-\tilde{W}\|_{L^2}$, therefore,

$$\|W-\tilde{W}\|_{L^2} \le Mh\|W-\tilde{W}\|_{H^1} \le Mh^{k+1}\|C\|_{H^{k+1}}.$$

□

Subtract (3.30) from (3.28), we get

$$(\nabla(W-W_h), \nabla v_h) + (\boldsymbol{b}\cdot\nabla W - \boldsymbol{b_h}\cdot\nabla W_h, v_h) = (f-f_h, v_h). \tag{3.41}$$

Let $\eta = W-\tilde{W}$ and $\xi = \tilde{W}-W_h$, choose $v_h = \xi$ and use (3.39), that is,

$$(\nabla\xi, \nabla\xi) + \Big((\boldsymbol{b}-\boldsymbol{b_h})\cdot\nabla\tilde{W}, \xi\Big) + (\boldsymbol{b_h}\cdot\nabla\xi, \xi) = (f-f_h, \xi). \tag{3.42}$$

Use the bounds given in (3.21) and (3.22), when C and C_h are both greater than or both less than C_{sat},

$$\|\boldsymbol{b}(C, \nabla p) - \boldsymbol{b}(C_h, \nabla p_h)\|_{L^2} \le B_c \|C - C_h\|_{L^2} + B_q \|\nabla(p - p_h)\|_{L^2}$$
$$\le M(\|C - C_h\|_{L^2} + h^k \|p\|_{H^{k+1}}). \quad (3.43)$$

When C_{sat} is between C and C_h,

$$\begin{aligned}
& \|\boldsymbol{b}(C, \nabla p) - \boldsymbol{b}(C_h, \nabla p_h)\|_{L^2} \\
\le\ & \|\boldsymbol{b}(C, \nabla p) - \boldsymbol{b}(C_{sat}, \nabla p_h)\|_{L^2} + \|\boldsymbol{b}(C_{sat}, \nabla p) - \boldsymbol{b}(C_h, \nabla p_h)\|_{L^2} \\
\le\ & B_c \|C - C_{sat}\|_{L^2} + B_c \|C_{sat} - C_h\|_{L^2} + 2B_q \|\nabla(p - p_h)\|_{L^2} \\
\le\ & M(\|C - C_h\|_{L^2} + h^k \|p\|_{H^{k+1}}). \quad (3.44)
\end{aligned}$$

Without loss of generality, this technique can be applied to f as well. Next we also have

$$\begin{aligned}
& (f(C, \nabla p, \Delta p) - f(C_h, \nabla p_h, \Delta p_h), \xi) \\
=\ & -(\nabla \cdot (\gamma(C)\nabla p)\, C - \nabla \cdot (\gamma(C_h)\nabla p_h)\, C_h, \xi) \\
=\ & (\gamma(C)\nabla p, \nabla(C\xi)) - (\gamma(C_h)\nabla(p - p_h), \nabla((C - C_h)\xi)) \\
+\ & (\gamma(C_h)\nabla(p - p_h), \nabla(C\xi)) + (\gamma(C_h)\nabla p, \nabla((C - C_h)\xi)) - (\gamma(C_h)\nabla p, \nabla(C\xi)) \\
\le\ & M\left(h^{2k} + \|\xi\|_{L^2}^2 + \epsilon\|\nabla\xi\|_{L^2}^2 + \|\eta\|_{L^2}^2 + \|\nabla\eta\|_{L^2}^2\right). \quad (3.45)
\end{aligned}$$

Let $r = 3$ and $q = 6$ in Lemma 2.6, then from (3.42) we get that

$$\|\nabla\xi\|_{L^2}^2 \le \|\boldsymbol{b} - \boldsymbol{b_h}\|_{L^2} \|\nabla\tilde{W}\|_{W^{0,6}} \|\xi\|_{W^{0,3}} + B\|\nabla\xi\|_{L^2}\|\xi\|_{L^2}$$
$$+ M\left(h^{2k} + \|\xi\|_{L^2}^2 + \epsilon\|\nabla\xi\|_{L^2}^2 + \|\eta\|_{L^2}^2 + \|\nabla\eta\|_{L^2}^2\right). \quad (3.46)$$

Since by Lemma 3.5, $\|\nabla\tilde{W}\|_{W^{0,6}} \leq \|\nabla(W-\tilde{W})\|_{W^{0,6}} + \|\nabla W\|_{W^{0,6}} \leq (h^k + 1)\|C\|_{H^{k+1}}$. Also by Lemma 2.7 and Young's inequality with ϵ, we have

$$\|\xi\|_{W^{0,3}} \leq \|\xi\|_{L^2}^{\frac{1}{2}}\|\xi\|_{H^1}^{\frac{1}{2}} \leq \epsilon\|\xi\|_{H^1} + M\|\xi\|_{L^2}.$$

Thus, (3.46) now reads as below:

$$\|\nabla\xi\|_{L^2}^2 \leq M\left(h^{2k} + \|\xi\|_{L^2}^2 + \epsilon\|\nabla\xi\|_{L^2}^2 + \|\eta\|_{L^2}^2 + \|\nabla\eta\|_{L^2}^2\right),$$

then,

$$\|\nabla\xi\|_{L^2} \leq M\left(\|C-C_h\|_{L^2} + h^k\right).$$

Therefore

$$\|\nabla(W-W_h)\|_{L^2} \leq \|\nabla\xi\|_{L^2} + \|\nabla\eta\|_{L^2} \leq M\left(\|C-C_h\|_{L^2} + h^k\right). \tag{3.47}$$

Let $\psi = W - W_h$, define ϕ to be the solution satisfying the adjoint problem of (3.20):

$$\begin{aligned} -\Delta\phi - \nabla\cdot(\boldsymbol{b}\phi) + \frac{1}{D(C)}\partial_c\boldsymbol{b}\cdot\nabla W\phi - \frac{1}{D(C)}\partial_c f\phi = \psi, &\qquad \text{in } \Omega, \\ \phi = 0, &\qquad \text{on } \partial\Omega, \end{aligned}$$

where we used the facts

$$\begin{aligned} \tfrac{\partial\boldsymbol{b}}{\partial W} &= \partial_c\boldsymbol{b}\tfrac{\partial C}{\partial W} = \tfrac{\partial_c\boldsymbol{b}}{D(C)}, \\ \tfrac{\partial f}{\partial W} &= \partial_c f\tfrac{\partial C}{\partial W} = \tfrac{\partial_c f}{D(C)}. \end{aligned}$$

Then we have

$$\|\psi\|_0^2 = (\nabla\psi, \nabla\phi) + (\nabla\psi, \boldsymbol{b}\phi) + \left(\psi, \frac{1}{D(C)}\partial_c\boldsymbol{b}\cdot\nabla W\phi\right) - \left(\psi, \frac{1}{D(C)}\partial_c f\phi\right).$$

Use (3.41), that is,

$$\|\psi\|_0^2 = (f - f_h, \phi) - (\boldsymbol{b} \cdot \nabla W - \boldsymbol{b}_h \cdot \nabla W_h, \phi) + (\boldsymbol{b} \cdot \nabla \psi, \phi) + \left(\psi, \frac{1}{D(C)} \partial_c \boldsymbol{b} \cdot \nabla W \phi\right) - \left(\psi, \frac{1}{D(C)} \partial_c f \phi\right).$$

Because

$$\begin{aligned}
&(\nabla\psi, \boldsymbol{b}\phi) + \left(\psi, \frac{1}{D(C)} \partial_c \boldsymbol{b} \cdot \nabla W \phi\right) - (\boldsymbol{b} \cdot \nabla W - \boldsymbol{b}_h \cdot \nabla W_h, \phi) \\
&= (\boldsymbol{b}_h \nabla\psi, \phi) + ((\boldsymbol{b} - \boldsymbol{b}_h)\nabla\psi, \phi) + (\psi, \partial_c \boldsymbol{b} \cdot \nabla W \phi) - (\boldsymbol{b}\nabla W - \boldsymbol{b}_h \nabla W_h, \phi) \\
&= (\boldsymbol{b}_h \nabla\psi, \phi - \phi_h) - ((\boldsymbol{b} - \boldsymbol{b}_h)\nabla W, \phi_h - \phi) \\
&-((\boldsymbol{b} - \boldsymbol{b}_h)\nabla W, \phi) + ((\boldsymbol{b} - \boldsymbol{b}_h)\nabla\psi, \phi) + (\frac{1}{D(C)} \partial_c \boldsymbol{b}\psi, \nabla W \phi) \\
&\leq (\boldsymbol{b}_h \nabla\psi, \phi - \phi_h) - (\partial_c \boldsymbol{b}(\zeta_c, \nabla p)(C - C_h)\nabla W, \phi_h - \phi) \\
&-(\partial_p \boldsymbol{b}(C_h, \nabla\zeta_p)(p - p_h)\nabla W, \phi_h - \phi) - (\partial_c \boldsymbol{b}(\zeta_c, \nabla p)(C - C_h)\nabla W, \phi) \\
&-(\partial_p \boldsymbol{b}(C_h, \nabla\zeta_p)(p - p_h)\nabla W, \phi) + (\partial_c \boldsymbol{b}(\zeta_c, \nabla p)(C - C_h)\nabla\psi, \phi) \\
&+(\partial_p \boldsymbol{b}(C_h, \nabla\zeta_p)(p - p_h)\nabla\psi, \phi) + (\partial_c \boldsymbol{b}(C, \nabla p)\psi, \nabla W \phi) \\
&\leq (\boldsymbol{b}_h \nabla\psi, \phi - \phi_h) - (\partial_c \boldsymbol{b}(\zeta_c, \nabla p)\psi\nabla W, \phi_h - \phi) + \frac{1}{d}(\partial_{cc} \boldsymbol{b}(\zeta_c, \nabla p)\psi^2 \nabla W, \phi) \\
&+(\partial_c \boldsymbol{b}\psi, \nabla\psi\phi) - (\partial_p \boldsymbol{b}(C_h, \nabla\zeta_p)(p - p_h)\nabla W, \phi_h) + (\partial_p \boldsymbol{b}(C_h, \nabla\zeta_p)(p - p_h)\nabla\psi, \phi),
\end{aligned}$$

where ζ_c is between C and C_h and ζ_p is between p and p_h. Thus, with a constant difference,

$$\begin{aligned}
&\|\psi\|_0^2 \leq (\boldsymbol{b}_h \nabla\psi, \phi - \phi_h) - (\partial_c \boldsymbol{b}(\zeta_c, \nabla p)\psi\nabla W, \phi_h - \phi) \\
&+(\partial_c^2 \boldsymbol{b}(\zeta_c, \nabla p)\psi^2 \nabla W, \phi) + (\partial_c \boldsymbol{b}(C, \nabla p)\psi, \nabla\psi\phi) \\
&-(\partial_p \boldsymbol{b}(C_h, \nabla\zeta_p)(p - p_h)\nabla W, \phi_h) + (\partial_p \boldsymbol{b}(C_h, \nabla\zeta_p)(p - p_h)\nabla\psi, \phi) \\
&+(\partial_c^2 f(\zeta_c, \nabla p, \Delta p)\psi^2, \phi)
\end{aligned}$$

$$\leq \|\nabla\psi\|_0\|\phi-\phi_h\|_{L^2}+\|\psi\|_{L^3}\|\nabla W\|_{L^6}\|\phi-\phi_h\|_{L^2}+\|\psi\|_{L^3}^2\|\nabla W\|_{L^6}\|\phi\|_{L^2}$$

$$+\|\psi\|_{L^3}\|\nabla\psi\|_{L^6}\|\phi\|_{L^2}+\|p-p_h\|_{L^3}\|\nabla W\|_{L^6}\|\phi-\phi_h\|_{L^2}$$

$$+\|p-p_h\|_{L^3}\|\nabla W\|_{L^6}\|\phi\|_{L^2}+\|p-p_h\|_{L^3}\|\nabla\psi\|_{L^6}\|\phi\|_{L^2}+\|\psi\|_{L^2}^2\|\phi\|_{L^2}$$

$$\leq h^2\|\psi\|_{H^1}\|\psi\|_{L^2}+\|\psi\|_{H^1}^2\|\psi\|_{L^2}+h^{k+2}\|\psi\|_{L^2}+h^k\|\psi\|_{L^2}+h^k\|\psi\|_{H^1}\|\psi\|_{L^2}$$

$$+\|\psi\|_{L^2}^3$$

$$\leq M(h^k+h^2\|\psi\|_{H^1}+\|\psi\|_{H^1}^2+\|\psi\|_{L^2}^2). \tag{3.48}$$

Substitute (3.47) into the above inequality (3.48),

$$\|\psi\|_{L^2}\leq M(h^k+h^2\|\psi\|_{L^2}+\|\psi\|_{L^2}^2).$$

By the compactness argument [Krolyi (2005); Thomson et al. (2001)], we know that $\|\psi\|_0\to 0$, then $\|\psi\|_0^2\to 0$ quadratically as $h\to 0$ in contrast to $\|\psi\|_0\to 0$, therefore

$$\|W-W_h\|_{L^2}+\|W-W_h\|_{H^1}\leq Mh^k.$$

Finally by Lemma 3.1,

$$\|C-C_h\|_{L^2}+\|C-C_h\|_{H^1}\leq Mh^k.$$

Now we give the final analysis result in the following theorem.

Theorem 3.1. *Let (W,p) be the solution of (3.28)-(3.29) and (W_h,p_h) be the solution of (3.30)-(3.31). Suppose W and C satisfy the relation (3.14) and $\tilde{W}$ is the projection defined in (3.39), then we have following error estimates*

$$\|p-p_h\|_{L^2}+\|p-p_h\|_{H^1}+\|C-C_h\|_{L^2}+\|C-C_h\|_{H^1}\leq Mh^k(\|p\|_{H^{k+1}}+\|C\|_{H^{k+1}}). \tag{3.49}$$

3.2.5 Numerical results

In this section, we implement the finite element method for a practical case in PEMFC by taking $\boldsymbol{b}(C, \nabla p) = 0$ and $f(C, \nabla p, \Delta p) = -\nabla \cdot (\bar{\gamma}_c \nabla p C)$ in the generalized steady state PEMFC transport equation (3.20), and further in its finite element discretization scheme (3.30) on the computational domain shown in Figure 3.5 with boundary conditions given in Section 3.2.2. We simply give the L^2 norm convergence tests for water concentration C and pressure p to verify the theoretical results.

To simulate a 2D PEMFC model with the numerical discretizations and algorithms demonstrated in Section 3.2.4, we generate a considerable resolution: 15617 grid points, 30720 triangle elements, and 31234 degrees of freedom in the systems. The entire numerical simulations are carried out stably and quickly, as we expect for an efficient iteration. The convergent results are eventually obtained within 10 nonlinear iteration steps under the stopping criterion: the relative iterative error is less than the tolerance, 10^{-6}.

We carry out the following numerical convergence study by doing simulations for the aforementioned simplified steady state two-phase transport PEMFC model on a sequence of nested grids produced by a grid doubling, e.g. from 10×6 to 160×96 (five levels of grids), and compare the obtained number of iteration and convergence errors on different mesh levels with increasing DOFs, as shown in Table 3.3 and 3.4.

To investigate the convergence error for the obtained numerical solution u_h, we carry out the following error estimates based on the numerical solutions on a sequence of nested grids $\|u_{2^{j-1}h} - u_{2^j h}\|_{L^2} \leq \|u - u_{2^{j-1}h}\|_{L^2} + \|u - u_{2^j h}\|_{L^2}$. We use linear

Mesh Size	Error	Order
$h = 2.5 \times 10^{-5}$	$1.89E-06$	-
$h = 1.25 \times 10^{-5}$	$4.00E-07$	$2.24E+00$
$h = 6.25 \times 10^{-6}$	$1.00E-07$	$2.00E+00$
$h = 3.125 \times 10^{-6}$	$2.55E-08$	$1.97E+00$

Table 3.3. Convergence test for water concentration C

Mesh Size	Error	Order
$h = 2.5 \times 10^{-5}$	$8.04E-04$	-
$h = 1.25 \times 10^{-5}$	$2.28E-04$	$1.82E+00$
$h = 6.25 \times 10^{-6}$	$6.28E-05$	$1.86E+00$
$h = 3.125 \times 10^{-6}$	$1.70E-05$	$1.88E+00$

Table 3.4. Convergence test for pressure p

interpolation and apply Theorem 3.1 to two adjacent mesh levels with the mesh size $2^{j-1}h$ and $2^j h$, respectively, and get $\|C_{2^{j-1}h} - C_{2^j h}\|_{L^2} = 3 \times 2^{j-1}h$ and $\|p_{2^{j-1}h} - p_{2^j h}\|_{L^2} = 3 \times 2^{j-1}h$. Here $j = 1, 2, \ldots,$ denotes the mesh level number. $j = 1$ means the finest mesh with mesh size h, and the mesh size of j-th level mesh is $2^{j-1}h$. Thus, in the discretization level

$$\ln\left(\frac{\|C_{2^j h} - C_{2^{j+1}h}\|_{L^2}}{\|C_{2^{j-1}h} - C_{2^j h}\|_{L^2}}\right) / \ln 2 \approx 1 \quad \text{and} \quad \ln\left(\frac{\|p_{2^j h} - p_{2^{j+1}h}\|_{L^2}}{\|p_{2^{j-1}h} - p_{2^j h}\|_{L^2}}\right) / \ln 2 \approx 1.$$

Even though the numerical errors and convergence orders appear to have a super convergence for water concentration C and pressure p (as shown in Table 3.3 and in Table 3.4) compared to the theoretical results in theorem 3.1, it is obvious that the convergence orders have a trend of decreasing in Table 3.3 and slight increasing in Table 3.4, which shall be able to be accepted as a reasonable verification of our theoretical results.

3.3 Numerical analysis of finite element method for a transient two-phase transport model of proton exchange membrane fuel cell

3.3.1 Introduction

This section continues our effort in [Sun and Sun (2014)] where the error estimates of finite element method with Kirchhoff transformation have been given for steady state PEMFC model. The goal of this section is to accurately analyze the error estimates of the semi-discrete finite element scheme and fully discrete finite element method with Crank-Nicolson scheme for a simplified transient two-phase transport model in the cathode gas diffusion layer (GDL) of PEMFC. We obtain the optimal error estimate in $L^\infty(H^1)$ norm and the sub-optimal error estimate in $L^\infty(L^2)$ norm for both finite element schemes in spatial discretization, and second order approximation in temporal discretization for the fully discrete scheme.

The rest of this section is organized as follows. In Section 3.3.2, a simplified 2D two-phase transport model in the cathode GDL of PEMFC is studied. Then Kirchhoff transformation is introduced to describe the reformulated water concentration equation, and its efficiency is demonstrated on dealing with the discontinuous and degenerate diffusivity. The semi-discrete finite element scheme is presented and its error estimate is given in Section 3.3.3. A fully discrete finite element method with Crank-Nicolson scheme is designed and analyzed correspondingly in Section 3.3.4.

3.3.2 A simplified 2D transient two-phase transport model in the cathode GDL of PEMFC

In this section, the governing equations for a simplified 2D transient two-phase transport problem in the cathode GDL of PEMFC are described, together with the computational domain and the corresponding boundary conditions. To define a simplified 2D transient isothermal two-phase transport model in the cathode GDL, we only need to address a pressure equation using Darcy's law, and water concentration equation in which Darcy's velocity is used. As mentioned in the introduction in Section 1.1, water management is the most important and challenging problem in PEMFC model. The physical feature of water determines that the two-phase zone and the single-phase zone are co-existing. For water concentration equation, in order to present a unified model that encompasses both the single- and two-phase regimes, and to ensure a smooth transition between the two, a discontinuous and degenerate function is introduced [Wang et al. (2001)] as diffusivity of the transport equation in terms of water concentration. In gaseous water region, the water concentration is below a fixed value called saturated water concentration ($16 mol/m^3$ at $80^o C$), coinciding with nonzero constant diffusivity. Once water concentration exceeds this fixed value, excess gaseous water is generated and condensed to liquid water. Correspondingly, the diffusivity suddenly jumps down to zero and then grows up into a smooth diffusivity function with respect to liquid water concentration. Thus a degenerate and discontinuous diffusivity is introduced. Nevertheless, GDL is the major component in PEMFC that contains both liquid water and gaseous water vapor, while gas channel only contains water vapor. Therefore, in this chapter the attention is put on the water species only in GDL instead of all species spreading everywhere. Based on the M^2 model, the two-phase transport model is defined as follows with respect to water's molar concentration C and pressure p [Sun et al. (2009b); Wang and Cheng (1996)]:

$$\epsilon_0 \partial_t C - \nabla \cdot (D(C) \nabla C) + \nabla \cdot (\gamma_c \boldsymbol{u} C) = 0, \tag{3.50}$$

$$\nabla \cdot \left(\frac{K}{\epsilon_0 \nu(C)} \nabla p \right) = 0, \tag{3.51}$$

where $\partial_t = \partial / \partial t$. Here ϵ_0 is the porosity of GDL, the Darcy's velocity $\boldsymbol{u}$ is defined as $\boldsymbol{u} = -\frac{K}{\epsilon_0 \rho \nu} \nabla p$. We assume $\nabla \cdot (\rho \boldsymbol{u}) = 0$, thus the pressure equation (3.51) is introduced. All the parameters relations and values are defined the same as in Section 3.2.2. By defining a similar new advection correction factor in Section 3.2.2 as $\bar{\gamma}_c = -\frac{K \gamma_c}{\epsilon_0 \rho \nu}$, the governing equations (3.50)-(3.51) can be written as

$$\epsilon_0 \partial_t C - \nabla \cdot (D(C) \nabla C) + \nabla \cdot (\bar{\gamma}_c \nabla p C) = 0 \tag{3.52}$$

$$\nabla \cdot \left(\frac{K}{\epsilon_0 \nu(C)} \nabla p \right) = 0. \tag{3.53}$$

The governing equations (3.52)-(3.53) take place in the cathode GDL of PEMFC, as shown in Figure 3.5. The computational domain and boundary conditions are the same as given in Section 3.2.2.

As discussed in Section 3.3.2, $D(C)$ is degenerate and also discontinuous at C_{sat}, which causes the numerical simulation to be inefficient and unstable. In order to resolve such computational difficulties, we use the Kirchhoff transformation [Sun et al. (2009b)] used in Section 3.2.3 (3.13). Thus with similar techiniques, we are able to reformulate the water concentration equation (3.52) with Kirchhoff transformation as follows

$$\frac{\epsilon_0}{D(C)+\delta}\partial_t W - \Delta W = -\nabla\cdot(\bar{\gamma}_c \nabla p C) \qquad \text{in } \Omega, \tag{3.54}$$

$$W = \int_0^{C_b} D(w)dw \qquad \text{on } (\partial\Omega)_1, \tag{3.55}$$

$$\partial_{\boldsymbol{n}} W = 0 \qquad \text{on } (\partial\Omega)_2 \text{ and } (\partial\Omega)_3, \tag{3.56}$$

$$\nabla W\cdot\boldsymbol{n} - \bar{\gamma}_c \nabla p C(W)\cdot\boldsymbol{n} = \frac{I(x)}{2F} \qquad \text{on } (\partial\Omega)_4.. \tag{3.57}$$

Here δ is a sufficiently small positive number for the sake of avoidance of possible zero denominator at $C = C_{\text{sat}}$.

In order to extend the numerical analysis on error estimates of finite element method, which will be given in Section 3.3.3, to a more general case, the reformulated water concentration equation can be generalized to the following form of convection-diffusion-reaction equation

$$r(C)\partial_t W - \Delta W + \boldsymbol{b}(C,\nabla p)\cdot\nabla W = f(C,\nabla p,\Delta p), \tag{3.58}$$

where

$$r(C) = \frac{\epsilon_0}{D(C)+\delta},\ \boldsymbol{b}(C,\nabla p) = \frac{\bar{\gamma}_c\nabla p}{D(C)+\delta},\ f(C,\nabla p,\Delta p) = -\nabla\cdot(\bar{\gamma}_c\nabla p)\,C(W).$$

Obviously, (3.54) is just special cases of (3.58). Without loss of generality, in what follows, we will carry out the error estimates of finite element method for (3.58) instead of (3.54).

We also define that $g(C) = \frac{K}{\epsilon_0 \nu(C)}$. All the necessary coefficient functions and their proper derivatives are Lipschitz continuous, and their upper and lower bounds satisfy the following conditions for $C \geq 0$,

$$d \leq D(C) \leq D, 0 < r \leq r(C) \leq R, b < |\boldsymbol{b}(C,\phi)| < B, |\gamma(C)| < \Gamma,$$

$$0 < g_0 \leq g(C), \frac{\partial g(C)}{\partial C} \leq G_c, b_p < \left|\frac{\partial \boldsymbol{b}(C,\phi)}{\partial \phi}\right| < B_p, b_{pp} < \left|\frac{\partial^2 \boldsymbol{b}(C,\phi)}{\partial \phi^2}\right| < B_{pp}. \quad (3.59)$$

However, since $D(C)$ is discontinuous at C_{sat}, $r(C)$ and $\boldsymbol{b}(C, \nabla p)$ are also discontinuous at C_{sat}. Therefore the following conditions are to be satisfied when C is on either side of C_{sat},

$$|r'(C)| \leq R',\ |r''(C)| \leq R'',\ b_c < \left|\frac{\partial \boldsymbol{b}(C,\phi)}{\partial C}\right| < B_c,$$

$$b_{cc} < \left|\frac{\partial^2 \boldsymbol{b}(C,\phi)}{\partial C^2}\right| < B_{cc},\ b_{cp} < \left|\frac{\partial \boldsymbol{b}(C,\phi)}{\partial \phi \partial C}\right| < B_{cp}. \quad (3.60)$$

In order to simplify notation, in what follows, we denote $r(C)$ as r, $\boldsymbol{b}(C, \nabla p)$ as $\boldsymbol{b}$, $f(C, \nabla p, \Delta p)$ as f, and $g(C)$ as g.

Since the expression for C in Kirchhoff transformation (3.14) is not explicit, we use the same Kirchhoff inverse transformation defined in (3.25) and (3.26).

3.3.3 Semi-discrete scheme and its error estimate

First of all, we assume the following regularity properties hold for W and p in the semi-discretization analysis:

$$C \in W^{1,\infty}(0, T; H^{k+1} \cap W^{1,\infty}(\Omega)) \text{ and } p \in W^{1,\infty}(0, T; W^{k+1,\infty}(\Omega)). \quad (3.61)$$

Then we define spaces

$$H_w = \left\{ W \in H^1\left(0, T; H^{k+1}(\Omega) \cap W^{1,\infty}(\Omega)\right); W|_{(\partial\Omega)_1} = \int_0^{C_b} D(w)dw \right\},$$

$$
\begin{aligned}
\bar{H_w} &= \{W \in H_w; W|_{\partial\Omega} = 0\}, \\
H_p &= \left\{p \in H^{k+1}(\Omega) \cap W^{1,\infty}(\Omega); p|_{(\partial\Omega)_1} = p_1 - (p_1 - p_2)x/l_{\mathrm{PEMFC}}\right\}, \\
\bar{H_p} &= \{p \in H_p; p|_{\partial\Omega} = 0\}.
\end{aligned}
$$

Since after applying Kirchhoff transformation (3.14), the water concentration equation is given as (3.54), here we for the convenience of referencing, we rewrite the governing equations as follows

$$
\frac{\epsilon_0}{D(C)+\delta}\partial_t W - \Delta W = -\nabla \cdot (\bar{\gamma}_c \nabla p C), \tag{3.62}
$$

$$
\nabla \cdot (g \nabla p) = 0. \tag{3.63}
$$

Apply standard finite element method to (3.62)-(3.63), their weak form is given as: find $(W, p) \in H_w \times H_p$, such that for any $(v, q) \in H_w \times H_p$:

$$
\begin{aligned}
\left(\frac{\epsilon_0}{D(C)+\delta}\partial_t W, v\right) + (\nabla W, \nabla v) &= (\bar{\gamma}_c \nabla p C, \nabla v) + \int_{\Omega_4} \frac{I(x)}{2F} v ds, \\
(g \nabla p, \nabla q) &= 0.
\end{aligned}
$$

Define piecewise linear polynomial finite element spaces, $S_h \subseteq H_w$, $T_h \subseteq H_p$, $\bar{S}_h \subseteq \bar{H}_w$ and $\bar{T}_h \subseteq \bar{H}_p$. Given $C_h^n \in S_h$, find $(W_h^{n+1}, p_h^{n+1}) \in S_h \times T_h$ such that for any $(v_h, q_h) \in \bar{S}_h \times \bar{T}_h$,

$$
\begin{aligned}
\left(\frac{\epsilon_0}{D(C_h^n)+\delta}\partial_t W_h^{n+1}, v_h\right) + \left(\nabla W_h^{n+1}, \nabla v_h\right) &= (\bar{\gamma}_c \nabla p C_h^n, \nabla v_h) + \int_{\Omega_4} \frac{I(x)}{2F} v_h ds, \\
\left(g_h \nabla p_h^{n+1}, \nabla q_h\right) &= 0.
\end{aligned}
$$

For the purpose of error estimate, as mentioned in Section 3.2.3, the more general governing equation (3.58) will be used in place of (3.62). Apply the standard finite element method to (3.58) and (3.63), their weak form is given as: find $(W, p) \in H_w \times H_p$, such that

$$(r\partial_t W, v) + (\nabla W, \nabla v) + (\boldsymbol{b} \cdot \nabla W, v) = (f, v), \qquad \forall v \in \bar{H}_w, \tag{3.64}$$

$$(g\nabla p, \nabla q) = 0, \qquad \forall q \in \bar{H}_p. \tag{3.65}$$

The semi-discretization form of (3.58) and (3.63) is given as follows: Find $(W_h, p_h) \in S_h \times T_h$, such that

$$(r_h\partial_t W_h, v_h) + (\nabla W_h, \nabla v_h) + (\boldsymbol{b}_h \cdot \nabla W_h, v_h) = (f_h, v_h), \qquad \forall v_h \in \bar{S}_h, \tag{3.66}$$

$$(g_h\nabla p_h, \nabla q_h) = 0, \qquad \forall q_h \in \bar{T}_h. \tag{3.67}$$

where r_h, $\boldsymbol{b}_h$ and f_h represents $r(C_h)$, $\boldsymbol{b}(C_h, \nabla p_h)$ and $f(C_h, \nabla p_h, \Delta p_h)$, respectively.

Similar to Lemma 3.4 from Section 3.2.4, we can get the following lemma.

Lemma 3.6. *Let (W, p) be the solution of (3.64)-(3.65), and (W_h, p_h) be the solution of (3.66)-(3.67). Suppose W and C satisfy the relation (3.14), then we have the following error estimates:*

$$\|p - p_h\|_{L^2} \le Mh^{k+1}\|p\|_{H^{k+1}} + M\|C - C_h\|_{L^2}, \tag{3.68}$$

and

$$\|\nabla(p - p_h)\|_{L^2} \le Mh^k\|p\|_{H^{k+1}} + M\|C - C_h\|_{L^2}. \tag{3.69}$$

Also similar to Lemma 3.1 in Section 3.2.4, we can get the following lemma.

Lemma 3.7. *Suppose W and C satisfy the relation (3.14), then their norms have the following relation*

$$d\|C\|_{H^{k+1}\cap W^{1,\infty}} \le \|W\|_{H^{k+1}\cap W^{1,\infty}} \le D\|C\|_{H^{k+1}\cap W^{1,\infty}}. \tag{3.70}$$

Define a projection $\tilde{W} \in S_h$ to satisfy

$$(\nabla(W-\tilde{W}), \nabla v_h) + (\boldsymbol{b} \cdot \nabla(W-\tilde{W}), v_h) = 0, \ \forall v_h \in \bar{S}_h, \tag{3.71}$$

then (3.64) also reads: Find $W \in H_w$, such that

$$(r\partial_t W, v) + (\nabla\tilde{W}, \nabla v) + (\boldsymbol{b} \cdot \nabla\tilde{W}, v) = (f, v), \ \forall v \in \bar{H}_w. \tag{3.72}$$

Lemma 3.8. *Let (W,p) be the solution of (3.64)-(3.65) and (W_h, p_h) be the solution of (3.66)-(3.67). Suppose W and C satisfy the relation (3.14) and $\tilde{W}$ is the projection defined in (3.71), then we have following error estimates*

$$\|W-\tilde{W}\|_{L^2} + h\|W-\tilde{W}\|_{H^1} \le Mh^{k+1}\|C\|_{H^{k+1}}, \tag{3.73}$$

$$\|\partial_t(W-\tilde{W})\|_{L^2} + h\|\partial_t(W-\tilde{W})\|_{H^1} \le Mh^{k+1}\left(\|C\|_{H^{k+1}} + \|\partial_t C\|_{H^{k+1}}\right). \tag{3.74}$$

Proof. Let $\Pi_h W$ be the finite element nodal interpolation of W. Since $\Pi_h W - \tilde{W} \in \bar{S}_h$, by (3.71),

$$\begin{aligned}&\left(\nabla\left(W-\tilde{W}\right), \nabla\left(W-\tilde{W}\right)\right) + \left(\boldsymbol{b}\cdot\nabla\left(W-\tilde{W}\right), W-\tilde{W}\right)\\ &\qquad = \left(\nabla\left(W-\tilde{W}\right), \nabla\left(W-\Pi_h W\right)\right) + \left(\boldsymbol{b}\cdot\nabla\left(W-\tilde{W}\right), W-\Pi_h W\right).\end{aligned}$$

Thus by (3.59),

$$\begin{aligned}&\|\nabla(W-\tilde{W})\|_{L^2}^2 \le B\|\nabla(W-\tilde{W})\|_{L^2}\|W-\tilde{W}\|_{L^2}\\ &\quad + \|\nabla(W-\tilde{W})\|_{L^2}\|\nabla\left(W-\Pi_h W\right)\|_{L^2} + B\|\nabla(W-\tilde{W})\|_{L^2}\|W-\Pi_h W\|_{L^2}.\end{aligned} \tag{3.75}$$

Divide (3.75) by $\|\nabla(W-\tilde{W})\|_{L^2}^2$ on both side, we have

$$\|\nabla(W-\tilde{W})\|_{L^2} \le B\|W-\tilde{W}\|_{L^2} + \|\nabla\left(W-\Pi_h W\right)\|_{L^2} + B\|W-\Pi_h W\|_{L^2}.$$

By the error of finite element nodal interpolation, we can get

$$\|W-\tilde{W}\|_{H^1} \le M\|W-\tilde{W}\|_{L^2}+Mh^k\|W\|_{H^{k+1}} \le M\|W-\tilde{W}\|_{L^2}+Mh^k\|C\|_{H^{k+1}}. \quad (3.76)$$

Next, we consider the L^2 error estimate of $W-\tilde{W}$ by using Aubin-Nitsche duality argument. Let $e = W - \tilde{W}$, and define $w \in H^2(\Omega) \cap H_0^1(\Omega)$ to satisfy the adjoint problem of (3.71) as follows,

$$\begin{cases} -\Delta w - \nabla \cdot (\boldsymbol{b} w) = e, \\ w = 0. \end{cases}$$

Let $\Pi_h w$ be the finite element nodal interpolation of w, then we have that

$$\begin{aligned} \|e\|_{L^2}^2 &= -(e, \Delta w) - (e, \nabla \cdot (\boldsymbol{b} w)) \\ &= (\nabla e, \nabla (w - \Pi_h w + \Pi_h w)) + (\nabla e, \boldsymbol{b}(w - \Pi_h w + \Pi_h w)) \\ &= (\nabla e, \nabla (w - \Pi_h w)) - (\nabla e, \boldsymbol{b}(w - \Pi_h w)) \\ &\le M\|e\|_{H^1}\|w - \Pi_h w\|_{H^1}. \end{aligned}$$

Since $\|w - \Pi_h w\|_{H^1} \le Mh\|w\|_{H^2}$ and $\|w\|_{H^2} \le \|e\|_{L^2}$, it is easy to see that

$$\|e\|_{L^2}^2 \le Mh\|e\|_{H^1}\|e\|_{L^2}.$$

Therefore by (3.76) and (3.70),

$$\|W - \tilde{W}\|_{L^2} \le Mh\|W - \tilde{W}\|_{H^1} \le Mh^{k+1}\|W\|_{H^{k+1}} \le Mh^{k+1}\|C\|_{H^{k+1}}.$$

Lastly, we obtain the L^2 and H^1 error estimates of $\partial_t(W-\tilde{W})$ by taking derivative with respect to t in (3.71),

$$\Big(\partial_t \nabla (W - \tilde{W}), \nabla v_h\Big) + \Big(\partial_t \boldsymbol{b} \cdot \nabla (W - \tilde{W}), v_h\Big) + \Big(\boldsymbol{b} \cdot \partial_t \nabla (W - \tilde{W}), v_h\Big) = 0.$$

Similar to the process above, (3.74) can be obtained.

□

Next we give the error estimate in max norm for $W - \tilde{W}$ as below.

Lemma 3.9. *Let W be the solution of (3.64) and W_h be the solution of (3.66). Suppose W and C satisfy the relation (3.14) and $\tilde{W}$ is the projection defined in (3.71), then we have following error estimates:*

$$\|W - \tilde{W}\|_{W^{0,\infty}} \leq Mh^{k+1} |\ln h|^{\frac{3}{2}} \|C\|_{H^{k+1}}, \tag{3.77}$$

$$\|W - \tilde{W}\|_{W^{1,\infty}} \leq Mh^{k} |\ln h| \|C\|_{H^{k+1}}. \tag{3.78}$$

Proof. Define a projection operator P_h to satisfy $\tilde{W} = P_h W \in \bar{S}_h$, then by (3.71),

$$W - \tilde{W} = W - P_h W = (I - P_h)W = (I - P_h)(W - \Pi_h W),$$

where I is the identity operator and $P_h \Pi_h W = \Pi_h W$. Since from [Ciarlet (1978)], we know

$$|\ln h|^{-\frac{1}{2}} \|P_h W\|_{W^{0,\infty}} + h |P_h W|_{W^{1,\infty}} \leq M \left(\|W\|_{W^{0,\infty}} + h |\ln h| |W|_{W^{1,\infty}}\right),$$

so when h is small enough, one can obtain

$$\begin{aligned} &\|W - \tilde{W}\|_{W^{0,\infty}} \leq \|W - \Pi_h W\|_{W^{0,\infty}} + \|P_h(W - \Pi_h W)\|_{W^{0,\infty}} \\ \leq\ & M \left(|\ln h|^{\frac{1}{2}} + 1\right) \|W - \Pi_h W\|_{W^{0,\infty}} + Mh |\ln h|^{\frac{3}{2}} |W - \Pi_h W|_{W^{1,\infty}} \\ \leq\ & M |\ln h|^{\frac{3}{2}} h^{k+1} \|W\|_{H^{k+1}}, \end{aligned}$$

and

$$\begin{aligned} &h|W - \tilde{W}|_{W^{1,\infty}} \leq h|W - \Pi_h W|_{W^{1,\infty}} + h|P_h(W - \Pi_h W)|_{W^{1,\infty}} \\ \leq\ & M\|W - \Pi_h W\|_{W^{0,\infty}} + Mh (1 + |\ln h|) |W - \Pi_h W|_{W^{1,\infty}} \\ \leq\ & M |\ln h| h^{k+1} \|W\|_{H^{k+1}}, \end{aligned}$$

therefore

$$\|W - \tilde{W}\|_{W^{1,\infty}} \le Mh^k |\ln h| \left(|\ln h|^{\frac{1}{2}} h + 1 \right) \|W\|_{H^{k+1}} \le Mh^k |\ln h| \|C\|_{H^{k+1}}.$$

□

Remark 3.1. When $h \to 0$, $h|\ln h| < 1$ and $h|\ln h|^{1/2} < 1$. Since $k \ge 1$, we know that $h^k|\ln h| < 1$ and $h^{k+1}|\ln h|^{3/2} < 1$, thus $\|W - \tilde{W}\|_{W^{1,\infty}}$ and $\|W - \tilde{W}\|_{W^{0,\infty}}$ are bounded.

Corollary 3.1. *Let W be the solution of (3.64) and W_h be the solution of (3.66). Suppose W and C satisfy the relation (3.14) and $\tilde{W}$ is the projection defined in (3.71), then $\|\tilde{W}\|_{L^\infty}$ and $\|\nabla \tilde{W}\|_{L^\infty}$ are bounded.*

Proof. Since

$$\|\tilde{W}\|_{L^\infty} + \|\nabla \tilde{W}\|_{L^\infty} \le \|W - \tilde{W}\|_{W^{1,\infty}} + \|W\|_{W^{1,\infty}},$$

use (3.78), we can get the boundedness of $\|\tilde{W}\|_{L^\infty}$ and $\|\nabla \tilde{W}\|_{L^\infty}$. □

Theorem 3.2. *Let (W, p) be the solution of (3.64)-(3.65) and (W_h, p_h) be the solution of (3.66)-(3.67). Suppose W and C satisfy the relation (3.14) and $\tilde{W}$ is the projection defined in (3.71). With (3.59) and (3.60), we have the error estimates as follows:*

$$\|p - p_h\|_{L^\infty(L^2)} + \|p - p_h\|_{L^\infty(H^1)} + \|C - C_h\|_{L^\infty(L^2)} + \|C - C_h\|_{L^\infty(H^1)} \le Mh^k. \quad (3.79)$$

Proof. Let $\eta = W - \tilde{W}$ and $\xi = \tilde{W} - W_h$. Choose $v_h = \xi$, the error equation of (3.58) can be achieved by subtracting (3.66) from (3.72) as follows,

$$(r_h \partial_t \xi, \xi) + (r_h \partial_t \eta, \xi) + ((r - r_h)\partial_t W, \xi) + (\nabla \xi, \nabla \xi)$$
$$\left((\boldsymbol{b} - \boldsymbol{b}_h) \cdot \nabla \tilde{W}, \xi \right) + (\boldsymbol{b}_h \cdot \nabla \xi, \xi) = (f - f_h, \xi). \quad (3.80)$$

Since the first term on the left hand side in (3.80) can be written as

$$\int_\Omega r_h(\partial_t\xi)\xi dx = \int_\Omega r_h\partial_t\left(\frac{1}{2}\xi^2\right)dx = \int_\Omega \partial_t\left(\frac{1}{2}r_h\xi^2\right)dx - \int_\Omega r_h'\partial_t C_h\left(\frac{1}{2}\xi^2\right)dx.$$

Use the same techiniques in (3.43), (3.44) and (3.45), integrate both sides of (3.80) with respect to t. By (3.73) and (3.74), we can get

$$\|\xi\|_{L^2}^2 + \int_0^t \|\nabla\xi\|_{L^2}^2 \leq M\left(\epsilon\int_0^t \|\nabla\xi\|_{L^2}^2 + \int_0^t \|\xi\|_{L^2}^2 + h^{2k}\right). \tag{3.81}$$

Then apply Gronwall's inequality to (3.81),

$$\|\xi\|_{L^\infty(L^2)} + \|\nabla\xi\|_{L^2(L^2)} \leq Mh^k.$$

Use (3.73) again, we have,

$$\|W - W_h\|_{L^\infty(L^2)} + \|\nabla(W - W_h)\|_{L^2(L^2)} \leq Mh^k. \tag{3.82}$$

Lastly, we let $v_h = \partial_t\xi$ in (3.80) and use a similar approach as above to obtain the error estimate of $\|\nabla(W - W_h)\|_{L^\infty(L^2)}$ as follows,

$$\|\nabla(W - W_h)\|_{L^\infty(L^2)} + \|\partial_t(W - W_h)\|_{L^2(L^2)} \leq Mh^k. \tag{3.83}$$

Finally, combine (3.70), (3.82), (3.83), (3.68) and (3.69), we can get (3.79).

□

3.3.4 Fully discrete scheme and its error estimate

In this section, a fully discrete scheme is designed for the model using Crank-Nicolson Scheme. The error estimates in $L^\infty(H^1)$ and $L^\infty(L^2)$ norms are also given. First we give regularity assumptions for C and p in the full discretization analysis:

$$C \in W^{3,\infty}(0,T; H^{k+1} \cap W^{1,\infty}(\Omega)) \text{ and } p \in W^{2,\infty}(0,T; W^{k+1,\infty}(\Omega)). \tag{3.84}$$

In order to give the full discretization of the system (3.64)-(3.65), we first define a uniform partition $0 = t^0 < t^1 < \cdots < t^N = T$, with time-step size $\Delta t = T/N$, and $t^\sigma = \sigma \Delta t$, $\sigma \in \mathbb{R}$. Also, for any function φ, denote $\varphi^n \equiv \varphi(x, t^n)$, $\varphi^{n+\frac{1}{2}} \equiv (\varphi^{n+1} + \varphi^n)/2$, and $d_t \varphi^n \equiv (\varphi^{n+1} - \varphi^n)/\Delta t$. We use Crank-Nicolson scheme for the time discretization of (3.58) and (3.63), i.e., given (W_h^n, p_h^n), we seek (W_h^{n+1}, p_h^{n+1}) such that for any $(v_h, q_h) \in \bar{S}_h \times \bar{T}_h$

$$\left(r_h^{n+\frac{1}{2}} d_t W_h^n, v_h\right) + \left(\nabla W_h^{n+\frac{1}{2}}, \nabla v_h\right) + \left(\boldsymbol{b}_h^{n+\frac{1}{2}} \cdot \nabla W_h^{n+\frac{1}{2}}, v_h\right) = \left(f_h^{n+\frac{1}{2}}, v_h\right), \tag{3.85}$$

$$\left(g_h^{n+\frac{1}{2}} \nabla p_h^{n+\frac{1}{2}}, \nabla q_h\right) = 0. \tag{3.86}$$

Next, use the similar analysis for Lemma 3.6 and Lemma 3.8, we can prove the following results.

Lemma 3.10. *Let (W, p) be the solution of (3.64)-(3.65) and (W_h, p_h) be the solution of (3.66)-(3.67). Suppose $\tilde{W}$ is the projection defined in (3.71). For any $n = 0, 1, ..., N$, we have the following error estimates:*

$$\|p^n - p_h^n\|_{L^2} + \|p^n - p_h^n\|_{H^1} \leq M\left(h^k + \|C^n - C_h^n\|_{L^2}\right),$$

and

$$\|\partial_t^\alpha (W^n - \tilde{W}^n)\|_{L^2} + h\|\partial_t^\alpha \nabla (W^n - \tilde{W}^n)\|_{L^2} \leq M h^{k+1},$$

where $\alpha = 0, 1, 2, 3$.

Theorem 3.3. *Let (W, p) be the solution of (3.64)-(3.65) and (W_h, p_h) be the solution of (3.66)-(3.67). Suppose W and C satisfy the relation (3.14) and $\tilde{W}$ is the projection defined in (3.71). Then there exists a constant M depending only on the regularity of*

C and p, such that

$$\|C^N - C_h^N\|_{L^2} + \|\nabla(C^N - C_h^N)\|_{L^2}^2 \le M\left(h^k + (\Delta t)^2\right). \tag{3.87}$$

Proof. Let (3.64) and (3.71) take value at $t^{n+\frac{1}{2}}$, $0 \le n \le N-1$, we have

$$\left(r(t^{n+\frac{1}{2}})\partial_t W(t^{n+\frac{1}{2}}), v\right) + \left(\nabla\tilde{W}(t^{n+\frac{1}{2}}), \nabla v\right) + \left(\boldsymbol{b}(t^{n+\frac{1}{2}}) \cdot \nabla\tilde{W}(t^{n+\frac{1}{2}}), v\right) = \left(f(t^{n+\frac{1}{2}}), v\right). \tag{3.88}$$

Thus the error equation of the fully discrete scheme is achieved by subtracting (3.85) from (3.88), given as below,

$$\left(r(t^{n+\frac{1}{2}})\partial_t W(t^{n+\frac{1}{2}}) - r_h^{n+\frac{1}{2}} d_t W_h^n, v_h\right) + \left(\nabla\tilde{W}(t^{n+\frac{1}{2}}) - \nabla W_h^{n+\frac{1}{2}}, \nabla v_h\right) + \left(\boldsymbol{b}(t^{n+\frac{1}{2}}) \cdot \nabla\tilde{W}(t^{n+\frac{1}{2}}) - \boldsymbol{b}_h^{n+\frac{1}{2}} \cdot \nabla W_h^{n+\frac{1}{2}}, v_h\right) = \left(f(t^{n+\frac{1}{2}}) - f_h^{n+\frac{1}{2}}, v_h\right). \tag{3.89}$$

Let $\eta^n = W^n - \tilde{W}^n$ and $\xi^n = \tilde{W}^n - W_h^n$, then (3.89) becomes:

$$\sum_1^{11} G_i^n = 0, \tag{3.90}$$

where

$$\begin{aligned}
G_1^n &= \left(\left(r(t^{n+\frac{1}{2}}) - r_h^{n+\frac{1}{2}}\right)\partial_t W(t^{n+\frac{1}{2}}), v_h\right), \\
G_2^n &= \left(r_h^{n+\frac{1}{2}}\left(\partial_t W(t^{n+\frac{1}{2}}) - d_t W^n\right), v_h\right), \\
G_3^n &= \left(r_h^{n+\frac{1}{2}}\left(d_t \eta^n - \partial_t \eta(t^{n+\frac{1}{2}})\right), v_h\right), \\
G_4^n &= \left(r_h^{n+\frac{1}{2}}\partial_t \eta(t^{n+\frac{1}{2}}), v_h\right), \\
G_5^n &= \left(r_h^{n+\frac{1}{2}} d_t \xi^n, v_h\right), \\
G_6^n &= \left(\nabla\tilde{W}(t^{n+\frac{1}{2}}) - \nabla\tilde{W}^{n+\frac{1}{2}}, \nabla v_h\right),
\end{aligned}$$

$$
\begin{aligned}
G_7^n &= \left(\nabla \xi^{n+\frac{1}{2}}, \nabla v_h\right), \\
G_8^n &= \left(\left(\boldsymbol{b}(t^{n+\frac{1}{2}}) - \boldsymbol{b}_h^{n+\frac{1}{2}}\right) \cdot \nabla \tilde{W}(t^{n+\frac{1}{2}}), v_h\right), \\
G_9^n &= \left(\boldsymbol{b}_h^{n+\frac{1}{2}} \cdot \nabla \left(\tilde{W}(t^{n+\frac{1}{2}}) - \tilde{W}^{n+\frac{1}{2}}\right), v_h\right), \\
G_{10}^n &= \left(\boldsymbol{b}_h^{n+\frac{1}{2}} \cdot \nabla \xi^{n+\frac{1}{2}}, v_h\right), \\
G_{11}^n &= -\left(f(t^{n+\frac{1}{2}}) - f_h^{n+\frac{1}{2}}, v_h\right) = 0.
\end{aligned}
$$

We have the following results from Taylor's expansions: $\partial_t \varphi(t^{n+\frac{1}{2}}) - d_t \varphi^n = M(\Delta t)^2 \|\partial_{ttt}\varphi\|_{L^\infty(L^2)}$ and $\varphi(t^{n+\frac{1}{2}}) - \varphi^{n+\frac{1}{2}} = M(\Delta t)^2 \|\partial_{tt}\varphi\|_{L^\infty(L^2)}$. The also introduce the following technique for full discretization that is similar to the technique (3.43) as follows,

$$
\begin{aligned}
& \|\boldsymbol{b}(t^{n+\frac{1}{2}}) - \boldsymbol{b}_h^{n+\frac{1}{2}}\|_{L^2} \\
\leq\ & \|\boldsymbol{b}(t^{n+\frac{1}{2}}) - \boldsymbol{b}^{n+\frac{1}{2}}\|_{L^2} + \|\boldsymbol{b}^{n+\frac{1}{2}} - \boldsymbol{b}_h^{n+\frac{1}{2}}\|_{L^2} \\
\leq\ & M\,(\Delta t)^2 + M\left(\|\xi^{n+\frac{1}{2}}\|_{L^2} + \|\eta^{n+\frac{1}{2}}\|_{L^2} + \|\nabla p^{n+\frac{1}{2}} - \nabla p_h^{n+\frac{1}{2}}\|_{L^2}\right) \\
\leq\ & M\left((\Delta t)^2 + h^k + \|\xi^{n+\frac{1}{2}}\|_{L^2} + \|\eta^{n+\frac{1}{2}}\|_{L^2}\right). \qquad (3.91)
\end{aligned}
$$

Here by (3.59), (3.60) and Corollary 3.1, the choice of constant M in (3.91) is possible. Choose $v_h = \xi^{n+\frac{1}{2}}$ in (3.90), then

$$
G_{11}^n \leq M\left(\|\xi^{n+\frac{1}{2}}\|_{L^2}^2 + \epsilon\|\nabla\xi^{n+\frac{1}{2}}\|_{L^2}^2 + \|\eta^{n+\frac{1}{2}}\|_{L^2}^2 + \|\nabla\eta^{n+\frac{1}{2}}\|_{L^2}^2 + h^{2k} + (\Delta t)^4\right).
$$

Apply Taylor's expansion to G_2, G_3, G_6 and G_9; and apply the similar technique as (3.91) to G_1 and G_8. Keep only G_5 and G_7 on the left hand side and neglect all the constants. Take the sum from 0 to J on (3.90), $0 \leq J \leq N-1$. By using the telescoping skill and Young's inequality with ϵ, (3.89) now becomes:

$$\begin{aligned}
&\frac{1}{2\Delta t}\left(\|\xi^{J+1}\|_{L^2}^2 - \|\xi^0\|_{L^2}^2\right) + \sum_{n=0}^{J}\|\nabla\xi^{n+\frac{1}{2}}\|_{L^2}^2 \\
\leq\ & M\sum_{n=0}^{J}\left(\|\xi^{n+\frac{1}{2}}\|_{L^2}^2 + \|\eta^{n+\frac{1}{2}}\|_{L^2}^2 + \|\nabla\eta^{n+\frac{1}{2}}\|_{L^2}^2 + (\Delta t)^4 + h^{2k}\right) + \epsilon\sum_{n=0}^{J}\|\nabla\xi^{n+\frac{1}{2}}\|_{L^2}^2.
\end{aligned}$$

Since

$$\begin{aligned}
\left\|\sum_{n=0}^{J}\nabla\xi^n\right\|_{L^2} &\leq \sum_{n=0}^{J-1}\|\nabla\xi^{n+\frac{1}{2}}\|_{L^2} + \frac{1}{2}\|\nabla\xi^0\|_{L^2} + \frac{1}{2}\|\nabla\xi^J\|_{L^2} \\
&\leq \sum_{n=0}^{J}\|\nabla\xi^{n+\frac{1}{2}}\|_{L^2} + \frac{1}{2}\|\nabla\xi^0\|_{L^2},
\end{aligned}$$

use Gronwall's inequality,

$$\|\xi^{J+1}\|_{L^2} + (\Delta t)^{\frac{1}{2}}\left\|\sum_{n=0}^{J}\nabla\xi_i^n\right\|_{L^2} \leq M\left(h^k + (\Delta t)^2 + \|\xi^0\|_{L^2} + \|\nabla\xi^0\|_{L^2}\right).$$

Because $\tilde{W}^0$ and W_h^0 are both defined in their approximation forms, appropriately, one can pick up an appropriate initial values for both, such that $\|\nabla\xi^0\|_{L^2} + \|\xi^0\|_{L^2} \leq M((\Delta t)^2 + h^k)$. Thus

$$\|\xi^{J+1}\|_0 + (\Delta t)^{\frac{1}{2}}\left\|\sum_{n=0}^{J}\nabla\xi_i^n\right\|_{L^2} \leq M\left(h^k + (\Delta t)^2\right).$$

Therefore,

$$\begin{aligned}
&\|W^{J+1} - W_h^{J+1}\|_{L^2} + (\Delta t)^{\frac{1}{2}}\left\|\sum_{n=0}^{J}\nabla\left(W^n - W_h^n\right)\right\|_{L^2} \\
\leq\ & M\left((\Delta t)^2 + h^k\right) + \|\eta^{J+1}\|_{L^2} + (\Delta t)^{\frac{1}{2}}\left\|\sum_{n=0}^{J}\nabla\eta^n\right\|_{L^2} \\
\leq\ & M\left((\Delta t)^2 + h^k + (\Delta t)^{\frac{1}{2}}h^k\right).
\end{aligned}$$

Since $\Delta t < 1$, we can get

$$\|W^{J+1} - W_h^{J+1}\|_{L^2} + (\Delta t)^{\frac{1}{2}}\left\|\sum_{n=0}^{J}\nabla\left(W^n - W_h^n\right)\right\|_{L^2} \leq M\left((\Delta t)^2 + h^k\right).$$

Let $J = N - 1$, we get

$$\|W^N - W_h^N\|_{L^2} \le M\left((\Delta t)^2 + h^k\right). \tag{3.92}$$

Choosing $v_h = d_t\xi^n$ in (3.90) instead of $\xi^{n+\frac{1}{2}}$ and follow an analogous proof for $\|\nabla(W - W_h)\|_{L^\infty(L^2)}$ in Theorem 4.1, we can prove the error estimate in $L^\infty(H^1)$ norm, i.e.,

$$\|\nabla(W^N - W_h^N)\|_{L^2} \le M\left((\Delta t)^2 + h^k\right). \tag{3.93}$$

Finally, (3.87) follows from (3.92) and (3.93).

□

3.4 Modeling study and numerical analysis of Brinkman model

3.4.1 Introduction

It is well known that the free fluid flow in an open channel and the seepage flow in a porous medium can be modeled by the Stokes (or Navier-Stokes) equations and Darcy's law, respectively. However, when the porous medium is adjacent to the clear fluid in the open channel, the clear fluid can freely flow through the interface between the open channel and the porous medium, thus a coupled Stokes-Darcy (or Navier-Stokes-Darcy) system shall be formed in order to model such fluid dynamics phenomenon. To couple the two different problems defined in two different domains together, one usually connects them via the interface of the clear fluid and the porous medium by introducing some proper interface conditions. One can simply match the seepage velocity in the porous medium with the velocity in the clear fluid on the interface. The interface of the porous medium contains both pores and solid particles. In the pores, the fluid velocity in the porous medium matches with the fluid velocity outside the medium. Over the solid portion of the interface, the velocity is obviously zero in the porous medium. On the other hand, if we assume that the no-slip condition holds for the clear fluid on the surface of solid portion of the porous medium, then the velocity is zero as well at the solid portion of the interface in the neighboring clear fluid. The average velocity in the porous medium thus matches with the average velocity in the neighboring clear fluid, resulting in the continuity of normal velocity and tangential velocity, and the continuity of normal stress and shear stress. However, if the slip condition is applied to the clear fluid on the solid portion of the interface, then the tangential velocity in the neighboring clear fluid no longer matches with the tangential velocity in the porous medium, leading to the so-called Beavers-Joseph interface condition [Beavers and Joseph (1967); Cai et al. (2009); Mu and Xu (2007)] which states that the jump of the tangential velocities is proportional to the jump of shear stresses along the interface. Beavers-Joseph interface condition contains an empirical constant, to be determined experimentally, and this permits the needed flexibility in modeling the shear stress requirement. Also, unfortunately, from a mathematical point of view, the Beavers-Joseph interface condition poses some difficulties because this condition makes an indefinite contribution to the total energy budget. Consequently, many simplified versions of this interface conditions have emerged, among which the Beavers-Joseph-Saffman-Jones interface condition [Jones (1973); Layton et al. (2003); Saffman (1971)] is wildly used. Despite the convenience for mathematical analysis, models using the Beavers-Joseph-Saffman-Jones interface condition can lead to an inaccurate accounting of the exchange of fluid between the porous media and open channel.

In this section, we consider the no-slip condition on the solid portion of the interface of the clear fluid and porous medium, which is usually true when the clear fluid is viscous. Motivated by the qualitative difference between the descriptions of the above two different fluid flow problems occurring in the clear fluid and porous medium, Brinkman [Brinkman (1949)] suggested a general equation, later called Brinkman (or Forchheimer) model, to redefine the entire coupled system of the Stokes (or Navier-Stokes) flow and Darcy flow in a unified single domain by adding a so-called Darcy's force term to the momentum equation, in which a piecewise constant permeability K defined in each sub-domain plays the role to relate flow in a porous medium (finite K) with flow in a clear fluid ($K \to \infty$). It can be considered as an interpolation between the Stokes (or Navier-Stokes) equations and Darcy's law. It is worthnoting that similar to Brinkman model, the Forchheimer model is one continuum equation defined in one region with piecewise parameters that is used to describe a Navier-Stokes equation and Darcy's system in two regions. Though Brinkman's derivation was heuristic, he compared his results with an experimental relation due to Carman [Carman (1937)]. [Kim and Russel (1985)] also shows that theoretical predictions of permeability based on the Brinkman equation agree well with experimentally measured values from [Carman (1937)]. Subsequent investigators have rigorously established the validity of this equation at low volume fraction of solids [Tam (1969); Childress (1972); Howells (1974); Hinch (1977); Freed and Muthukumar (1978); Muthukumar and Freed (1979); Rubinstein (1986)]. A comparison was done in [Durlofsky and

Brady (1987)] between the solutions of the Brinkman model and the fundamental solution or Green's function for flow in porous media, and it showed that the Brinkman model accurately describes the flow in porous media when the volume fraction is below 0.05. The efficiency of such single domain approach is even more significant in three dimensions. The comparisons on the simplicity and accuracy between Brinkman (or Forchheimer) model and the coupled Navier-Stokes-Darcy system has only been seen in some limited literature such as [Chen et al. (2010); Shi and Wang (2007); Nield (1983)]. Asymptotic analysis was given by [Chen et al. (2010)] by comparing the real solutions of the partial differential equations. Though the results was accurate in [Chen et al. (2010)], but the authors were limited by the techniques of finding the analytic solutions of PDEs and therefore were only able to discuss the one dimensional case.

An important application of the coupled Stokes-Darcy (or Navier-Stokes-Darcy) system arises from the Proton Exchange Membrane fuel cell (PEMFC) model [Wang (2004); Wang and Cheng (1997, 1996); Wang et al. (2001); Pasaogullari et al. (2007); Pasaogullari and Wang (2004); Wang et al. (1999); Liu and Wang (2007a,b); Sun (2011)], on the coupling of gas diffusion layer (GDL) and gas channel (GC), where the momentum transport in GDL is treated as the flow in the porous media. In addition, two forms of Brinkman (or Forchheimer) model have been used. One has the porosity to square power appearing [Sun (2011); Jiang (2009)], while the other has the porosity to the first power [Discacciati and Quarteroni (2004)]. More recently, base on a PEMFC model, [Shi and Wang (2007)] gave a detailed numerical comparison between four models: Darcy's Law, Navier-Stokes equation, the Brinkman equation and the pure diffusion model and showed when the Brinkman parameter K was chosen as different small values, there was no visible difference on the fuel cell's performance between the prediction from Brinkman model and the experiment data obtained from [He et al. (2000)]. However, this paper did not give a quantitative measure of the differences.

In this section, we study the Brinkman model obtained from applying a parameter re-scaling technique on the traditional Brinkman model, to overcome the numerical difficulties raised from the discontinuous pressure and flux across the interface between the Darcy and Stoke domains. We apply mixed finite element method on both the Brinkman model and the Forchheimer model to achieve the optimal convergence rate in all parameters. We also conduct the asymptotic analysis between Brinkman model, Darcy's law and Stokes equation, and obtain the convergence result with respect to the piecewise constant permeability. Such quantitative measure of the difference between the models is first proved here to the author's best knowledges. We eventually gave numerical experiments to verify the error analysis by mixed finite element method and the quantitative measure of differences by asymptotic analysis.

The rest of this section is organized as follows. The Brinkman model and its relationship with Darcy's law and Stokes equation is studies in Section 3.4.2, and a parameter re-scaling technique is also introduced in Section 3.4.2. Then, in Section 3.4.3, the asymptotic analyses are introduced between the Stokes system and Brinkman model and between the Darcy's law and Brinkman model. In Section 3.4.4 and Section 3.4.5, the mixed finite element schemes are described and the approximation theorems are proved for Brinkman model and Forchheimer model, respectively.

In Section 3.4.6, the numerical experiment is carried out, in which a series of numerical convergence tests are given to verify the error estimate results proved in Section 3.4.4 and Section 3.4.5.

3.4.2 Model Development

Let $\Omega \in \mathbb{R}^d$, $(d = 2, 3)$, be a bounded domain. The classical Brinkman model was introduced by H. C. Brinkman [Brinkman (1949)] using a general equation that interpolates between the Stokes equation and Darcy's system to describe the two different types of fluid flow, laminar flow and porous media flow, as follows

$$\begin{cases} -\Delta \boldsymbol{u} + \nabla p + \frac{1}{K}\boldsymbol{u} = \boldsymbol{f}, & \text{in } \Omega, \\ \nabla \cdot \boldsymbol{u} = g, & \text{in } \Omega, \\ \int_\Omega p dx = 0, & \text{in } \Omega, \\ \boldsymbol{u} = \boldsymbol{u}_B, & \text{on } \partial\Omega, \end{cases} \tag{3.94}$$

where $\Omega = \Omega_D \cup \Omega_S$, Ω_D denotes the Darcy domain and Ω_S the Stokes domain, $\Gamma = \partial\Omega_D \cap \partial\Omega_S$ represents the interface of Ω_D and Ω_S. $\boldsymbol{u} \in H^2(\Omega)$ is the velocity and $p \in H^1(\Omega)$ is the pressure. The parameter K is a piecewise constant defined as

$$K = \begin{cases} K_D, & \text{in } \Omega_D, \\ K_S, & \text{in } \Omega_S, \end{cases}$$

where $0 < K_{min} \leq K_D < 1$ and $1 < K_S \leq K_{max} < \infty$. As a consequence, the right hand side $\boldsymbol{f}$ turns out to be a piecewise function defined as

$$\boldsymbol{f} = \begin{cases} \boldsymbol{f}_D, & \text{in } \Omega_D, \\ \boldsymbol{f}_S, & \text{in } \Omega_S. \end{cases}$$

For the compatibility purpose, we require $\int_{\partial\Omega} u_B ds = \int_\Omega g dx$ due to the divergence theorem. For the simplicity, we let $g(x)$ be zero in this dissertation to model the case of an incompressible laminar flow. We will discuss about the compressible case of

$g(x) \neq 0$ in the latter section as a remark. And, without loss of generality, we assume $u_B = 0$ in the rest of this section. Therefore the governing equation now is given as

$$\begin{cases} -\Delta \boldsymbol{u} + \nabla p + \frac{1}{K}\boldsymbol{u} = \boldsymbol{f}, & \text{in } \Omega, \\ \nabla \cdot \boldsymbol{u} = 0, & \text{in } \Omega, \\ \int_\Omega p dx = 0, & \text{in } \Omega, \\ \boldsymbol{u} = 0, & \text{on } \partial\Omega. \end{cases} \tag{3.95}$$

Remark 3.2. Obviously, Brinkman model is a one-continuum-system defined in a single domain, in contrast to Stokes-Darcy coupling system [Mehdaoui et al. (2008); Chen et al. (2010); Durlofsky and Brady (1987); Shi and Wang (2007)] which has two systems of equations defined in two different domains connecting through the interfacial conditions (Beavers-Joseph conditions) on the interface [Beavers and Joseph (1967); Chen et al. (2010)].

One of the applications of Brinkman model is to describe the fluid motion in the gas diffusion layers and gas channels of proton exchange membrane (PEM) fuel cell [Wang (2004)], where, the steady state momentum equation of Brinkman model is defined as (see also [Chen et al. (2010)])

$$-\nabla \cdot (\rho\nu\phi\nabla\boldsymbol{u}) + \phi\nabla p + \frac{\rho\nu\phi}{K}\boldsymbol{u} = \boldsymbol{f}. \tag{3.96}$$

Here the density ρ, the two-phase mixture viscosity ν of liquid phase and gaseous phase of water, the porosity of porous media ϕ and the permeability K are constants in the single-phase region. ρ and ν are not constants in the two-phase region, but could be roughly considered as constants under a certain circumstance such as the liquid saturation $s \leq 20\%$ under which a single-phase case could be approximated admitted [Wang (2004)].

Therefore by re-scaling the pressure by $\frac{p}{\rho\nu}$, we could derive (3.95), where K in

(3.95) actually is not just a mathematical parameter but the physical permeability.

Theorem 3.4. *(3.95) is an equivalent development from the system below,*

$$\begin{cases} -\Delta \boldsymbol{u} + \frac{1}{K^\alpha}\nabla \tilde{p} + \frac{1}{K}\boldsymbol{u} = \boldsymbol{f}, & \text{in } \Omega, \\ \nabla \cdot \boldsymbol{u} = 0, & \text{in } \Omega, \\ \int_\Omega p dx = 0, & \text{in } \Omega, \\ \boldsymbol{u} = 0, & \text{on } \partial\Omega, \end{cases} \tag{3.97}$$

where $0 < \alpha < 1$ *is a properly chosen parameter.*

Though (3.95) is more wildly used as Brinkman model, (3.97) is the model that allows the approximation for Darcy and Stokes models as K *approaches zero and infinity, respectively.*

Proof. First, it is obvious when $K_D \to 0$ and $K_S \to \infty$, for a properly chosen $\alpha \in (0, 1)$, (3.97) approximates the following Stokes-Darcy coupling system

$$\begin{cases} \frac{1}{K_D^\alpha}\nabla \tilde{p} + \frac{1}{K_D}\boldsymbol{u} = 0, & \text{in } \Omega_D, \\ -\Delta \boldsymbol{u} + \frac{1}{K_S^\alpha}\nabla \tilde{p} = \boldsymbol{f}_S, & \text{in } \Omega_S, \\ \nabla \cdot \boldsymbol{u} = 0, & \text{in } \Omega, \end{cases} \tag{3.98}$$

which are essentially Darcy's and Stokes models defined in Ω_D and Ω_S, respectively. The approximation rate between (3.97) and (3.98) with respect to the parameter $\epsilon = K_D^\alpha$ will be discussed in Section 3.4.3. Now for $i = D, S$, we re-scale (3.97) and (3.98) in Ω_i, respectively, using

$$\tilde{p} = K_i^\alpha p, \tag{3.99}$$

then we get the equivalent system (3.95) and the following re-scaled Stokes-Darcy coupling system

$$\begin{cases} \nabla p + \frac{1}{K_D}\boldsymbol{u} = 0, & \text{in } \Omega_D, \\ -\Delta \boldsymbol{u} + \nabla p = \boldsymbol{f}_S, & \text{in } \Omega_S, \\ \nabla \cdot \boldsymbol{u} = 0, & \text{in } \Omega. \end{cases} \tag{3.100}$$

□

Remark 3.3. From the proof of Theorem 3.4, we can see that (3.95) does not directly approximate (3.100) when K approaches zero, i.e., in the aspect of Darcy's system, although (3.95) and (3.100) are re-scaled from (3.97) and (3.98), respectively, and at the same time (3.97) approximates (3.98). The approximation of (3.95) to (3.100) only exists for the case of Stokes, i.e., when K approaches infinity.

Remark 3.4. Due to (3.99), $\tilde{p}$ is not a continuous function in Ω, i.e., it is discontinuous across the interface Γ, while the solutions of Brinkman model (3.95), both p and $\boldsymbol{u}$, are continuous functions in Ω.

Remark 3.5. Although (3.97) is a more accurate form to approximate Darcy and Stokes models (3.98) with different values of K, we always use (3.95) as Brinkman model but not (3.97) to describe the scenario of Stokes-Darcy coupling. The reason is that the flux of (3.97) across the interface Γ, $(\nabla \boldsymbol{u} - 1/K\tilde{p}I) \cdot \boldsymbol{n}$, is not continuous at all, and there exists a jump due to the difference of the values of K across Γ; however, the flux of (3.95), $(\nabla \boldsymbol{u} - pI) \cdot \boldsymbol{n}$, is always continuous across Γ. Because of the discontinuous flux of (3.97), It is much harder to solve (3.97) than (3.95) in an accurate manner. More complicated and advanced numerical method and/or locally much finer mesh have to be considered in order to resolve the difficulty arising from the jump coefficient K across Γ. Nevertheless, in contrast, (3.95) can be solved with the standard Stokes element and less computational cost, the desired pressure solution is then easily obtained by the re-scaling (3.99).

Remark 3.6. In Theorem 3.4, $\alpha \neq 1$, otherwise then the first equation in (3.97) approximates $\boldsymbol{u} = -\nabla \tilde{p}$ in Ω_D as K approaches zero, which is inconsistent with the well-known Darcy's law defined for the seepage flow in the porous media as follows:

$$\boldsymbol{u} = -\frac{K}{\nu\phi}\nabla\tilde{p}, \text{ in } \Omega_D. \tag{3.101}$$

Obviously, $K/(\nu\phi) \neq 1$ in reality for the seepage flow in the porous media, where, for instance, in the gas diffusion layers of PEM fuel cells, the magnitude of permeability K could be as small as 10^{-12}, in contrast with the magnitude of the mixture viscosity of water ν, 10^{-6}, and of the porosity ϕ, 10^{-1}, as shown in Table 3.5 in Section 3.4.6.

Corollary 3.2. *Let $\epsilon = K_D^{\alpha}$ be small enough and $K_D = K_S^{-\beta}$, where $0 < \alpha < 1$ and $\beta \geq 1$, then (3.97) can be rewritten as*

$$\begin{cases} -\epsilon^{\frac{1}{\alpha}}\Delta\boldsymbol{u} + \epsilon^{\frac{1}{\alpha}-1}\nabla\tilde{p} + \boldsymbol{u} = \epsilon^{\frac{1}{\alpha}}\boldsymbol{f}_D, & \text{in } \Omega_D, \\ -\Delta\boldsymbol{u} + \epsilon^{\frac{1}{\beta}}\nabla\tilde{p} + \epsilon^{\frac{1}{\alpha\beta}}\boldsymbol{u} = \boldsymbol{f}_S, & \text{in } \Omega_S, \\ \nabla\cdot\boldsymbol{u} = 0, & \text{in } \Omega. \end{cases} \tag{3.102}$$

which approximates the following systems in Ω_D and Ω_S, respectively, as $\epsilon \to 0$,

$$\begin{cases} \epsilon^{\frac{1}{\alpha}-1}\nabla\tilde{p} + \boldsymbol{u} = 0, & \\ \nabla\cdot\boldsymbol{u} = 0, & \text{in } \Omega_D, \end{cases} \tag{3.103}$$

and

$$\begin{cases} -\Delta\boldsymbol{u} + \epsilon^{\frac{1}{\beta}}\nabla\tilde{p} = \boldsymbol{f}_S, & \\ \nabla\cdot\boldsymbol{u} = 0, & \text{in } \Omega_S. \end{cases} \tag{3.104}$$

Proof. Since $\beta \geq 1$, when K_D approaches zero, K_S approaches infinity. Thus, with the help of the sufficiently small positive number $\epsilon = K_D^{\alpha}$ $(0 < \alpha < 1)$ as K_D approaches zero, we can equivalently reformulate (3.97) to (3.102), and (3.98) to (3.103) and (3.104) in terms of a single parameter $\epsilon \in (0, 1)$. Therefore, by dropping the high order terms of ϵ, (3.102) approximates (3.103) and (3.104) in Ω_D and Ω_S, respectively, as $\epsilon \to 0$. □

In order to avoid any confusion on the notations, in the rest of the section, we denote the solutions to (3.103) as $(\boldsymbol{u}_D, \tilde{p}_D)$ and the solutions to (3.104) as $(\boldsymbol{u}_S, \tilde{p}_S)$.

3.4.3 Asymptotic analysis of the difference between Brinkman model and Darcy/Stokes system

(I) Between Brinkman model and Darcy's system

The weak formulation of Darcy equation (3.103) is given as follows: find $(\boldsymbol{u}_D, \tilde{p}_D) \in (H^1(\Omega_D))^d \times L^2(\Omega_D)$ such that for any $(\boldsymbol{v}, q) \in (H^1(\Omega_D))^d \times L^2(\Omega_D)$,

$$- \epsilon^{\frac{1}{\alpha}-1}(\nabla \cdot \boldsymbol{v}, \tilde{p}_D) + (\boldsymbol{u}_D, \boldsymbol{v}) = 0, \tag{3.105}$$

$$(\nabla \cdot \boldsymbol{u}_D, q) = 0. \tag{3.106}$$

And the above weak forms (3.105)-(3.106) are approximated by the weak formulation of $(3.102)_1$ as follows: find $(\boldsymbol{u}, \tilde{p}) \in (H^1(\Omega_D))^d \times L^2(\Omega_D)$ such that for any $(\boldsymbol{v}, q) \in (H^1(\Omega_D))^d \times L^2(\Omega_D)$,

$$\epsilon^{\frac{1}{\alpha}}(\nabla \boldsymbol{u}, \nabla \boldsymbol{v}) - \epsilon^{\frac{1}{\alpha}-1}(\nabla \cdot \boldsymbol{v}, \tilde{p}) + (\boldsymbol{u}, \boldsymbol{v}) = \epsilon^{\frac{1}{\alpha}}(\boldsymbol{f}_D, \boldsymbol{v}), \tag{3.107}$$

$$(\nabla \cdot \boldsymbol{u}, q) = 0. \tag{3.108}$$

Theorem 3.5. *Let $(\boldsymbol{u}_D, \tilde{p}_D)$ be the solution of (3.105)-(3.106) and $(\boldsymbol{u}, \tilde{p})$ be the solution of (3.107)-(3.108), we have the asymptotic approximation in Ω_D as follows,*

$$\|\boldsymbol{u} - \boldsymbol{u}_D\|_{L^2} \leq \epsilon^{\frac{1}{\alpha}} \left(\|\boldsymbol{u}\|_{H^2} + \|\boldsymbol{f}_D\|_{L^2}\right), \tag{3.109}$$

$$\|\tilde{p} - \tilde{p}_D\|_{L^2} \leq \epsilon \left(\|\boldsymbol{u}\|_{H^2} + \|\boldsymbol{f}_D\|_{L^2}\right). \tag{3.110}$$

Proof. By subtracting (3.105) and (3.106) from (3.107) and (3.108) respectively, we get the error equations as follows,

$$\epsilon^{\frac{1}{\alpha}}(\nabla \boldsymbol{u}, \nabla \boldsymbol{v}) - \epsilon^{\frac{1}{\alpha}-1}(\nabla \cdot \boldsymbol{v}, \tilde{p} - \tilde{p}_D) + (\boldsymbol{u} - \boldsymbol{u}_D, \boldsymbol{v}) = \epsilon^{\frac{1}{\alpha}}(\boldsymbol{f}_D, \boldsymbol{v}), \tag{3.111}$$

$$(\nabla \cdot (\boldsymbol{u} - \boldsymbol{u}_D), q) = 0. \tag{3.112}$$

Let $\boldsymbol{v} = \boldsymbol{u} - \boldsymbol{u}_D$ and $q = \tilde{p} - \tilde{p}_D$, we have

$$\epsilon^{\frac{1}{\alpha}}(\nabla \boldsymbol{u}, \nabla(\boldsymbol{u} - \boldsymbol{u}_D)) + (\boldsymbol{u} - \boldsymbol{u}_D, \boldsymbol{u} - \boldsymbol{u}_D) = \epsilon^{\frac{1}{\alpha}}(\boldsymbol{f}_D, \boldsymbol{u} - \boldsymbol{u}_D), \tag{3.113}$$

then

$$-\epsilon^{\frac{1}{\alpha}}(\Delta \boldsymbol{u}, \boldsymbol{u} - \boldsymbol{u}_D) + (\boldsymbol{u} - \boldsymbol{u}_D, \boldsymbol{u} - \boldsymbol{u}_D) = \epsilon^{\frac{1}{\alpha}}(\boldsymbol{f}_D, \boldsymbol{u} - \boldsymbol{u}_D), \tag{3.114}$$

thus

$$\|\boldsymbol{u} - \boldsymbol{u}_D\|_{L^2} \leq \epsilon^{\frac{1}{\alpha}} \left(\|\Delta \boldsymbol{u}\|_{L^2} + \|\boldsymbol{f}_D\|_{L^2}\right) \leq \epsilon^{\frac{1}{\alpha}} \left(\|\boldsymbol{u}\|_{H^2} + \|\boldsymbol{f}_D\|_{L^2}\right). \tag{3.115}$$

Use the error equation (3.111), we also get

$$\epsilon^{\frac{1}{\alpha}-1}(\nabla \cdot \boldsymbol{v}, \tilde{p} - \tilde{p}_D) = \epsilon^{\frac{1}{\alpha}}(\nabla \boldsymbol{u}, \nabla \boldsymbol{v}) + (\boldsymbol{u} - \boldsymbol{u}_D, \boldsymbol{v}) - \epsilon^{\frac{1}{\alpha}}(\boldsymbol{f}_D, \boldsymbol{v}).$$

By the LBB condition and the continuity conditions, we have

$$\epsilon^{\frac{1}{\alpha}-1}\|\boldsymbol{v}\|_{H^1}\|\tilde{p} - \tilde{p}_D\|_{L^2} \leq \epsilon^{\frac{1}{\alpha}} \left(\|\boldsymbol{u}\|_{H^1} + \|\boldsymbol{f}_D\|_{L^2}\right) \|\boldsymbol{v}\|_{H^1} + \|\boldsymbol{u} - \boldsymbol{u}_D\|_{L^2}\|\boldsymbol{v}\|_{H^1},$$

that is,

$$\epsilon^{\frac{1}{\alpha}-1}\|\tilde{p} - \tilde{p}_D\|_{L^2} \leq \epsilon^{\frac{1}{\alpha}} \left(\|\boldsymbol{u}\|_{H^2} + \|\boldsymbol{f}_D\|_{L^2}\right),$$

which then gives (3.110). □

Remark 3.7. Because (3.95) does not approximate (3.100), there does not exist any convergence between p and p_D. However, if we re-scale $\tilde{p}$ and $\tilde{p}_D$ in (3.110) using $\tilde{p} = K_D^{\alpha} p = \epsilon p$ and $\tilde{p}_D = \epsilon p_D$, then we would have

$$\|p - p_D\|_{L^2} \leq \|\boldsymbol{u}\|_{H^2} = O(1),$$

which actually illustrates that (3.95) does not converge to (3.100) in the aspect of Darcy's system as ϵ approaches zero.

(II) Between Brinkman model and Stokes system

The weak formulation of Stokes equations (3.104) is given as follows: find $(\boldsymbol{u}_S, \tilde{p}_S) \in (H^1(\Omega_S))^d \times L^2(\Omega_S)$ such that for any $(\boldsymbol{v}, q) \in (H^1(\Omega_S))^d \times L^2(\Omega_S)$,

$$(\nabla \boldsymbol{u}_S, \nabla \boldsymbol{v}) - \epsilon^{\frac{1}{\beta}}(\nabla \cdot \boldsymbol{v}, \tilde{p}_S) = (\boldsymbol{f}_S, \boldsymbol{v}), \tag{3.116}$$

$$(\nabla \cdot \boldsymbol{u}_S, q) = 0. \tag{3.117}$$

And the above weak forms (3.116)-(3.117) are approximated by the weak formulation of $(3.102)_2$ as follows: find $(\boldsymbol{u}, \tilde{p}) \in (H^1(\Omega_S))^d \times L^2(\Omega_S)$ such that for any $(\boldsymbol{v}, q) \in (H^1(\Omega_S))^d \times L^2(\Omega_S)$,

$$(\nabla \boldsymbol{u}, \nabla \boldsymbol{v}) - \epsilon^{\frac{1}{\beta}}(\nabla \cdot \boldsymbol{v}, \tilde{p}) + \epsilon^{\frac{1}{\alpha\beta}}(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{f}_S, \boldsymbol{v}), \tag{3.118}$$

$$(\nabla \cdot \boldsymbol{u}, q) = 0. \tag{3.119}$$

Theorem 3.6. *Let $(\boldsymbol{u}_S, \tilde{p}_S)$ be the solution of (3.116)-(3.117) and $(\boldsymbol{u}, \tilde{p})$ be the solution of (3.118)-(3.119), we have the asymptotic approximation in Ω_S as follows,*

$$\|\boldsymbol{u} - \boldsymbol{u}_S\|_{H^1} \leq C_\Omega \epsilon^{\frac{1}{\alpha\beta}} \|\boldsymbol{u}\|_{L^2}, \tag{3.120}$$

$$\|\tilde{p} - \tilde{p}_S\|_{L^2} \leq (1 + C_\Omega)\epsilon^{\frac{1}{\beta}(\frac{1}{\alpha}-1)} \|\boldsymbol{u}\|_{L^2}. \tag{3.121}$$

Proof. By subtracting (3.118) and (3.119) from (3.116) and (3.117), respectively, we get the error equations as follows,

$$(\nabla(\boldsymbol{u} - \boldsymbol{u}_S), \nabla \boldsymbol{v}) - \epsilon^{\frac{1}{\beta}}(\nabla \cdot \boldsymbol{v}, \tilde{p} - \tilde{p}_S) + \epsilon^{\frac{1}{\alpha\beta}}(\boldsymbol{u}, \boldsymbol{v}) = 0, \tag{3.122}$$

$$(\nabla \cdot (\boldsymbol{u} - \boldsymbol{u}_S), q) = 0. \tag{3.123}$$

Let $\boldsymbol{v} = \boldsymbol{u} - \boldsymbol{u}_S$ and $q = \tilde{p} - \tilde{p}_S$, we have

$$(\nabla(\boldsymbol{u} - \boldsymbol{u}_S), \nabla(\boldsymbol{u} - \boldsymbol{u}_S)) + \epsilon^{\frac{1}{\alpha\beta}}(\boldsymbol{u}, \boldsymbol{u} - \boldsymbol{u}_S) = 0, \tag{3.124}$$

thus

$$\|\nabla(\boldsymbol{u}-\boldsymbol{u}_S)\|_{L^2}^2 \leq \epsilon^{\frac{1}{\alpha\beta}}\|\boldsymbol{u}\|_{L^2}\|\boldsymbol{u}-\boldsymbol{u}_S\|_{L^2} \leq \epsilon^{\frac{1}{\alpha\beta}}C_\Omega\|\boldsymbol{u}\|_{L^2}\|\nabla(\boldsymbol{u}-\boldsymbol{u}_S)\|_{L^2}, \tag{3.125}$$

which then gives us (3.120).

Also by the error equation (3.122), we have

$$\epsilon^{\frac{1}{\beta}}(\nabla\cdot\boldsymbol{v}, \tilde{p}-p_S) = (\nabla(\boldsymbol{u}-\boldsymbol{u}_S), \nabla\boldsymbol{v}) + \epsilon^{\frac{1}{\alpha\beta}}(\boldsymbol{u}, \boldsymbol{v}). \tag{3.126}$$

By the LBB condition and the continuity conditions,

$$\epsilon^{\frac{1}{\beta}}\|\boldsymbol{v}\|_{H^1}\|\tilde{p}-p_S\|_{L^2} \leq \epsilon^{\frac{1}{\alpha\beta}}\|\boldsymbol{u}\|_{L^2}\|\boldsymbol{v}\|_{L^2} + \|\boldsymbol{u}-\boldsymbol{u}_S\|_{H^1}\|\boldsymbol{v}\|_{H^1}, \tag{3.127}$$

that is

$$\epsilon^{\frac{1}{\beta}}\|\tilde{p}-\tilde{p}_S\|_{L^2} \leq \epsilon^{\frac{1}{\alpha\beta}}\|\boldsymbol{u}\|_{L^2} + \|\boldsymbol{u}-\boldsymbol{u}_S\|_{H^1} \leq \epsilon^{\frac{1}{\alpha\beta}}(1+C_\Omega)\|\boldsymbol{u}\|_{L^2}. \tag{3.128}$$

□

Remark 3.8. Although (3.95) does not approximate (3.100) in the aspect of Darcy's system when K approaches zero, (3.95) does approximate (3.100) when K approaches infinity, namely, in the aspect of Stokes model. By using $\tilde{p} = K_S^\alpha p = \epsilon^{-\frac{1}{\beta}}p$ and $\tilde{p}_S = \epsilon^{-\frac{1}{\beta}}p_S$, we have

$$\|p-p_S\|_{L^2} \leq \epsilon^{\frac{1}{\alpha\beta}}(1+C_\Omega)\|\boldsymbol{u}\|_{L^2}. \tag{3.129}$$

(3.120) and (3.129) show that both velocity and pressure solutions of Brinkman model approximate those of Stokes model in the same convergence rate $O(\epsilon^{-\alpha\beta})$.

Remark 3.9. By (3.120) and (3.121), β shall be sufficiently small in order to get the best approximation of Brinkman equation to Stokes equation in Stokes domain. Since $\beta \geq 1$, we can safely choose $\beta = 1$.

Remark 3.10. In [Chen et al. (2010)], a parameter ϵ is used, which is the same as our ϵ when $\alpha = \frac{1}{2}$. Interestingly enough, as a result in [Chen et al. (2010)], the difference between the velocity in the conduit for the Stokes-Brinkman system and the Stokes-Darcy system with the Beavers-Joseph-Saffman-Jones (BJSJ) interface condition [Saffman (1971); Layton et al. (2003); Jones (1973)] is $O(\epsilon^2)$. This matches our results given in (3.109) and (3.120) perfectly though we only consider the two domains separately without introducing the BJSJ interface condition.

3.4.4 Mixed finite element approximation for Brinkman model

Now we define

$$U = (H_0^1(\Omega))^d, \quad Q = L_0^2(\Omega) = \{q \in L^2(\Omega), \int q dx = 0\}, \tag{3.130}$$

and

$$\begin{aligned}(f,g)_D &= \int_{\Omega_D} fg dx \quad , \quad (f,g)_S = \int_{\Omega_S} fg dx, \\ \|f\|^2_{L^2(\Omega_D)} &= \int_{\Omega_D} f^2 dx \quad , \quad \|f\|^2_{L^2(\Omega_S)} = \int_{\Omega_S} f^2 dx.\end{aligned}$$

The weak formulation of (3.95) is defined as: find $(\boldsymbol{u}, p) \in U \times Q$, such that

$$\frac{1}{K_D}(\boldsymbol{u},\boldsymbol{v})_D + \frac{1}{K_S}(\boldsymbol{u},\boldsymbol{v})_S + (\nabla\boldsymbol{u},\nabla\boldsymbol{v}) - (\nabla\cdot\boldsymbol{v},p) = (\boldsymbol{f},\boldsymbol{v}), \qquad \forall \boldsymbol{v} \in U, \tag{3.131}$$

$$(\nabla\cdot\boldsymbol{u},q) = 0, \qquad \forall q \in Q. \tag{3.132}$$

We now define the bilinear forms

$$a(\boldsymbol{u},\boldsymbol{v}) = \frac{1}{K_D}(\boldsymbol{u},\boldsymbol{v})_D + \frac{1}{K_S}(\boldsymbol{u},\boldsymbol{v})_S + (\nabla\boldsymbol{u},\nabla\boldsymbol{v}), \tag{3.133}$$

$$b(\boldsymbol{v},p) = -(\nabla\cdot\boldsymbol{v},p), \tag{3.134}$$

then (3.131)-(3.132) could be written as: Find $(\boldsymbol{u}, p) \in U \times Q$, such that

$$a(\boldsymbol{u}, \boldsymbol{v}) + b(\boldsymbol{v}, p) = (\boldsymbol{f}, \boldsymbol{v}), \qquad \boldsymbol{v} \in U, \tag{3.135}$$

$$b(\boldsymbol{u}, q) = 0, \qquad q \in Q. \tag{3.136}$$

Easily we have

$$\begin{aligned} |a(\boldsymbol{u}, \boldsymbol{v})| &\leq \frac{1}{K_D}\|\boldsymbol{u}\|_{L^2(\Omega_D)}\|\boldsymbol{v}\|_{L^2(\Omega_D)} + \frac{1}{K_S}\|\boldsymbol{u}\|_{L^2(\Omega_S)}\|\boldsymbol{v}\|_{L^2(\Omega_S)} + \|\nabla\boldsymbol{u}\|_{L^2}\|\nabla\boldsymbol{v}\|_{L^2} \\ &\leq \frac{1}{K_D}\|\boldsymbol{u}\|_{L^2(\Omega)}\|\boldsymbol{v}\|_{L^2(\Omega)} + \|\nabla\boldsymbol{u}\|_{L^2}\|\nabla\boldsymbol{v}\|_{L^2} \\ &\leq \frac{1}{K_D}\|\boldsymbol{u}\|_U\|\boldsymbol{v}\|_U, \forall \boldsymbol{u}, \boldsymbol{v} \in U, \qquad (3.137) \\ |b(\boldsymbol{u}, p)| &\leq \|\nabla\cdot\boldsymbol{u}\|_{L^2}\|p\|_{L^2} \leq \|\nabla\boldsymbol{u}\|_{L^2}\|p\|_{L^2} \leq \|\boldsymbol{u}\|_U\|p\|_Q, \forall \boldsymbol{u} \in U, \forall q \in Q, (3.138) \end{aligned}$$

and

$$\begin{aligned} |a(\boldsymbol{v}, \boldsymbol{v})| &= \frac{1}{K_D}\|\boldsymbol{v}\|^2_{L^2(\Omega_D)} + \frac{1}{K_S}\|\boldsymbol{v}\|^2_{L^2(\Omega_S)} + \|\nabla\boldsymbol{v}\|^2_{L^2} \\ &\geq \frac{1}{K_S}\|\boldsymbol{v}\|^2_{L^2} + \|\nabla\boldsymbol{v}\|^2_{L^2} \geq \min\{\frac{1}{K_S}, 1\}\left(\|\boldsymbol{v}\|^2_{L^2} + \|\nabla\boldsymbol{v}\|^2_{L^2}\right) \\ &\geq \frac{1}{K_S}\|\boldsymbol{v}\|^2_U. \qquad (3.139) \end{aligned}$$

Also, for any $q \in Q$, there exists $\boldsymbol{v} \in U$ such that $\nabla \cdot \boldsymbol{v} = -q$. Actually we just need to solve an adjoint problem as follows,

$$-\Delta\phi = q, \qquad \text{in } \Omega,$$

$$\phi = 0, \qquad \text{on } \partial\Omega,$$

where $\phi \in H^2 \cup H^1_0(\Omega)$. Then let $\boldsymbol{u} = \nabla\phi$. Then

$$\begin{aligned} b(\boldsymbol{v}, q) &= -(\nabla\cdot\boldsymbol{v}, q) = (q, q) = \|q\|^2_{L^2}, \\ \|\boldsymbol{v}\|_U &= \|\nabla\phi\|_{H^1} \leq C\|\phi\|_{H^2} \leq C\|q\|_{L^2} \end{aligned}$$

so that

$$\sup_{\boldsymbol{v}\in U}\frac{b(\boldsymbol{v},q)}{\|\boldsymbol{v}\|_U}\geq\frac{\|q\|_{L^2}^2}{\|\boldsymbol{v}\|_U}\geq\frac{\|q\|_{L^2}^2}{C\|q\|_{L^2}}\geq C\|q\|_Q.$$

Therefore,

$$\inf_{q\in Q}\sup_{\boldsymbol{v}\in U}\frac{b(\boldsymbol{v},q)}{\|\boldsymbol{v}\|_U\|q\|_Q}\geq\gamma>0. \tag{3.140}$$

By the Ladyzhenskaya-Babuska-Brezzi (LBB) condition, there exists a unique solution to (3.135)-(3.136).

We define

$$Z = \{\boldsymbol{u}\in U|\nabla\cdot\boldsymbol{u}=0\}, \tag{3.141}$$

$$Z_h = \{\boldsymbol{u}_h\in U_h|b(\boldsymbol{u}_h,q_h)=0,q_h\in Q_h\}, \tag{3.142}$$

then (3.135)-(3.136) can be reformulated as follows: Find $\boldsymbol{u}\in Z$ such that

$$a(\boldsymbol{u},\boldsymbol{v})=(\boldsymbol{f},\boldsymbol{v}),\forall\boldsymbol{v}\in Z, \tag{3.143}$$

Let U_h, Q_h be finite dimensional subspaces of U and Q, respectively. We look for a solution to the following problem: given $\boldsymbol{f}\in U'$, find $(\boldsymbol{u}_h,p_h)\in U_h\times Q_h$, such that

$$a(\boldsymbol{u}_h,\boldsymbol{v}_h)+b(\boldsymbol{v}_h,p_h)=(\boldsymbol{f},\boldsymbol{v}_h),\qquad \boldsymbol{v}_h\in U_h, \tag{3.144}$$

$$b(\boldsymbol{u}_h,q_h)=0,\qquad q_h\in Q_h. \tag{3.145}$$

We can similarly obtain the coercivity of the bilinear form $a(\cdot,\cdot)$ in $U_h\times U_h$ and the continuity of the bilinear forms $a(\cdot,\cdot)$ over $U_h\times U_h$ and $b(\cdot,\cdot)$ over $U_h\times Q_h$. Also we have the LBB condition

$$\forall q_h\in Q_h,\exists\boldsymbol{u}_h\in U_h,\boldsymbol{u}_h\neq 0: b(\boldsymbol{u}_h,q_h)\geq\beta\|\boldsymbol{u}_h\|_U\|q_h\|_Q.$$

Therefore, (3.144)-(3.145) has a unique solution. Moreover, we choose to use P^sP^{s-1} element, which is the well known Taylor Hood mixed element that is a stable pair for Stokes and Navier Stokes equations, and is also stable for Brinkman equations (3.95). By Brezzi's theory [Brezzi (1974)], we have the following Lemma.

Lemma 3.11. *Using $P^{s+1}P^s$ element, $s \geq 1$, we have the following finite element error estimate results for interpolations given by Brezzi's theory [Brezzi (1974)] as follows,*

$$\inf_{\boldsymbol{v}_h \in U_h} \|\boldsymbol{u} - \boldsymbol{v}_h\|_U \leq Ch^{s+1}\|\boldsymbol{u}\|_{H^{s+2}}, \tag{3.146}$$

$$\inf_{\boldsymbol{q}_h \in Q_h} \|p - q_h\|_Q \leq Ch^{s+1}\|p\|_{H^{s+1}}. \tag{3.147}$$

Theorem 3.7. *let $(\boldsymbol{u}, p)$ be the solution to (3.135)-(3.136) and let $(\boldsymbol{u}_h, p_h)$ be the solution to (3.144)-(3.145), then we have*

$$\|\boldsymbol{u} - \boldsymbol{u}_h\|_{L^2} + h\|\boldsymbol{u} - \boldsymbol{u}_h\|_{H^1} \leq Ch^{s+2}\left(\left(\frac{K_S}{K_D} + 1\right)\|\boldsymbol{u}\|_{H^{s+2}} + K_S\|p\|_{H^{s+1}}\right) \tag{3.148}$$

$$\|p - p_h\|_{L^2} \leq Ch^{s+1}\left(\frac{K_S}{K_D} + 1\right)\left(\frac{1}{K_D}\|\boldsymbol{u}\|_{H^{s+2}} + \|p\|_{H^{s+1}}\right) \tag{3.149}$$

Proof. Let $\boldsymbol{v}_h \in U_h$ and $q_h \in Q_h$. Subtract (3.144) from (3.135), we have

$$a(\boldsymbol{u} - \boldsymbol{u}_h, \boldsymbol{v_h}) + b(\boldsymbol{v}_h, p - p_h) = 0,$$

and further let $\tilde{\boldsymbol{u}}_{\boldsymbol{h}} \in Z_h$,

$$a(\boldsymbol{u_h} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}, \boldsymbol{v_h}) + b(\boldsymbol{v}_h, p_h - q_h) = a(\boldsymbol{u} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}, \boldsymbol{v_h}) + b(\boldsymbol{v}_h, p - q_h). \tag{3.150}$$

Choose $\boldsymbol{v}_h = \boldsymbol{u_h} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}} \in Z_h$. Since $\tilde{\boldsymbol{u}}_{\boldsymbol{h}} \in Z_h$, we have $b(\boldsymbol{u_h} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}, p_h - q_h) = 0$, so

$$a(\boldsymbol{u_h} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}, \boldsymbol{u_h} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}) = a(\boldsymbol{u} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}, \boldsymbol{u_h} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}) + b(\boldsymbol{u_h} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}, p - q_h).$$

from the continuity and coercivity of $a(\boldsymbol{u}_h, \boldsymbol{v}_h)$, we get

$$\begin{aligned} \frac{1}{K_S}\|\boldsymbol{u_h} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}\|_U^2 &\leq a(\boldsymbol{u_h} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}, \boldsymbol{u_h} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}) \\ \leq \quad & \frac{1}{K_D}\|\boldsymbol{u} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}\|_U \|\boldsymbol{u_h} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}\|_U + \|\boldsymbol{u_h} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}\|_U \|p - q_h\|_Q, \end{aligned}$$

thus

$$\|\boldsymbol{u_h} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}\|_U \leq K_S \left(\frac{1}{K_D}\|\boldsymbol{u} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}\|_U + \|p - q_h\|_Q \right),$$

and then

$$\begin{aligned} \|\boldsymbol{u} - \boldsymbol{u}_h\|_U &\leq \|\boldsymbol{u_h} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}\|_U^2 + \|\boldsymbol{u} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}\|_U^2 \\ &\leq K_S \left(\left(\frac{1}{K_D} + \frac{1}{K_S} \right) \|\boldsymbol{u} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}\|_U + \|p - q_h\|_Q \right) \end{aligned} \qquad (3.151)$$

.

For each $\boldsymbol{v}_h \in U_h$, there exists a unique $\boldsymbol{z}_h \in (Z_h)^\perp$ [Brezzi (1974); Quarteroni and Valli (2008)], such that

$$b(\boldsymbol{z}_h, q_h) = b(\boldsymbol{u} - \boldsymbol{v}_h, q_h), \forall q_h \in Q_h,$$

thus

$$\|\boldsymbol{z}_h\|_U \|q_h\|_Q \leq \frac{1}{\gamma}\|\boldsymbol{u} - \boldsymbol{v}_h\|_U \|q_h\|_Q.$$

Setting $\tilde{\boldsymbol{u}}_{\boldsymbol{h}} := \boldsymbol{z}_h + \boldsymbol{v}_h$, we see that

$$\|\boldsymbol{u} - \tilde{\boldsymbol{u}}_{\boldsymbol{h}}\|_U \leq \|\boldsymbol{u} - \boldsymbol{v}_h\|_U + \|\boldsymbol{z}_h\|_U \leq \left(1 + \frac{1}{\gamma}\right) \|\boldsymbol{u} - \boldsymbol{v}_h\|_U$$

Together with (3.151), consequently we have

$$\|\boldsymbol{u} - \boldsymbol{u}_h\|_U \leq C K_S \left(\left(\frac{1}{K_D} + \frac{1}{K_S} \right) \|\boldsymbol{u} - \boldsymbol{v}_h\|_U + \|p - q_h\|_Q \right),$$

therefore

$$\|\boldsymbol{u}-\boldsymbol{u}_h\|_{H^1} \leq Ch^{s+1}\left(\left(\frac{K_S}{K_D}+1\right)\|\boldsymbol{u}\|_{H^{s+2}} + K_S\|p\|_{H^{s+1}}\right). \tag{3.152}$$

Now we shall use the Aubin-Nitche duality argument to obtain the L^2 error estimate of $\boldsymbol{u}-\boldsymbol{u}_h$. We define the adjoint problem of the strong form of (3.143): find $w \in H^2(\Omega) \cap U$ such that,

$$\begin{aligned}
-\Delta \boldsymbol{w} + \frac{1}{K_D}\boldsymbol{w} &= \boldsymbol{u}-\boldsymbol{u}_h, && \text{in } \Omega_D\\
-\Delta \boldsymbol{w} + \frac{1}{K_S}\boldsymbol{w} &= \boldsymbol{u}-\boldsymbol{u}_h, && \text{in } \Omega_S\\
\boldsymbol{w} &= 0, && \text{on } \partial\Omega.
\end{aligned}$$

Then by the regularity theory of PDE, $\|\boldsymbol{w}\|_{H^2} \leq \|\boldsymbol{u}-\boldsymbol{u}_h\|_{L^2}$. Let $\Pi_h \boldsymbol{w} \in Z_h$ be the finite element nodal interpolation of $\boldsymbol{w}$,

$$\begin{aligned}
\|\boldsymbol{u}-\boldsymbol{u}_h\|_{L^2}^2 &= (\nabla \boldsymbol{w}, \nabla(\boldsymbol{u}-\boldsymbol{u}_h)) + \frac{1}{K_D}(\boldsymbol{w}, \boldsymbol{u}-\boldsymbol{u}_h)_D + \frac{1}{K_S}(\boldsymbol{w}, \boldsymbol{u}-\boldsymbol{u}_h)_S\\
&= (\nabla(\boldsymbol{w}-\Pi_h\boldsymbol{w}), \nabla(\boldsymbol{u}-\boldsymbol{u}_h)) + (\nabla\Pi_h\boldsymbol{w}, \nabla(\boldsymbol{u}-\boldsymbol{u}_h))\\
&+ \frac{1}{K_D}((\boldsymbol{w}-\Pi_h\boldsymbol{w}), \boldsymbol{u}-\boldsymbol{u}_h)_D + \frac{1}{K_D}(\Pi_h\boldsymbol{w}, \boldsymbol{u}-\boldsymbol{u}_h)_D\\
&+ \frac{1}{K_S}((\boldsymbol{w}-\Pi_h\boldsymbol{w}), \boldsymbol{u}-\boldsymbol{u}_h)_S + \frac{1}{K_S}(\Pi_h\boldsymbol{w}, \boldsymbol{u}-\boldsymbol{u}_h)_S\\
&\leq (\nabla(\boldsymbol{w}-\Pi_h\boldsymbol{w}), \nabla(\boldsymbol{u}-\boldsymbol{u}_h)) + \frac{1}{K_D}((\boldsymbol{w}-\Pi_h\boldsymbol{w}), \boldsymbol{u}-\boldsymbol{u}_h)\\
&\leq h\|\boldsymbol{w}\|_{H^2}\|\nabla(\boldsymbol{u}-\boldsymbol{u}_h)\|_{L^2} + \frac{1}{K_D}h^2\|\boldsymbol{w}\|_{H^2}\|\boldsymbol{u}-\boldsymbol{u}_h\|_{L^2}\\
&\leq h\|\boldsymbol{u}-\boldsymbol{u}_h\|_{L^2}\|\nabla(\boldsymbol{u}-\boldsymbol{u}_h)\|_{L^2} + \frac{1}{K_D}h^2\|\boldsymbol{u}-\boldsymbol{u}_h\|_{L^2}^2
\end{aligned}$$

So we have

$$\|\boldsymbol{u}-\boldsymbol{u}_h\|_{L^2} \leq h\|\nabla(\boldsymbol{u}-\boldsymbol{u}_h)\|_{L^2} + \frac{1}{K_D}h^2\|\boldsymbol{u}-\boldsymbol{u}_h\|_{L^2}.$$

Since we can always pick a sufficiently small parameter h whenever K_D is determined, we can have (3.148).

From the LBB condition (3.140), for each $q_h \in Q_h$, we have

$$\|p_h - q_h\|_Q \leq \frac{1}{\gamma} \sup_{\boldsymbol{v}_h \in U_h, \boldsymbol{v}_h \neq 0} \frac{b(\boldsymbol{v}_h, p_h - q_h)}{\|\boldsymbol{v}_h\|_U}.$$

From (3.150),

$$b(\boldsymbol{v}_h, p_h - q_h) = a(\boldsymbol{u} - \boldsymbol{u}_h, \boldsymbol{v}_h) + b(\boldsymbol{v}_h, p - q_h).$$

By the continuity of $b(\boldsymbol{v}_h, p_h)$ we obtain

$$\begin{aligned} \|p_h - q_h\|_Q &\leq \frac{1}{\gamma} \sup_{\boldsymbol{v}_h \in U_h, \boldsymbol{v}_h \neq 0} \frac{a(\boldsymbol{u} - \boldsymbol{u}_h, \boldsymbol{v}_h) + b(\boldsymbol{v}_h, p - q_h)}{\|\boldsymbol{v}_h\|_U} \\ &\leq \frac{1}{\gamma} \left(\frac{1}{K_D} \|\boldsymbol{u} - \boldsymbol{u}_h\|_U + \|p - q_h\|_Q \right), \end{aligned}$$

then

$$\begin{aligned} \|p - p_h\|_Q \leq \|p_h - q_h\|_Q + \|p - q_h\|_Q \\ \leq \frac{1}{\gamma} \left(\frac{1}{K_D} \|\boldsymbol{u} - \boldsymbol{u}_h\|_U + (1+\gamma) \|p - q_h\|_Q \right). \end{aligned}$$

Therefore we get (3.149). □

For the non-divergence free case of Brinkman model (3.94), we can follow [Brezzi (1974); Quarteroni and Valli (2008)] to analyze its wellposedness and get the same results as Theorem 3.7. We give a sketch of such analysis in the following remark.

Remark 3.11. We first give the weak form of the non-divergence free Brinkman system (3.94) as follows: Find $(\boldsymbol{u}, p) \in U \times Q$, such that

$$a(\boldsymbol{u}, \boldsymbol{v}) + b(\boldsymbol{v}, p) = (\boldsymbol{f}, \boldsymbol{v}), \qquad \boldsymbol{v} \in U, \tag{3.153}$$

$$b(\boldsymbol{u}, q) = (g, q), \qquad q \in Q, \tag{3.154}$$

where $a(\cdot,\cdot)$ and $b(\cdot,\cdot)$ are defined the same in (3.133) and (3.134). Then the continuity and coercivity of the bilinear form $a(\cdot,\cdot)$ over $U \times Q$ remain as in (3.137) and (3.139), and the continuity and LBB condition of $b(\cdot,\cdot)$ over $U \times Q$ also remain as in (3.138) and (3.140). Therefore by Brezzi's theory [Brezzi (1974)], there is a unique solution to (3.153)-(3.154).

Then the discretization of (3.153)-(3.154) is given as follows: Find $(\boldsymbol{u}_h, p_h) \in U_h \times Q_h$, such that

$$a(\boldsymbol{u}_h, \boldsymbol{v}_h) + b(\boldsymbol{v}_h, p_h) = (\boldsymbol{f}, \boldsymbol{v}_h), \qquad \boldsymbol{v}_h \in U_h, \tag{3.155}$$

$$b(\boldsymbol{u}_h, q_h) = (g, q_h), \qquad q_h \in Q_h. \tag{3.156}$$

As defined in (3.142), Z_h is the space of discretely divergence-free functions associated with the finite dimensional spaces. The bilinear form $a(\cdot,\cdot)$ remains coercive in Z_h as it is coercive in U and Z_h is a subspace of U. Moreover, the continuity of the bilinear forms $a(\cdot,\cdot)$ over $U \times Q$ and $b(\cdot,\cdot)$ over $U \times Q$ also remains. Thus once more by Brezzi's theory [Brezzi (1974)], there is a unique solution to (3.155)-(3.156).

Define $Z^g = \{\boldsymbol{v} \in U | b(\boldsymbol{v}, q) = (g, q), \forall q \in Q\}$ and $Z_h^g = \{\boldsymbol{v}_h \in U_h | b(\boldsymbol{v}_h, q_h) = (g, q_h), \forall q_h \in Q_h\}$. Then choose $\tilde{\boldsymbol{u}}_{\boldsymbol{h}} \in Z_h^g$ and follow the proof of Theorem 3.7, we can get the same convergence results as (3.148) and (3.149).

Corollary 3.3. *When $\epsilon = K_D^\alpha$ and $K_D = K_S^{-\beta}$,*

$$\begin{aligned} \|\boldsymbol{u} - \boldsymbol{u}_h\|_{L^2} + h\|\boldsymbol{u} - \boldsymbol{u}_h\|_{H^1} &\leq C\epsilon^{-\frac{1}{\alpha}(\frac{1}{\beta}+1)} h^{s+2}(\|\boldsymbol{u}\|_{H^{s+2}} + \|p\|_{H^{s+1}}), & (3.157) \\ \|p - p_h\|_{L^2} &\leq C\epsilon^{-\frac{1}{\alpha}(\frac{1}{\beta}+2)} h^{s+1}(\|\boldsymbol{u}\|_{H^{s+2}} + \|p\|_{H^{s+1}}). & (3.158) \end{aligned}$$

Proof. Substitute $\epsilon = K_D^\alpha = K_S^{-\alpha\beta}$ into (3.148) and (3.149), and because $0 < K_D < 1$,

$0 < \alpha < 1$ and $\beta \geq 1$, we have $0 < \epsilon < 1$. Therefore we obtain (3.157) and (3.158).

□

For a fixed mesh size h, from (3.157) and (3.158), we know that the finite element approximation requires a bigger ϵ in order to get a better numerical approximation, while the PDE asymptotic analysis results in (3.109), (3.110), (3.120) and (3.121) imply that a smaller ϵ will produce a better approximation from the Brinkman model to the Darcy's and Stokes model. So overall, we proceed to find an optimal ϵ in the following corollary for a fixed mesh size h.

Corollary 3.4. *When $\beta = 1$, and*

$$\epsilon = \begin{cases} \left((1+\dfrac{3}{\alpha})h^{s+1}(h+2)\right)^{\frac{\alpha}{2\alpha+3}}, \text{ when } 0 < \alpha \leq \dfrac{1}{2}, \\ \left(\dfrac{3+\alpha}{1-\alpha}h^{s+1}(h+2)\right)^{\frac{\alpha}{4}}, \text{ when } \dfrac{1}{2} \leq \alpha < 1, \end{cases} \tag{3.159}$$

the re-scaled finite element solution $(\boldsymbol{u}_h, \tilde{p}_h)$ of Brinkman model (3.95) has the best approximation to both the solution $(\boldsymbol{u}_S, \tilde{p}_S)$ of Stokes equations (3.103) in Ω_S and the solution $(\boldsymbol{u}_D, \tilde{p}_D)$ of Darcy's equations (3.104) in Ω_D in the sense that both numerical and PDE's asymptotic accuracy are achieved at the same time, where $\tilde{p}_h$ equals ϵp_h in Ω_D and $\epsilon^{-1}p_h$ in Ω_S.

Proof. By Remark 3.9, we know it is optimal to choose $\beta = 1$. And when $\beta = 1$, (3.157) and (3.158) give that

$$\|\boldsymbol{u} - \boldsymbol{u}_h\|_{L^2} + \|p - p_h\|_{L^2} \leq C\epsilon^{-\frac{2}{\alpha}}(h + \epsilon^{-\frac{1}{\alpha}})h^{s+1}. \tag{3.160}$$

When $0 < \alpha \leq \frac{1}{2}$, (3.109), (3.110), (3.120) and (3.121) show that

$$\|\boldsymbol{u} - \boldsymbol{u}_D\|_{L^2(\Omega_D)} + \|\boldsymbol{u} - \boldsymbol{u}_S\|_{L^2(\Omega_S)} + \|\tilde{p} - \tilde{p}_D\|_{L^2(\Omega_D)} + \|\tilde{p} - \tilde{p}_S\|_{L^2(\Omega_S)} \leq C\epsilon. \tag{3.161}$$

Thus, by adding (3.160) and (3.161) together, and considering the re-scaling identity (3.99) which results in $\tilde{p}_D = \epsilon p$ in Ω_D and $\tilde{p}_S = \epsilon^{-1} p$ in Ω_S, we have

$$\|\boldsymbol{u}_D - \boldsymbol{u}_h\|_{L^2(\Omega_D)} + \|\boldsymbol{u}_S - \boldsymbol{u}_h\|_{L^2(\Omega_S)} + \|\tilde{p}_D - \tilde{p}_h\|_{L^2(\Omega_D)} + \|\tilde{p}_S - \tilde{p}_h\|_{L^2(\Omega_S)} \leq C\tilde{e}(\epsilon), \quad (3.162)$$

where

$$\tilde{e}(\epsilon) = \epsilon + \epsilon^{-\frac{2}{\alpha}}(h + \epsilon^{1-\frac{1}{\alpha}} + \epsilon^{-1-\frac{1}{\alpha}})h^{s+1}.$$

As long as $\tilde{e}(\epsilon)$ reaches its minimum at a certain value of ϵ, we know the approximation on the left hand side of (3.162) is the best. Since

$$\frac{d\tilde{e}}{d\epsilon} = 1 + \big(-\frac{2h}{\alpha}\epsilon^{-1-\frac{2}{\alpha}} + (1 - \frac{3}{\alpha})\epsilon^{-\frac{3}{\alpha}} - (1 + \frac{3}{\alpha})\epsilon^{-2-\frac{3}{\alpha}}\big)h^{s+1}, \quad (3.163)$$

it is not difficult to verify that $\frac{d^2\tilde{e}}{d\epsilon^2} > 0$ for all $\epsilon > 0$, thus $\tilde{e}(\epsilon)$ must exist a minimum value at its critical number. However, it is very hard to solve the equation $\frac{d\tilde{e}}{d\epsilon} = 0$ as defined in (3.163) for a critical number ϵ. In order to easily find an optimal ϵ at which the right hand side of (3.162) reaches its minimum, we further magnify $\tilde{e}(\epsilon)$ as

$$\tilde{e}(\epsilon) < e(\epsilon) = \epsilon + h^{s+1}(h + 2)\epsilon^{-1-\frac{3}{\alpha}}.$$

Hence, instead of $\tilde{e}(\epsilon)$, we deal with $e(\epsilon)$ which is simpler than $\tilde{e}(\epsilon)$ and is still held the right hand side of (3.162). Since $\frac{de}{d\epsilon} = 1 - (1 + \frac{3}{\alpha})\epsilon^{-2-\frac{3}{\alpha}} h^{s+1}(h + 2)$, and $\frac{d^2 e}{d\epsilon^2} > 0$ for all $\epsilon > 0$, we know that $e(\epsilon)$ reaches its minimum at

$$\epsilon = \left((1 + \frac{3}{\alpha})h^{s+1}(h + 2)\right)^{\frac{\alpha}{2\alpha+3}},$$

which means, at this value of ϵ the approximation on the left hand side of (3.162) becomes the best for $0 < \alpha \leq \frac{1}{2}$, i.e., both finite element approximation and PDE's asymptotic property of Brinkman model (3.95) achieve their accuracy at the same time.

When $\frac{1}{2} \leq \alpha < 1$, (3.109), (3.110), (3.120) and (3.121) show that

$$\|\boldsymbol{u} - \boldsymbol{u}_D\|_{L^2(\Omega_D)} + \|\boldsymbol{u} - \boldsymbol{u}_S\|_{L^2(\Omega_S)} + \|\tilde{p} - \tilde{p}_D\|_{L^2(\Omega_D)} + \|\tilde{p} - \tilde{p}_S\|_{L^2(\Omega_S)} \leq C\epsilon^{\frac{1}{\alpha}-1}.$$

Following the same analysis approach, we can attain the following optimal value of ϵ

$$\epsilon = \left(\frac{3+\alpha}{1-\alpha} h^{s+1}(h+2)\right)^{\frac{\alpha}{4}}$$

at which the approximation on the left hand side of (3.162) becomes the best for $\frac{1}{2} \leq \alpha < 1$. □

3.4.5 Mixed finite element approximation for Forchheimer model

Similarly to Brinkman model, the Forchheimer model is one equation defined in one region with piecewise parameters that is used to describe a Navier Stokes equation and Darcy's system in two regions. Though our main focus in this paper is Brinkman model, we still give the finite element error approximation for the Forchheimer model since they use very similar techniques. We define the governing equations as follows

$$\begin{cases} -\Delta \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} + \nabla p + \frac{1}{K}\boldsymbol{u} = \boldsymbol{f}, & \text{in } \Omega, \\ \nabla \cdot \boldsymbol{u} = 0, & \text{in } \Omega, \\ \int_\Omega p dx = 0, & \text{in } \Omega, \\ \boldsymbol{u} = 0, & \text{on } \partial\Omega. \end{cases} \tag{3.164}$$

The parameter K is a piecewise constant defined as

$$K = \begin{cases} K_D, & \text{in } \Omega_D, \\ K_S, & \text{in } \Omega_S, \end{cases}$$

where $0 < K_{min} \leq K_D < 1$ and $1 < K_S \leq K_{max} < \infty$.

Let U and P be the same as in (3.130) and $a(\boldsymbol{u}, \boldsymbol{v})$ and $b(\boldsymbol{v}, p)$ be the same as in (3.133) and (3.134). Define

$$c(\boldsymbol{w}; \boldsymbol{z}, \boldsymbol{v}) = \int_{\Omega} ((\boldsymbol{w} \cdot \nabla)\boldsymbol{z}) \cdot \boldsymbol{v}.$$

Then we have the weak formulation of (3.166) as: Find $(\boldsymbol{u}, p) \in U \times Q$, so that

$$a(\boldsymbol{u}, \boldsymbol{v}) + c(\boldsymbol{u}; \boldsymbol{u}, \boldsymbol{v}) + b(\boldsymbol{v}, p) = (\boldsymbol{f}, \boldsymbol{v}), \qquad \forall \boldsymbol{v} \in U, \tag{3.165}$$

$$b(\boldsymbol{u}, q) = 0, \qquad \forall q \in Q. \tag{3.166}$$

Define $U_{div} \subset U$ and $U_{div} = \{\boldsymbol{v} \in U | \nabla \cdot \boldsymbol{v} = 0\}$, so U_{div} is the subspace of U of divergence-free functions. The Forchheimer equations (3.167)-(3.168) can be reformulated as follows: Find $\boldsymbol{u} \in U_{div}$ such that

$$a(\boldsymbol{u}, \boldsymbol{v}) + c(\boldsymbol{u}; \boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{f}, \boldsymbol{v}), \forall \boldsymbol{v} \in U_{div}. \tag{3.167}$$

Lemma 3.12. *If $\boldsymbol{u}$ is a solution to problem (3.169), then there exists a unique $p \in Q$ such that $(\boldsymbol{u}, p)$ is a solution of problem (3.167)-(3.168).*

Now we give the proof of the existence and uniqueness of a solution to (3.169). We define the space

$$H_{div} := \{\boldsymbol{v} \in (L^2(\Omega))^d | \nabla \cdot \boldsymbol{v} = 0 \text{ in } \Omega, \boldsymbol{v} \cdot \boldsymbol{n} = 0 \text{ on } \partial\Omega\},$$

where $\boldsymbol{n}$ is the unit outward normal vector on $\partial\Omega$.

Theorem 3.8. *Let $\boldsymbol{f} \in H_{div}$ with $\|\boldsymbol{f}\|_{L^2} < 1/C_{\Omega}$, where C_{Ω} only depends on the Poincaré constant, then there exists a unique solution $\boldsymbol{u} \in U_{div}$ to problem (3.169).*

Proof. For each $\boldsymbol{w} \in U_{div}$, we define

$$A_{\boldsymbol{w}}(\boldsymbol{z}, \boldsymbol{v}) = a(\boldsymbol{z}, \boldsymbol{v}) + c(\boldsymbol{w}; \boldsymbol{z}, \boldsymbol{v}), \forall \boldsymbol{v}, \boldsymbol{z} \in U.$$

Since

$$
\begin{aligned}
|c(\boldsymbol{w};\boldsymbol{z},\boldsymbol{v})| &\leq \sum |\int w_j \frac{\partial z_j}{\partial x_j} v_j dx| \\
&\leq \|w_j\|_{L^4} \|\frac{\partial z_j}{\partial x_j}\|_{L^2} \|v_j\|_{L^4}, (H^1 \hookrightarrow L^4 \text{ for } d = 2,3) \\
&\leq C\|\boldsymbol{w}\|_U \|\boldsymbol{z}\|_U \|\boldsymbol{v}\|_U,
\end{aligned}
$$

we get that $A_{\boldsymbol{w}}(\boldsymbol{z},\boldsymbol{v})$ is continuous. By using Poincaré inequality for $\boldsymbol{v} \in U$ and because $\boldsymbol{w} \in U_{div}$, we also have

$$
\begin{aligned}
A_{\boldsymbol{w}}(\boldsymbol{v},\boldsymbol{v}) &= \|\nabla \boldsymbol{v}\|_{L^2}^2 + ((\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\cdot\boldsymbol{w}) + \frac{1}{K_D}\|\boldsymbol{v}\|_{L^2(\Omega_D)}^2 + \frac{1}{K_S}\|\boldsymbol{v}\|_{L^2(\Omega_S)}^2 \\
&\geq \frac{1}{C_\Omega}\|\boldsymbol{v}\|_U^2 - \frac{1}{2}\int_\Omega \nabla\cdot\boldsymbol{w}|\boldsymbol{v}|^2 dx + \frac{1}{2}\int_{\partial\Omega} \boldsymbol{w}\cdot\boldsymbol{n}|\boldsymbol{v}|^2 dx \\
&= \frac{1}{C_\Omega}\|\boldsymbol{v}\|_U^2,
\end{aligned}
$$

where C_Ω only depends on the Poincaré constant, then by Lax-Milgram theorem, for each $\boldsymbol{w} \in U_{div}$, there is a unique solution $\boldsymbol{z} \in U_{div}$ to the equation

$$A_{\boldsymbol{w}}(\boldsymbol{z},\boldsymbol{v}) = (\boldsymbol{f},\boldsymbol{v}), \forall \boldsymbol{v} \in U_{div}. \tag{3.168}$$

Further, we have $\|\boldsymbol{z}\|_U^2 \leq C_\Omega |A_{\boldsymbol{w}}(\boldsymbol{z},\boldsymbol{z})| \leq C_\Omega \|\boldsymbol{f}\|_{L^2}\|\boldsymbol{z}\|_{L^2} \leq C_\Omega \|\boldsymbol{f}\|_{L^2}\|\boldsymbol{z}\|_U$, and thus

$$\|\boldsymbol{z}\|_U \leq C_\Omega \|\boldsymbol{f}\|_{L^2}. \tag{3.169}$$

Now we define a map $\Phi(\boldsymbol{w}) = \boldsymbol{z}$, and define $\Lambda = \{\boldsymbol{v} \in U_{div} | \|\boldsymbol{v}\|_U \leq C_\Omega \|\boldsymbol{f}\|_{L^2}\}$, so we have $\Phi(U_{div}) \subset \Lambda$. Assume for $\boldsymbol{w}_1, \boldsymbol{w}_2 \in U_{div}$, $\boldsymbol{z}_1$ and $\boldsymbol{z}_2$ are the solutions to (3.170), respectively, that is

$$A_{\boldsymbol{w}_1}(\boldsymbol{z}_1,\boldsymbol{v}) = (\boldsymbol{f},\boldsymbol{v}) \tag{3.170}$$

and

$$A_{\boldsymbol{w}_2}(\boldsymbol{z}_2,\boldsymbol{v}) = (\boldsymbol{f},\boldsymbol{v}). \tag{3.171}$$

Subtract (3.173) from (3.172), we get

$$a((\boldsymbol{z}_1 - \boldsymbol{z}_2), \boldsymbol{v}) + c(\boldsymbol{w}_1; \boldsymbol{z}_1 - \boldsymbol{z}_2, \boldsymbol{v}) - c(\boldsymbol{w}_1 - \boldsymbol{w}_2; \boldsymbol{z}_2, \boldsymbol{v}) = 0.$$

Let $\boldsymbol{v} = \boldsymbol{z}_1 - \boldsymbol{z}_2 \in U_{div}$, then

$$\|\boldsymbol{z}_1 - \boldsymbol{z}_2\|_U^2 + \frac{1}{K_D}\|\boldsymbol{z}_1 - \boldsymbol{z}_2\|_{L^2(\Omega_D)}^2 + \frac{1}{K_S}\|\boldsymbol{z}_1 - \boldsymbol{z}_2\|_{L^2(\Omega_S)}^2 \\ + c(\boldsymbol{w}_1; \boldsymbol{z}_1 - \boldsymbol{z}_2, \boldsymbol{z}_1 - \boldsymbol{z}_2) - c(\boldsymbol{w}_1 - \boldsymbol{w}_2; \boldsymbol{z}_2, \boldsymbol{z}_1 - \boldsymbol{z}_2) = 0. \quad (3.172)$$

Since

$$\begin{aligned} c(\boldsymbol{w}_1; \boldsymbol{z}_1 - \boldsymbol{z}_2, \boldsymbol{z}_1 - \boldsymbol{z}_2) &= \frac{1}{2}\int \boldsymbol{w}_1 \nabla \cdot (\boldsymbol{z}_1 - \boldsymbol{z}_2)^2 \\ &= -\frac{1}{2}\int \nabla \cdot \boldsymbol{w}_1 (\boldsymbol{z}_1 - \boldsymbol{z}_2)^2 + \frac{1}{2}\int_{\partial\Omega} \boldsymbol{w}_1 \cdot \boldsymbol{n}(\boldsymbol{z}_1 - \boldsymbol{z}_2)^2 dx = 0, \end{aligned}$$

(3.174) gives,

$$\|\boldsymbol{z}_1 - \boldsymbol{z}_2\|_U^2 + \frac{1}{K_D}\|\boldsymbol{z}_1 - \boldsymbol{z}_2\|_{L^2(\Omega_D)}^2 + \frac{1}{K_S}\|\boldsymbol{z}_1 - \boldsymbol{z}_2\|_{L^2(\Omega_S)}^2 = -c(\boldsymbol{w}_1 - \boldsymbol{w}_2; \boldsymbol{z}_2, \boldsymbol{z}_1 - \boldsymbol{z}_2),$$

and then

$$\|\boldsymbol{z}_1 - \boldsymbol{z}_2\|_U^2 \leq \hat{C}\|\boldsymbol{w}_1 - \boldsymbol{w}_2\|_U \|\boldsymbol{z}_2\|_U \|\boldsymbol{z}_1 - \boldsymbol{z}_2\|_U.$$

Since also $\boldsymbol{z}_1, \boldsymbol{z}_2 \in \Lambda$, we have the following from (3.171),

$$\|\boldsymbol{z}_1 - \boldsymbol{z}_2\|_U \leq C_\Omega \|\boldsymbol{w}_1 - \boldsymbol{w}_2\|_U \|\boldsymbol{f}\|_{L^2}.$$

Thus when $C\|\boldsymbol{f}\|_{L^2} < 1$,

$$\|\Phi(\boldsymbol{w}_1) - \Phi(\boldsymbol{w}_2)\|_U = \|\boldsymbol{z}_1 - \boldsymbol{z}_2\|_U < \|\boldsymbol{w}_1 - \boldsymbol{w}_2\|_U.$$

This means Φ is a contraction mapping, so there is a fixed point to $\Phi(\boldsymbol{w}) = \boldsymbol{z}$, that is $\Phi(\boldsymbol{u}) = \boldsymbol{u} \in \Lambda$ as the unique solution to (3.169). □

Furthermore, when using $P^{s+1}P^s$ element, that is, Taylor - Hood element, by Brezzi's theory [Brezzi (1974)], the following result holds.

Corollary 3.5. *There exist two operators* $\boldsymbol{r}_h : (H^1(\Omega))^d \to U_h$ *and* $s_h : L^2(\Omega) \to Q_h$ *such that*

$$\|\boldsymbol{v} - \boldsymbol{r}_h(\boldsymbol{v})\|_U \leq Ch^{s+1}\|\boldsymbol{v}\|_{H^{s+2}}, \qquad \forall \boldsymbol{v} \in (H^{s+2}(\Omega))^d, \tag{3.173}$$

$$\|q - s_h(q)\|_Q \leq Ch^{s+1}\|q\|_{H^{s+1}}, \qquad \forall q \in H^{s+1}(\Omega). \tag{3.174}$$

Now we look for a solution to the following problem: given $\boldsymbol{f} \in U'$, find $(\boldsymbol{u}_h, p_h) \in U_h \times Q_h$, such that

$$a(\boldsymbol{u}_h, \boldsymbol{v}_h) + c(\boldsymbol{u}_h; \boldsymbol{u}_h, \boldsymbol{v}_h) + b(\boldsymbol{v}_h, p_h) = (\boldsymbol{f}, \boldsymbol{v}_h), \qquad \forall \boldsymbol{v}_h \in U_h, \tag{3.175}$$

$$b(\boldsymbol{u}_h, q_h) = 0, \qquad \forall q_h \in Q_h, \tag{3.176}$$

where U_h, Q_h are the finite dimensional subspaces of U and Q, respectively. We can similarly obtain the wellposedness of (3.177)-(3.178) as in Section 3.4.4. For what concerns the convergence estimate, we obtain the following theorem using the techniques introduced in Section 10.2.2 in [Quarteroni and Valli (2008)] and the similar error analysis we did in Theorem 3.7 for the zero-order term of $\boldsymbol{u}$ involving the parameter K in (3.167).

Theorem 3.9. *let* $(\boldsymbol{u}, p)$ *be the solution to (3.167)-(3.168) and let* $(\boldsymbol{u}_h, p_h)$ *be the solution to (3.177)-(3.178), then we have*

$$\begin{aligned}
&\|p - p_h\|_{L^2} + \|\boldsymbol{u} - \boldsymbol{u}_h\|_{H^1} \\
&\leq Ch^{s+1}\left(\left(\left(\frac{K_S}{K_D} + 1\right)\left(\frac{1}{K_D} + 1\right) + 1\right)\|\boldsymbol{u}\|_{H^{s+2}} + \left(\frac{K_S}{K_D} + K_S + 2\right)\|p\|_{H^{s+1}}\right).
\end{aligned} \tag{3.177}$$

Proof. Define $W = U \times Q$, $Y = U' = (H^{-1}(\Omega))^d$ and $\Lambda = \mathbb{R}^+$. Define linear operator T as follows: given $\boldsymbol{f}^* \in U'$, we denote by

$$T\boldsymbol{f}^* := (\boldsymbol{u}^*, p^*) \in U \times Q$$

the solution of the following Stokes problem

$$\frac{1}{K_D}(\boldsymbol{u}^*, \boldsymbol{v})_D + \frac{1}{K_S}(\boldsymbol{u}^*, \boldsymbol{v})_S + (\nabla \boldsymbol{u}^*, \nabla \boldsymbol{v}) - (\nabla \cdot \boldsymbol{v}, p^*) = (\boldsymbol{f}^*, \boldsymbol{v}), \qquad \forall \boldsymbol{v} \in U, \tag{3.178}$$

$$-(\nabla \cdot \boldsymbol{u}^*, q) = 0, \qquad \forall q \in Q. \tag{3.179}$$

A C^∞-mapping from $\Lambda \times W$ into Y defined by

$$G : (\mu, \boldsymbol{z}) \to G(\mu, \boldsymbol{z}) = \mu \left(\sum_{j=1}^{d} v_j \frac{\partial \boldsymbol{v}}{\partial x_j} - \boldsymbol{f} \right)$$

is associated to $\boldsymbol{f} \in (L^2(\Omega))^d$. Here $\boldsymbol{z} = (\boldsymbol{v}, q) \in W$.

Then (3.167)-(3.168) can be regarded as particular cases of the following class of problems: given $\lambda \in \Lambda$, find $\boldsymbol{w}(\lambda) \in W$ such that

$$F(\lambda, \boldsymbol{w}(\lambda)) := \boldsymbol{w}(\lambda) + TG(\lambda, \boldsymbol{w}(\lambda)) = 0.$$

(3.177)-(3.178) can be represented in the following form: given $\lambda \in \Lambda$, find $\boldsymbol{w}_h(\lambda) \in W_h$ such that

$$F_h(\lambda, \boldsymbol{w}_h(\lambda)) := \boldsymbol{w}_h(\lambda) + T_h G(\lambda, \boldsymbol{w}_h(\lambda)) = 0.$$

Indeed, we set $W_h = U_h \times Q_h$ and define $T_h : (H^{-1}(\Omega))^d \to W_h$ as follows: for any $\boldsymbol{f}^* \in (H^{-1}(\Omega))^d$, $T_h \boldsymbol{f}^* := (\boldsymbol{u}_h^*, p_h^*) \in U_h \times Q_h$ is such that

$$\frac{1}{K_D}(\boldsymbol{u}_h^*, \boldsymbol{v}_h)_D + \frac{1}{K_S}(\boldsymbol{u}_h^*, \boldsymbol{v}_h)_S + (\nabla \boldsymbol{u}_h^*, \nabla \boldsymbol{v}_h) - (\nabla \cdot \boldsymbol{v}_h^*, p_h) = (\boldsymbol{f}^*, \boldsymbol{v}_h), \qquad \forall \boldsymbol{v}_h \in U_h,$$

$$-(\nabla \cdot \boldsymbol{u}_h^*, q_h) = 0, \qquad \forall q_h \in Q_h.$$

Obviously, (3.182)-(3.182) is the finite dimensional approximation to the Stokes problem (3.180)-(3.181). If we set $\boldsymbol{w}_h := (\boldsymbol{u}_h, p_h)$ we deduce from (3.177)-(3.178) that

$$\boldsymbol{w}_h = -T_h G(1, \boldsymbol{w}_h),$$

or equivalently,

$$F_h(\lambda, \boldsymbol{w}_h) := \boldsymbol{w}_h + T_h G(\lambda, \boldsymbol{w}_h) = 0,$$

with $\lambda = 1$. This is specifically for the viscosity $\nu = 1$. If $\nu \neq 1$, then we choose $\boldsymbol{w}_h = -T_h G(1/\lambda, \boldsymbol{w}_h)$. [Quarteroni and Valli (2008)].

The conditions in Theorem 10.2.1 in [Quarteroni and Valli (2008)] are all satisfied in our case, hence we conclude that, for h small enough, there exists a unique branch of non-singular solutions of (3.177)-(3.178). Moreover, the following convergence inequality holds

$$\|\boldsymbol{w}(\lambda) - \boldsymbol{w}_h(\lambda)\|_W \leq C\left(\|\boldsymbol{w}(\lambda) - \Pi_h \boldsymbol{w}_h(\lambda)\|_W + \|(T - T_h)G(\lambda, \boldsymbol{w}(\lambda))\|_W\right), \quad (3.180)$$

where for each $(\boldsymbol{v}, q) \in U \times Q$, $\Pi_h(\boldsymbol{v}, q)$ is defined as

$$\Pi_h(\boldsymbol{v}, q) := (\boldsymbol{\Pi}_{U_h}(\boldsymbol{v}), \Pi_{Q_h}(q)).$$

Here $\boldsymbol{\Pi}_{U_h}$ and Π_{Q_h} are the orthogonal projections over U_h and Q_h with respect to the scalar product of $(H^1(\Omega))^d$ and $L^2(\Omega)$, respectively. For any $\boldsymbol{w} = (\boldsymbol{u}, p)$, define $\|\boldsymbol{w}\|_W = \|\boldsymbol{u}\|_U + \|p\|_Q$. Then by (3.175) and (3.176),

$$\begin{aligned} & \|\boldsymbol{w}(\lambda) - \Pi_h \boldsymbol{w}(\lambda)\|_W = \|\boldsymbol{u}(\lambda) - \boldsymbol{\Pi}_{U_h}(\boldsymbol{u}(\lambda))\|_U + \|p(\lambda) - \Pi_{Q_h}(p(\lambda))\|_Q \\ \leq \ & \|\boldsymbol{u}(\lambda) - \boldsymbol{r}_h(\boldsymbol{u}(\lambda))\|_U + \|p(\lambda) - s_h(p(\lambda))\|_Q \\ \leq \ & Ch^{s+1}\left(\|\boldsymbol{u}\|_{H^{s+2}} + \|p\|_{H^{s+1}}\right) \qquad (3.181) \end{aligned}$$

Moreover $\|(T-T_h)G(\lambda, \boldsymbol{w}(\lambda))\|_W$ is nothing but error arising from the finite element approximation to a Stokes problem whose right hand side is $G(\lambda, \boldsymbol{w}(\lambda))$. By (3.152) and (3.149), we have

$$\begin{aligned}
&\|(T-T_h)G(\lambda, \boldsymbol{w}(\lambda))\|_W \\
&\leq Ch^{s+1}\left(\left(\frac{K_S}{K_D}+1\right)\left(\frac{1}{K_D}+1\right)\|\boldsymbol{u}\|_{H^{s+2}}+\left(\frac{K_S}{K_D}+K_S+1\right)\|p\|_{H^{s+1}}\right). \quad (3.182)
\end{aligned}$$

Thus by (3.182), (3.183) and (3.184), we have (3.179). □

Corollary 3.6. *Given* $0<\alpha<1$ *and* $\beta \geq$, *for* $\epsilon = K_D^{\alpha}$ *and* $K_D = K_S^{-\beta}$,

$$\|\boldsymbol{u}-\boldsymbol{u}_h\|_{H^1}+\|p-p_h\|_{L^2} \leq C\epsilon^{-\frac{1}{\alpha}(\frac{1}{\beta}+2)}h^{s+1}(\|\boldsymbol{u}\|_{H^{s+2}}+\|p\|_{H^{s+1}}). \quad (3.183)$$

3.4.6 Numerical Experiment

Remark 3.12. Actually, the first equation in (3.97) approximates $\boldsymbol{u} = -K^{1-\alpha}\nabla\tilde{p}$ as K approaches zero in Ω_D, which implies that, in order to be consistent with Darcy's law (3.101), $K^{1-\alpha} = K/(\nu\phi)$, i.e., $\alpha = \ln(\nu\phi)/\ln K$.

For instance, in the case of PEM fuel cells, since ν is the mixture viscosity of liquid phase and gaseous phase of water, $\nu = s\nu_l + (1-s)\nu_g$, where $0 \leq s \leq 1$ is the liquid saturation, thus ν can be estimated by average as $(\nu_l+\nu_g)/2$. Given the values of parameters in Table 3.5, we are able to evaluate the value of $\alpha \approx 0.449$ in the case of PEM fuel cell.

For the convenience of numerical experiment, without loss of generality, we choose the mean value of α in its range $(0,1)$, i.e., $1/2$, as a specific value of α to carry out the numerical experiment. $\alpha = 1/2$ is also close to the physical value of α shown in

Parameter	Symbol	Value	Unit
Kinematic viscosity of fluid	ν_l	3.533×10^{-7}	m^2/s
Kinematic viscosity of gas	ν_g	3.59×10^{-5}	m^2/s
Permeability of porous media	K	8.69×10^{-12}	m^2
Porosity of porous media	ϕ	0.6	

Table 3.5. Values of parameters in PEMFC [Sun (2011)]

Remark 3.12. As shown in Remark 3.9, $\beta = 1$ is optimal for the value of β to get the best approximation. Then (3.102) can be particularly rewritten as

$$\begin{cases} -\epsilon^2 \Delta \boldsymbol{u} + \epsilon \nabla \tilde{p} + \boldsymbol{u} = \epsilon^2 \boldsymbol{f}_D, & \text{in } \Omega_D, \\ -\Delta \boldsymbol{u} + \epsilon \nabla \tilde{p} + \epsilon^2 \boldsymbol{u} = \boldsymbol{f}_S, & \text{in } \Omega_S, \\ \nabla \cdot \boldsymbol{u} = 0, & \text{in } \Omega, \end{cases} \tag{3.184}$$

which approximates

$$\begin{cases} \epsilon \nabla \tilde{p}_D + \boldsymbol{u}_D = \epsilon^2 \boldsymbol{f}_D, & \text{in } \Omega_D, \\ -\Delta \boldsymbol{u}_S + \epsilon \nabla \tilde{p}_S = \boldsymbol{f}_S, & \text{in } \Omega_S, \\ \nabla \cdot \boldsymbol{u} = 0, & \text{in } \Omega. \end{cases} \tag{3.185}$$

(I) Convergence with respect to h for Brinkman model

We first choose $s = 1$, that is, we choose to use $P^{s+1}P^s = P^2P^1$ element. We choose the real solutions as

$$\begin{cases} u_1 = -\cos x \sin y, \\ u_2 = \sin x \cos y, \\ p = \frac{1}{2} - \frac{\cos 2x + \cos 2y}{4}, \end{cases} \tag{3.186}$$

where $\boldsymbol{u} = (u_1, u_2)^T$. On a uniform rectangular mesh, we investigate the error estimates in L^2 and H^1 norms of velocity and L^2 norm of pressure.

	L^2 for velocity	H^1 for velocity	L^2 for pressure
$\epsilon = 10^{-1}$	3.00	2.00	2.00
$\epsilon = 10^{-2}$	3.01	2.00	2.09
$\epsilon = 10^{-3}$	3.01	2.01	3.73
$\epsilon = 10^{-4}$	3.01	2.01	3.98
$\epsilon = 10^{-5}$	3.01	2.01	3.88
$\epsilon = 10^{-6}$	3.01	2.01	2.32
$\epsilon = 10^{-7}$	3.01	2.01	1.97
$\epsilon = 10^{-8}$	3.01	2.01	1.96

Table 3.6. Convergence rate of $\boldsymbol{u}$ and p

For each ϵ chosen, Table 3.6 shows that the convergence rates are optimal in L^2 and H^1 norms of velocity and L^2 norm of pressure. This matches our theoretical results proved in Theorem 3.7.

(II) Convergence with respect to h for Forchheimer model

Same as in Brinkman model, we choose $s = 1$ and use the same real solutions as (**??**). On a uniform rectangular mesh, we investigate the error estimates in L^2 and H^1 norms of velocity and L^2 norm of pressure.

	H^1 for velocity	L^2 for pressure
$\epsilon = 10^{-1}$	2.00	1.93
$\epsilon = 10^{-2}$	2.00	1.86
$\epsilon = 10^{-3}$	2.01	3.68
$\epsilon = 10^{-4}$	2.01	3.98
$\epsilon = 10^{-5}$	2.01	3.88
$\epsilon = 10^{-6}$	2.01	2.32
$\epsilon = 10^{-7}$	2.01	1.97
$\epsilon = 10^{-8}$	2.01	1.96

Table 3.7. Convergence rate of $\boldsymbol{u}$ and p

For each ϵ chosen, Table 3.7 shows that the convergence rates are optimal H^1 norm of velocity and L^2 norm of pressure. This matches our theoretical results proved in Theorem 3.9.

3.5 An innovation of Butler-Volmer equation for the electrochemical kinetic model

As shown in Section 3.1, the fuel cell model involves the species transport (convection-diffusion-reaction) equations (3.1)-(3.2), fluid flow (Navier-Stokes-Darcy) equations (3.4)-(3.5), energy (heat conduction) equation (3.6), and electrostatic potential (Poisson) equations (3.7)-(3.8). An assumption of local equilibrium of the diffuse (polarization) layer must hold for such model since the source terms of (3.1)-(3.8) are all characterized by a simplified electrochemical kinetics, Butler-Volmer equation (3.3). However, such strong equilibrium assumption for the diffuse charge distribution does not always hold. The standard Butler-Volmer equation no longer fits the mathematical description without arbitrary assumptions such as local equilibrium or electroneutrality of the electrolyte or for instance a prescribed, constant surface charge, thus it can no be applied in such situations as thin electrolyte films (where diffusion layers overlap and/or the bulk electrical field is a significant portion of the field strength in the polarization layer), operation at large, super-limiting currents or large AC frequencies, which are all situations where the diffuse charge distribution loses its quasi-equilibrium structure. On the other hand, the full, non-equilibrium Poisson-Nernst-Planck (PNP) model for the transport rates of all mobile ions through the electrolyte [Smith and White (1993)] describes the electrochemical kinetic system when ions can be considered as point charges, without excluded volume, the structure of the electrolyte including the polarization layer that forms on the electrodes.

The PNP model describes ion concentration and potential profiles both in the electrolyte bulk, as well as in the diffusion layers, all the way up to the reaction planes. The resulting PNP-fuel cell model can be generally used, for the equilibrium and non-equilibrium situation, as well as for steady-state and fully dynamic transport problems. In the next Chapter 4, we will first study PNP equations, and its numerical methodologies and analyses, then develop a new fuel cell model with the replacement of Butler-Volmer equation by PNP equations in Chapter 5.

CHAPTER 4

POISSON-NERNST-PLANCK (PNP) MODEL

4.1 Introduction to Poisson-Nernst-Planck (PNP) model

Poisson-Nernst-Planck (PNP) equations provide a mean-field continuum electrodiffusion model for the flows of charged particles in terms of the average density distributions and the electrostatic potential. This model has been widely used to describe the transport of charged particles in semiconductors [Jerome (1996); Markowich (1986); Newman (1991); Rouston (1990); Selberherr (1984)], electrochemical systems [Bazant et al. (2009); Ciucci and Lai (2011); Marcicki et al. (2012); Richardson and King (2007); Rubinstein (1990); Soestbergen et al. (2010)] and biological membrane channels [Bolintineanu et al. (2009); Cardenas et al. (2000); Coalson and Kurnikova (2005); Eisenberg (1998); Eisenberg et al. (2010); Eisenberg (1996); Hollerbach et al. (2000); Kurnikova et al. (1999); Lu et al. (2007); Singer and Norbury (2009)].

The mathematical analysis and numerical approximation of the PNP equations have attracted considerable interests. The existence of solutions to the PNP equations has been shown in [Jerome (1985); Mock (1972)]. In [Liu (2009)], the existence and local uniqueness of a solution to the one-dimensional steady-state PNP systems with multiple ion species has been shown. In [Gajewski and Gröger (1986); Mock (1972)], the existence and uniqueness of temporally global solutions have been proved for PNP systems based on maximum principle and compactness arguments. Analytic solutions have been found for one-dimensional case [Bicknell et al. (1977); Golovnev and Trimper (2010, 2011)].

Due to the nonlinearity of the coupled system of partial differential equations (PDEs), in general, it is mathematically challenging to find the analytic solution of PNP equations. Therefore, numerical methods are often employed to find the approximate solutions. There are many existing studies on the numerical techniques for solving PNP equations. Finite difference method has been widely used to solve PNP equations [Bolintineanu et al. (2009); Cardenas et al. (2000); Cohen and Cooley (1965); Eisenberg and Chen (1993); Im and Roux (2002); Kurnikova et al. (1999)]. In [Kurnikova et al. (1999)], a lattice relaxation scheme is used together with the finite difference scheme to solve three-dimensional PNP equations. A second-order finite difference method has been designed to solve PNP equations in ion channels [Zheng et al. (2011)]. The use of finite difference method has certain limitation on the description of ionic channel geometry. Finite volume method was then used in [Mathur and Murthy (2009); Wu et al. (2002)] to solve PNP equations in the irregular domains, but was still limited by the low convergence rate because of the difficulty of the design of high-order control volume. Finite element method has the advantage of handling ion channels with irregular surfaces [Gatti et al. (1998); Lu et al. (2007, 2010); Song et al. (2004a,b); Zhou et al. (2008); Jerome and Kerkhoven (1991)], and its convergence rate only depends on the regularity of the solution. In [Jerome and Kerkhoven (1991); Jerome (1996)], a convergence theory has been established for the finite element method by defining a fixed point mapping T, termed Gummel's map [Gummel (1964)], solving each of the decoupled PNP equations and substituting these solutions in successive PDEs in a Gauss-Seidel fashion. The fixed points of the mapping T then coincide with solutions to the PNP system, however, no convergence rate was given for this finite element approximation. Spectral element method [Hollerbach and Chen (2002)] and boundary element method [Zhou et al. (2008)] have also been studied for three-dimensional PNP equations, but their convergence analyses were not conducted. Recently, an error estimate of the standard finite element method was given in [Yang and Lu (2013)] for a type of steady-state PNP equations modeling the electrodiffusion of ions in a solvated biomolecular system, however, their error estimates for the potential and concentration in H^1 norm depend essentially on the L^2 error of the concentration, which was only numerically shown to be second order.

4.2 Error analysis of finite element method for Poisson-Nernst-Planck equations

4.2.1 Introduction

In this section, we study the a priori error estimates of the finite element approximation to a type of time-dependent Poisson-Nernst-Planck (PNP) equations. Two types of temporal semi-dicretization schemes for the time-dependent PNP equations are introduced in [Prohl and Schmuck (2009)] and employed to prove the existence and uniqueness of the solutions of the discretized PNP equations. An optimal error estimate for a fully discrete finite element discretization of the time-dependent Navier-Stokes-Poisson-Nernst-Planck system using linear element is claimed in [Prohl and Schmuck (2010)] without a complete proof. In fact, the techniques used in [Prohl and Schmuck (2010)] for the error analysis of the temporal semi-discretization cannot be carried over to either spatial semi-discretization or full discretization of the time-dependent PNP equations. So far, we have not seen a priori error estimate of the standard finite element method for time-dependent PNP equations with either semi- or full discretization schemes in a completely correct manner.

The main purpose of this section is to provide a complete a priori error analysis for the finite element discretization of the time-dependent PNP equations. We obtain optimal error estimates in $L^\infty(H^1)$ and $L^2(H^1)$ norms and a sub-optimal error estimate in the $L^\infty(L^2)$ norm for both semi- and fully discrete finite element discretization using linear elements. In addition, we also give an optimal error estimate in $L^\infty(L^2)$ norm for the quadratic or higher-order finite element discretization.

The rest of this section is organized as follows. Section 4.2.2 introduces the model problem. Section 4.2.3 describes the semi- and full discretization of the problem. The main error estimates for semi-discretization and full dicretization are given in Section 4.2.4 and Section 4.2.5, respectively. Numerical experiments are reported in Section 4.2.6.

4.2.2 PNP system and its variational form

Let $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$, be a convex bounded Lipschitz domain. The classic PNP system was introduced by W. Nernst [Nernst (1889)] and M. Planck [Planck (1890)]. It describes the mass concentration of ions $C_1, C_2 : \Omega \times (0, T] \to \mathbb{R}^+ \cup \{0\}$, and the electrostatic potential $\Phi : \Omega \times (0,T] \to \mathbb{R}$,

$$\begin{aligned} \partial_t C_i - \nabla \cdot (\nabla C_i + q_i C_i \nabla \Phi) &= F_i, \text{ for } i = 1, 2 && (4.1) \\ -\Delta \Phi &= \sum_{i=1}^{2} q_i C_i + F_3, && (4.2) \end{aligned}$$

where $\partial_t = \partial/\partial t$. The index i corresponds to the different ionic species, and q_i is the charge of the species i, for simplicity, in the following we choose $q_1 = 1$, $q_2 = -1$. F_i ($i = 1, 2, 3$) denote the reaction source terms. Note that the convection terms given in (4.1) are in divergence form.

Denote the initial concentrations and potential by (C_1^0, C_2^0, Φ^0). Either flux-free condition or Dirichlet type boundary conditions can be applied to the PNP equations [Burger et al. (2012)]. For simplicity, we shall consider the homogeneous Dirichlet boundary conditions as follows:

$$C_1 = C_2 = \Phi = 0, \text{ on } \partial\Omega \times (0,T].$$

The weak formulation of the system (4.1)-(4.2) is given as follows: find $C_i \in L^2(0,T; H_0^1(\Omega)) \cap L^\infty(0,T; L^\infty(\Omega))$, $i = 1, 2$, and $\Phi(t) \in H_0^1(\Omega)$ such that,

$$\begin{aligned} (\partial_t C_i, v) + (\nabla C_i, \nabla v) + (q_i C_i \nabla \Phi, \nabla v) &= (F_i, v), \qquad \forall v \in H_0^1(\Omega), && (4.3) \\ (\nabla \Phi, \nabla \phi) - \sum_{i=1}^{2} q_i (C_i, \phi) &= (F_3, \phi), \qquad \forall \phi \in H_0^1(\Omega). && (4.4) \end{aligned}$$

In [Gajewski and Gröger (1986)], it was proved that there exists a unique solution (C_1, C_2, Φ) satisfying (4.3)-(4.4) when $F_i \in L_+^\infty(0,T;\mathbb{R}^d)$.

4.2.3 Finite element discretization

Let $\mathcal{T}_h$ be a quasi-uniform mesh of Ω with mesh size $0 < h < 1$ [Brenner and Scott (2002)] and define the corresponding finite element space $S_h \subset H_0^1$ by

$$S_h = \{v \in H^1(\Omega) : v|_{\partial\Omega} = 0 \text{ and } v|_K \in P_k(K), \forall K \in \mathcal{T}_h\},$$

where $P_k(K)$ is the set of polynomials of degree k or less.

The semi-discretization to (4.3)-(4.4) is defined as follows: find $(C_{1,h}, C_{2,h}, \Phi) \in [S_h]^3$ such that,

$$(\partial_t C_{i,h}, v_h) + (\nabla C_{i,h}, \nabla v_h) + (q_i C_{i,h} \nabla\Phi_h, \nabla v_h) = (F_i, v_h), \qquad \forall v_h \in S_h, \quad (4.5)$$

$$(\nabla\Phi_h, \nabla\phi_h) - \sum_{i=1}^{2} q_i (C_{i,h}, \phi_h) = (F_3, \phi_h), \qquad \forall \phi_h \in S_h, \quad (4.6)$$

with the initial condition $(C_{1,h}^0, C_{2,h}^0, \Phi_h^0)$ given by the interpolation of (C_1^0, C_2^0, Φ^0) in $[S_h]^3$ and the Dirichlet boundary condition $C_{1,h} = C_{2,h} = \Phi_h = 0$.

In order to give the full discretization of the system (4.3)-(4.4), we first define a uniform partition $0 = t^0 < t^1 < \cdots < t^N = T$, with time-step size $\Delta t = T/N$, and $t^\sigma = \sigma\Delta t$, $\sigma \in \mathbb{R}$. Also, for any function φ, denote $\varphi^n \equiv \varphi(x, t^n)$, $\varphi^{n+\frac{1}{2}} \equiv (\varphi^{n+1} + \varphi^n)/2$, and $d_t\varphi^n \equiv (\varphi^{n+1} - \varphi^n)/\Delta t$.We use the Crank-Nicolson scheme for the time discretization, i.e., given $(C_{1,h}^n, C_{2,h}^n, \Phi_h^n)$, we seek $(C_{1,h}^{n+1}, C_{2,h}^{n+1}, \Phi_h^{n+1}) \in [S_h]^3$ such that, for any $v_h \in S_h$ and $\phi_h \in S_h$,

$$\left(d_t C_{i,h}^n, v_h\right) + \left(\nabla C_{i,h}^{n+\frac{1}{2}}, \nabla v_h\right) + \left(q_i C_{i,h}^{n+\frac{1}{2}} \nabla \Phi_h^{n+\frac{1}{2}}, \nabla v_h\right) = (F_i^{n+\frac{1}{2}}, v_h), \quad (4.7)$$

$$\left(\nabla \Phi_h^{n+\frac{1}{2}}, \nabla \phi_h\right) - \sum_{i=1}^{2} q_i \left(C_{i,h}^{n+\frac{1}{2}}, \phi_h\right) = (F_3^{n+\frac{1}{2}}, \phi_h). \quad (4.8)$$

The wellposedness of (4.7)-(4.8) can be proved by the approach given in [Prohl and Schmuck (2009)].

Finally, we use the Picard's linearization for the nonlinear term in (4.7) and obtain the following practical numerical algorithm:

Algorithm 4.1. *1. Initialization for time marching: Set time step $n = 0$, and take the initial value $(C^0_{1,h}, C^0_{2,h}, \Phi^0_h) \in [S_h]^3$.*

2. Initialization for nonlinear iteration: Let $\left(C^{n+1,0}_{1,h}, C^{n+1,0}_{2,h}, \Phi^{n+1,0}_h\right)$ take the value of $\left(C^n_{1,h}, C^n_{2,h}, \Phi^n_h\right)$ when $n \geq 0$.

3. Finite element computation on each nonlinear iteration: For $l \geq 0$, compute $\left(C^{n+1,l+1}_{1,h}, C^{n+1,l+1}_{2,h}, \Phi^{n+1,l+1}_h\right) \in [S_h]^3$, such that for all $(v_{1,h}, v_{2,h}, \phi_h) \in [S_h]^3$ and for $i = 1, 2$,

$$\left(\frac{1}{\Delta t}\left(C^{n+1,l+1}_{i,h} - C^n_{i,h}\right), v_h\right) + \left(\nabla C^{n+\frac{1}{2},l+1}_{i,h}, \nabla v_h\right) + \left(q_i C^{n+\frac{1}{2},l+1}_{i,h} \nabla \Phi^{n+\frac{1}{2},l}_h, \nabla v_h\right) = \left(F^{n+\frac{1}{2}}_i, v_h\right),$$

$$\left(\nabla \Phi^{n+\frac{1}{2},l+1}_h, \nabla \phi_h\right) - \sum_{i=1}^{2} q_i \left(C^{n+\frac{1}{2},l+1}_{i,h}, \phi_h\right) = \left(F^{n+\frac{1}{2}}_3, \phi_h\right).$$

4. Checking the stopping criteria for nonlinear iteration: For a fixed tolerance ε, stop the iteration if

$$\sum_{i=1}^{2} \|C^{n+1,l+1}_{i,h} - C^{n+1,l}_{i,h}\|_{L^2} + \|\Phi^{n+1,l+1}_h - \Phi^{n+1,l}_h\|_{L^2} \leq \varepsilon,$$

and set $\left(C^{n+1}_{1,h}, C^{n+1}_{2,h}, \Phi^{n+1}_h\right) = \left(C^{n+1,l+1}_{1,h}, C^{n+1,l+1}_{2,h}, \Phi^{n+1,l+1}_h\right)$. Otherwise, set $l \leftarrow l+1$ and go to Step 3 to continue the nonlinear iteration.

5. Time marching: Stop if $n+1 = N$. Otherwise set $n \leftarrow n+1$ and go to Step 2.

4.2.4 Error analysis for the semi-discretization

In this section, we give a priori error estimates for the semi - discrete solution $(C_{1,h}, C_{2,h}, \Phi_h)$. For the sake of simplicity, we sometimes drop the time dependence in $C_i(t)$, $C_{i,h}(t)$, $\Phi(t)$ and $\Phi_h(t)$ in the following sections. Denote M as a generic constant throughout this section.

First of all, we assume the following regularity properties hold for C_i $(i = 1, 2)$, and Φ in the semi-discretization analysis:

$$C_i \in W^{1,\infty}(0, T; H^{k+1} \cap W^{1,\infty}(\Omega)) \text{ and } \Phi \in W^{1,\infty}(0, T; W^{k+1,\infty}(\Omega)). \tag{4.9}$$

For any $\tau \in [0, T]$, let $\tilde{\Phi} \in S_h$ be the H^1 projection of $\Phi(\tau)$ satisfy

$$(\nabla(\Phi(\tau) - \tilde{\Phi}(\tau)), \nabla\phi_h) = 0, \forall \phi_h \in S_h. \tag{4.10}$$

We first recall the standard error estimates of the above H^1 projection in various norms [Ciarlet (1978); Wheeler (1973)], as shown in the following lemma.

Lemma 4.1. *Let (C_1, C_2, Φ) be the solution of (4.3)-(4.4) satisfying the regularity assumptions (4.9), and $(C_{1,h}, C_{2,h}, \Phi_h)$ be the solution of (4.5)-(4.6). Let $\tilde{\Phi}(\tau)$ be defined in (4.10), then for $\tau \in (0, T]$, we have the following error estimates:*

$$\begin{aligned} h\|\partial_t \nabla \left(\Phi(\tau) - \tilde{\Phi}(\tau)\right)\|_{L^2} + \|\partial_t(\Phi(\tau) - \tilde{\Phi}(\tau))\|_{L^2} + h\|\nabla \left(\Phi(\tau) - \tilde{\Phi}(\tau)\right)\|_{L^2} \\ + \|\Phi(\tau) - \tilde{\Phi}(\tau)\|_{L^2} \leq M h^{k+1} \left(\|\Phi(\tau)\|_{H^{k+1}} + \|\partial_t \Phi(\tau)\|_{H^{k+1}}\right), \end{aligned} \tag{4.11}$$

and

$$\begin{aligned} \|\nabla(\Phi(\tau) - \tilde{\Phi}(\tau))\|_{L^\infty} + \|\partial_t \nabla(\Phi(\tau) - \tilde{\Phi}(\tau))\|_{L^\infty} \\ \leq M h^k \left(\|\Phi(\tau)\|_{W^{k+1,\infty}} + \|\partial_t \Phi(\tau)\|_{W^{k+1,\infty}}\right). \end{aligned} \tag{4.12}$$

In the following lemma, we prove the error estimates of $\tilde{\Phi} - \Phi_h$ and $\partial_t \left(\tilde{\Phi} - \Phi_h\right)$.

Lemma 4.2. *Let (C_1, C_2, Φ) be the solution to (4.3)-(4.4), $(C_{1,h}, C_{2,h}, \Phi_h)$ be the solution to (4.5)-(4.6), and $\tilde{\Phi}$ be defined by (4.10). Then for $\tau \in (0, T]$,*

$$\|\tilde{\Phi}(\tau) - \Phi_h(\tau)\|_{L^2} + \|\nabla \left(\tilde{\Phi}(\tau) - \Phi_h(\tau)\right)\|_{L^2} \leq M \sum_{i=1}^{2} \|C_i(\tau) - C_{i,h}(\tau)\|_{L^2}, \quad (4.13)$$

and

$$\|\partial_t \left(\tilde{\Phi}(\tau) - \Phi_h(\tau)\right)\|_{L^2} + \|\partial_t \nabla \left(\tilde{\Phi}(\tau) - \Phi_h(\tau)\right)\|_{L^2} \leq M \sum_{i=1}^{2} \|\partial_t \left(C_i(\tau) - C_{i,h}(\tau)\right)\|_{L^2}. \quad (4.14)$$

Proof. Subtract (4.6) from (4.4), use (4.10), and let $\phi_h = \tilde{\Phi} - \Phi_h$, we have for $\tau \in (0, T]$,

$$(\nabla(\tilde{\Phi} - \Phi_h), \nabla(\tilde{\Phi} - \Phi_h)) - \sum_{i=1}^{2} q_i(C_i - C_{i,h}, \tilde{\Phi} - \Phi_h) = 0.$$

By Poincaré inequality,

$$\|\nabla(\tilde{\Phi} - \Phi_h)\|_{L^2}^2 \leq \sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2} \|\tilde{\Phi} - \Phi_h\|_{L^2}$$
$$\leq \tilde{M} \sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2} \|\nabla(\tilde{\Phi} - \Phi_h)\|_{L^2},$$

where $\tilde{M}$ is a constant depending on the size of the domain Ω. Hence, we get

$$\|\nabla \left(\tilde{\Phi} - \Phi_h\right)\|_{L^2} \leq M \sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2}.$$

Use the standard approach of Aubin-Nitsche duality argument for nonlinear elliptic equation [Douglas and Dupont (1975); Liu et al. (1996); Hlavacek et al. (1994); Harrell and Layton (24); Abdulle and Vilmart (2012)], we can get the the L^2 norm error estimate as follows,

$$\|\tilde{\Phi} - \Phi_h\|_{L^2} \leq Mh\|\nabla\left(\tilde{\Phi} - \Phi_h\right)\|_{L^2} + \sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2}.$$

Thus we get (4.13).

Differentiating (4.6) and (4.10) with respect to time, and following the similar process we can obtain the L^2 and H^1 error estimate of $\partial_t(\tilde{\Phi} - \Phi_h)$. Thus we get (4.14). □

By (4.11), (4.13), (4.14) and Poincaré inequality, we can easily get the error estimates of $\Phi - \Phi_h$ and $\partial_t(\Phi - \Phi_h)$ in L^2 and H^1 norms, as shown in the following lemma.

Lemma 4.3. *Let (C_1, C_2, Φ) be the solution of (4.3)-(4.4) satisfing the regularity assumptions (4.9) and $(C_{1,h}, C_{2,h}, \Phi_h)$ be the solution of (4.5)-(4.6). Then for $\tau \in (0, T]$, we now have the following error estimates:*

$$\|\Phi(\tau) - \Phi_h(\tau)\|_{L^2} \leq Mh^{k+1}\|\Phi(\tau)\|_{H^{k+1}} + M\sum_{i=1}^{2} \|C_i(\tau) - C_{i,h}(\tau)\|_{L^2}, \tag{4.15}$$

$$\|\nabla(\Phi(\tau) - \Phi_h(\tau))\|_{L^2} \leq Mh^{k}\|\Phi(\tau)\|_{H^{k+1}} + M\sum_{i=1}^{2} \|C_i(\tau) - C_{i,h}(\tau)\|_{L^2}, \tag{4.16}$$

$$\begin{aligned}\|\partial_t(\Phi(\tau) - \Phi_h(\tau))\|_{L^2} \leq{}& Mh^{k+1}\left(\|\Phi(\tau)\|_{H^{k+1}} + \|\partial_t\Phi(\tau)\|_{H^{k+1}}\right) \\ &+ M\sum_{i=1}^{2}\left(\|C_i(\tau) - C_{i,h}(\tau)\|_{L^2} + \|\partial_t(C_i(\tau) - C_{i,h}(\tau))\|_{L^2}\right),\end{aligned} \tag{4.17}$$

and

$$\begin{aligned}\|\partial_t\nabla(\Phi(\tau) - \Phi_h(\tau))\|_{L^2} \leq{}& Mh^{k}\left(\|\Phi(\tau)\|_{H^{k+1}} + \|\partial_t\Phi(\tau)\|_{H^{k+1}}\right) \\ &+ M\sum_{i=1}^{2}\left(\|C_i(\tau) - C_{i,h}(\tau)\|_{L^2} + \|\partial_t(C_i(\tau) - C_{i,h}(\tau))\|_{L^2}\right).\end{aligned} \tag{4.18}$$

Next we move our focus to C_i and introduce its H^1 projection. Define the finite element solution $\tilde{C}_i \in S_h$ to satisfy the following variational problem at any given time $\tau \in [0, T]$ as

$$\left(\nabla\left(C_i(\tau) - \tilde{C}_i(\tau)\right), \nabla v_h\right) + q_i\left(\left(C_i(\tau) - \tilde{C}_i(\tau)\right)\nabla\Phi(\tau), \nabla v_h\right) = 0, \forall v_h \in S_h \quad (4.19)$$

The well-posedness of (4.19) can be proved by a similar approach for (4.7) [Prohl and Schmuck (2009)], which shall be even simpler since (4.19) is linear with respect to $\tilde{C}_i$.

Now we consider the error estimates of $C_i - \tilde{C}_i$ in L^2 and H^1 norms.

Lemma 4.4. *Let (C_1, C_2, Φ) be the solution of (4.3)-(4.4) satisfing the regularity assumptions (4.9), and $\tilde{C}_i$ defined in (4.19). We have the following error estimates for $\tau \in [0, T]$:*

$$\|C_i(\tau) - \tilde{C}_i(\tau)\|_{L^2} + h\|\nabla\left(C_i(\tau) - \tilde{C}_i(\tau)\right)\|_{L^2} \leq Mh^{k+1}\|C_i(\tau)\|_{H^{k+1}}, \quad (4.20)$$

and further,

$$\|\partial_t\left(C_i(\tau) - \tilde{C}_i(\tau)\right)\|_{L^2} + h\|\partial_t\nabla\left(C_i(\tau) - \tilde{C}_i(\tau)\right)\|_{L^2} \leq Mh^{k+1}\left(\|C_i(\tau)\|_{H^{k+1}} + \|\partial_t C_i(\tau)\|_{H^{k+1}}\right). \quad (4.21)$$

Proof. Let $\Pi_h C_i \in S_h$ be the finite element nodal interpolation of C_i, use (4.19) we get

$$\left(\nabla\left(C_i - \tilde{C}_i\right), \nabla\left(C_i - \tilde{C}_i\right)\right) + q_i\left(\left(C_i - \tilde{C}_i\right)\nabla\Phi, \nabla\left(C_i - \tilde{C}_i\right)\right)$$
$$= \left(\nabla\left(C_i - \tilde{C}_i\right), \nabla\left(C_i - \Pi_h C_i\right)\right) + q_i\left(\left(C_i - \tilde{C}_i\right)\nabla\Phi, \nabla\left(C_i - \Pi_h C_i\right)\right). \quad (4.22)$$

Use Cauchy-Schwarz inequality and Young's inequality,

$$\begin{aligned}
\|\nabla(C_i - \tilde{C}_i)\|_{L^2}^2 &\leq \|\nabla(C_i - \tilde{C}_i)\|_{L^2}\|\nabla(C_i - \Pi_h C_i)\|_{L^2} \\
&\quad +\|\nabla\Phi\|_{L^\infty}\|\nabla(C_i - \Pi_h C_i)\|_{L^2}\|C_i - \tilde{C}_i\|_{L^2} \\
&\quad +\|\nabla\Phi\|_{L^\infty}\|\nabla(C_i - \tilde{C}_i)\|_{L^2}\|C_i - \tilde{C}_i\|_{L^2} \\
&\leq \left(\frac{1}{4\epsilon} + \frac{1}{2}\right)\left(\|\nabla(C_i - \Pi_h C_i)\|_{L^2}^2 + \|\nabla\Phi\|_{L^\infty}^2\|C_i - \tilde{C}_i\|_{L^2}^2\right) \\
&\quad +2\epsilon\|\nabla(C_i - \tilde{C}_i)\|_{L^2}^2,
\end{aligned}$$

hence

$$\begin{aligned}
\|\nabla(C_i - \tilde{C}_i)\|_{L^2} &\leq M\left(\|\nabla(C_i - \Pi_h C_i)\|_{L^2} + \|C_i - \tilde{C}_i\|_{L^2}\right) \qquad (4.23)\\
&\leq M\left(h^k\|C_i\|_{H^{k+1}} + \|C_i - \tilde{C}_i\|_{L^2}\right).
\end{aligned}$$

The last inequality comes from the interpolation error estimate in H^1 norm [Ciarlet (1978)].

Now we shall use Aubin-Nitsche duality argument to obtain the L^2 error estimate of $C_i - \tilde{C}_i$. We define the adjoint problem of (4.19) as below,

$$\begin{cases}
-\Delta u_i + q_i\nabla\Phi\cdot\nabla u_i &= C_i - \tilde{C}_i, \text{in } \Omega \\
u_i &= 0, \text{ on } \partial\Omega.
\end{cases}$$

By the regularity theory of partial differential equations [Evans (2010)], it is well known that $\|u_i\|_{H^2} \leq M\|C_i - \tilde{C}_i\|_{L^2}$ for $\Phi(\tau) \in W^{1,\infty}(\Omega)$.

Let $\Pi_h u_i \in S_h$ be the finite element nodal interpolation of u_i, and use (4.19), Cauchy-Schwartz inequality and Poincaré inequality, we have

$$\begin{aligned}
\|C_i - \tilde{C}_i\|_{L^2}^2 &= (\nabla(C_i - \tilde{C}_i), \nabla u_i) + q_i(C_i - \tilde{C}_i, \nabla\Phi\cdot\nabla u_i) \\
&= (\nabla(C_i - \tilde{C}_i), \nabla(u_i - \Pi_h u_i)) + (\nabla(C_i - \tilde{C}_i), \nabla\Pi_h u_i)
\end{aligned}$$

$$
\begin{aligned}
& +q_i(C_i - \tilde{C}_i, \nabla\Phi \cdot \nabla(u_i - \Pi_h u_i)) + q_i(C_i - \tilde{C}_i, \nabla\Phi \cdot \nabla\Pi_h u_i) \\
= \;& (\nabla(C_i - \tilde{C}_i), \nabla(u_i - \Pi_h u_i)) + q_i(C_i - \tilde{C}_i, \nabla\Phi \cdot \nabla(u_i - \Pi_h u_i)) \\
\leq \;& \|\nabla(C_i - \tilde{C}_i)\|_{L^2} \|\nabla(u_i - \Pi_h u_i)\|_{L^2} \\
& +\tilde{M}\|\nabla\Phi\|_{L^\infty} \|\nabla(C_i - \tilde{C}_i)\|_{L^2} \|\nabla(u_i - \Pi_h u_i)\|_{L^2} \\
\leq \;& Mh\|\nabla(C_i - \tilde{C}_i)\|_{L^2} \|u_i\|_{H^2} \\
\leq \;& Mh\|\nabla(C_i - \tilde{C}_i)\|_{L^2} \|C_i - \tilde{C}_i\|_{L^2},
\end{aligned}
$$

where $\tilde{M}$ is the Poincaré constant. Therefore,

$$
\|C_i - \tilde{C}_i\|_{L^2} \leq Mh\|\nabla(C_i - \tilde{C}_i)\|_{L^2}.
$$

Thus when h is sufficiently small, use (4.23), we get (4.20).

Take derivative with respect to t in (4.19), and similar to (4.22), for any $v_h \in S_h$, we have,

$$
\begin{aligned}
& (\partial_t \nabla(C_i - \tilde{C}_i), \partial_t \nabla(C_i - \tilde{C}_i)) + q_i(\partial_t((C_i - \tilde{C}_i)\nabla\Phi), \partial_t \nabla(C_i - \tilde{C}_i)) \\
& \quad = (\partial_t \nabla(C_i - \tilde{C}_i), \partial_t \nabla(C_i - \Pi_h C_i)) + q_i(\partial_t((C_i - \tilde{C}_i)\nabla\Phi), \partial_t \nabla(C_i - \Pi_h C_i))
\end{aligned}
$$

Therefore, by Poincaré inequality and Young's inequality,

$$
\begin{aligned}
\|\partial_t \nabla(C_i - \tilde{C}_i)\|_{L^2}^2 \;\leq\; & \frac{1}{4\epsilon}\|\nabla\Phi\|_{L^\infty}^2 \|\partial_t(C_i - \tilde{C}_i)\|_{L^2}^2 + \epsilon\|\partial_t \nabla(C_i - \tilde{C}_i)\|_{L^2}^2 \\
+ \;& \frac{1}{4\epsilon}\|\partial_t \nabla\Phi\|_{L^\infty}^2 \|C_i - \tilde{C}_i\|_{L^2}^2 + \epsilon\|\partial_t \nabla(C_i - \tilde{C}_i)\|_{L^2}^2 \\
+ \;& \frac{1}{4\epsilon}\|\partial_t \nabla(C_i - \Pi_h C_i)\|_{L^2}^2 + \epsilon\|\partial_t \nabla(C_i - \tilde{C}_i)\|_{L^2}^2 \\
+ \;& \frac{1}{2}\|\nabla\Phi\|_{L^\infty}^2 \|\partial_t(C_i - \tilde{C}_i)\|_{L^2}^2 + \frac{1}{2}\|\partial_t \nabla(C_i - \Pi_h C_i)\|_{L^2}^2 \\
+ \;& \frac{1}{2}\|\partial_t \nabla\Phi\|_{L^\infty}^2 \|C_i - \tilde{C}_i\|_{L^2}^2 + \frac{1}{2}\|\partial_t \nabla(C_i - \Pi_h C_i)\|_{L^2}^2.
\end{aligned}
$$

Since ϵ is arbitrary small, and $\Phi \in W^{1,\infty}(0,T;W^{k+1,\infty}(\Omega))$, we can get

$$\|\partial_t \nabla (C_i - \tilde{C}_i)\|_{L^2} \leq M \left(\|C_i - \tilde{C}_i\|_{L^2} + \|\partial_t \nabla (C_i - \Pi_h C_i)\|_{L^2} + \|\partial_t (C_i - \tilde{C}_i)\|_{L^2} \right).$$

Use (4.20) and the interpolation error estimate [Ciarlet (1978)], we have

$$\|\partial_t \nabla (C_i - \tilde{C}_i)\|_{L^2} \leq M \left(h^k \left(\|C_i\|_{H^{k+1}} + \|\partial_t C_i\|_{H^{k+1}} \right) + \|\partial_t (C_i - \tilde{C}_i)\|_{L^2} \right).$$

Again, by a simiar Aubin-Nitsche duality argument, we can obtain (4.21). □

For the maximum norm error estimates of $C_i - \tilde{C}_i$, we give the following lemma. The proof can be done using a similar fashion as Lemma 4.4 and some classic results of the error estimate in maximum norm given in [Brenner and Scott (2002); Ciarlet (1978); Wheeler (1973)].

Lemma 4.5. *Let (C_1, C_2, Φ) be the solution of (4.3)-(4.4) satisfing the regularity assumptions (4.9), and $(C_{1,h}, C_{2,h}, \Phi_h)$ be the solution of (4.5)-(4.6). Let $\tilde{C}_i(\tau)$ be defined in (4.19), then for $\tau \in (0,T]$, we have the following error estimates:*

$$\begin{aligned} &\|C_i(\tau) - \tilde{C}_i(\tau)\|_{L^\infty} + \|\partial_t \left(C_i(\tau) - \tilde{C}_i(\tau) \right) \|_{L^\infty} \\ &\qquad \leq \begin{cases} M h^{k+1-\frac{d}{2}} |\log h| \left(\|C_i(\tau)\|_{H^{k+1}} + \|\partial_t C_i(\tau)\|_{H^{k+1}} \right), & \textit{when } k = 1, \\ M h^{k+1-\frac{d}{2}} \left(\|C_i(\tau)\|_{H^{k+1}} + \|\partial_t C_i(\tau)\|_{H^{k+1}} \right), & \textit{when } k > 1. \end{cases} \end{aligned} \tag{4.24}$$

Finally, we give a priori error estimate for $C_i - C_{i,h}$ and $\Phi - \Phi_h$ in $L^\infty(L^2)$ and $L^\infty(H^1)$ norms in the following theorem.

Theorem 4.1. *Let (C_1, C_2, Φ) be the solution of (4.3) and (4.4) satisfying the regularity assumptions (4.9) and $(C_{1,h}, C_{2,h}, \Phi_h)$ be the solution of (4.5) and (4.6). Then* *when $k \geq d-1$, we have a priori error estimates for $\tau \in (0,T]$,*

$$\|C_i(\tau) - C_{i,h}(\tau)\|_{L^\infty(L^2)} + \|\nabla(C_i(\tau) - C_{i,h}(\tau))\|_{L^\infty(L^2)}$$
$$+ \|\Phi(\tau) - \Phi_h(\tau)\|_{L^\infty(L^2)} + \|\nabla(\Phi(\tau) - \Phi_h(\tau))\|_{L^\infty(L^2)} \leq Mh^k, \quad (4.25)$$

where $i = 1,2$ and M is a constant depending only on the regularities of C_i and Φ.

Proof. Subtract (4.5) from (4.3), and use the Galerkin orthogonality (4.19), we have

$$(\partial_t(C_i - C_{i,h}), v_h) + (\nabla(\tilde{C}_i - C_{i,h}), \nabla v_h) + q_i(\tilde{C}_i \nabla\Phi - C_{i,h}\nabla\Phi_h, \nabla v_h) = 0, \forall v_h \in S_h.$$

Hence,

$$(\partial_t(\tilde{C}_i - C_{i,h}), v_h) + (\nabla(\tilde{C}_i - C_{i,h}), \nabla v_h) = -(\partial_t(C_i - \tilde{C}_i), v_h) - q_i((\tilde{C}_i - C_{i,h})\nabla\Phi, \nabla v_h)$$
$$+ q_i((C_i - C_{i,h})\nabla(\Phi - \Phi_h), \nabla v_h) - q_i(C_i\nabla(\Phi - \Phi_h), \nabla v_h). \quad (4.26)$$

Let $\eta_i = C_i - \tilde{C}_i$ and $\xi_i = \tilde{C}_i - C_{i,h}$, choose $v_h = \xi_i \in S_h$, we can write (4.26) as

$$(\partial_t \xi_i, \xi_i) + (\nabla\xi_i, \nabla\xi_i) = \sum_{i=1}^{4} H_i, \quad (4.27)$$

where H_i, $i = 1,2,3,4$, are defined as

$$H_1 := -(\partial_t \eta_i, \xi_i),$$
$$H_2 := -q_i(\xi_i \nabla\Phi, \nabla\xi_i),$$
$$H_3 := q_i((C_i - C_{i,h})\nabla(\Phi - \Phi_h), \nabla\xi_i),$$
$$H_4 := -q_i(C_i\nabla(\Phi - \Phi_h), \nabla\xi_i).$$

In the following, we shall estimate H_1, H_2, H_3, and H_4, respectively.

$$\begin{aligned}
H_1 &\leq \|\partial_t \eta_i\|_{L^2}\|\xi_i\|_{L^2} \leq M h^{k+1}\|\xi_i\|_{L^2} \leq \frac{M}{2}h^{2k+2} + \frac{1}{2}\|\xi_i\|_{L^2}^2, && \text{(by (4.21))}\\
H_2 &\leq \|\nabla\Phi\|_{L^\infty}\|\xi_i\|_{L^2}\|\nabla\xi_i\|_{L^2} \leq \frac{1}{4\epsilon}\|\nabla\Phi\|_{L^\infty}^2\|\xi_i\|_{L^2}^2 + \epsilon\|\nabla\xi_i\|_{L^2}^2, &&\\
H_4 &\leq \|C_i\|_{L^\infty}\|\nabla(\Phi-\Phi_h)\|_{L^2}\|\nabla\xi_i\|_{L^2} &&\\
&\leq \|C_i\|_{L^\infty}\left(Mh^k\|\Phi\|_{H^{k+1}} + \sum_{i=1}^{2}\|C_i - C_{i,h}\|_{L^2}\right)\|\nabla\xi_i\|_{L^2} && \text{(by (4.16))}\\
&\leq Mh^k\|\nabla\xi_i\|_{L^2} + M\sum_{i=1}^{2}\|\xi_i\|_{L^2}^2 + 2\epsilon\|\nabla\xi_i\|_{L^2}^2. && \text{(by (4.20))}\\
H_3 &\leq q_i(\eta_i\nabla(\Phi-\Phi_h),\nabla\xi_i) + q_i(\xi_i\nabla(\Phi-\Phi_h),\nabla\xi_i) &&\\
&\leq M\|\eta_i\|_{L^2}(\|\nabla(\Phi-\tilde{\Phi})\|_{L^\infty} + \|\nabla(\tilde{\Phi}-\Phi_h)\|_{L^\infty})\|\nabla\xi_i\|_{L^2} &&\\
&\quad + M\|\xi_i\|_{L^2}(\|\nabla(\Phi-\tilde{\Phi})\|_{L^\infty} + \|\nabla(\tilde{\Phi}-\Phi_h)\|_{L^\infty})\|\nabla\xi_i\|_{L^2} &&\\
&\leq M\left(h^{2k+1}\|\nabla\xi_i\|_{L^2} + h^k\|\xi_i\|_{L^2}\|\nabla\xi_i\|_{L^2}\right) &&\\
&\quad + M\left(h^{k+1} + \|\xi_i\|_{L^2}\right)\|\nabla(\tilde{\Phi}-\Phi_h)\|_{L^\infty}\|\nabla\xi_i\|_{L^2}. && \text{(by (4.12),(4.20))}
\end{aligned}$$

By inverse inequality and (4.13), we have

$$\begin{aligned}
&\|\nabla(\tilde{\Phi}-\Phi_h)\|_{L^\infty} \leq Mh^{-\frac{d}{2}}\|\nabla(\tilde{\Phi}-\Phi_h)\|_{L^2}\\
\leq\; & Mh^{-\frac{d}{2}}\sum_{j=1}^{2}\|C_j - C_{j,h}\|_{L^2} \leq Mh^{-\frac{d}{2}}\sum_{j=1}^{2}\left(\|\xi_j\|_{L^2} + \|\eta_j\|_{L^2}\right),
\end{aligned}$$

also by (4.12) and (4.20),

$$\begin{aligned}
H_3 &\leq M\left(h^{2k+1}\|\nabla\xi_i\|_{L^2} + h^k\|\xi_i\|_{L^2}\|\nabla\xi_i\|_{L^2}\right)\\
&\quad + M\left(h^k + h^{-\frac{d}{2}}\|\xi_i\|_{L^2}\right)\sum_{j=1}^{2}\left(\|\xi_j\|_{L^2} + \|\eta_j\|_{L^2}\right)\|\nabla\xi_i\|_{L^2}\\
&\leq Mh^{2k+1}\|\nabla\xi_i\|_{L^2} + Mh^{k+1-\frac{d}{2}}\sum_{j=1}^{2}\|\xi_j\|_{L^2}\|\nabla\xi_i\|_{L^2}\\
&\quad + Mh^{-\frac{d}{2}}\|\xi_i\|_{L^2}\sum_{j=1}^{2}\|\xi_j\|_{L^2}\|\nabla\xi_i\|_{L^2}.
\end{aligned}$$

Now we conduct a mathematical induction process and propose the following induction hypothesis

$$h^{-\frac{d}{2}}\|\xi_i(t)\|_{L^2} \le M, \forall t \in [0,T]. \tag{4.28}$$

By the initial conditions and (4.20), we have

$$h^{-\frac{d}{2}}\|\xi_i(0)\|_{L^2} \le h^{-\frac{d}{2}}\|C_i(0) - C_{i,h}(0)\|_{L^2} + h^{-\frac{d}{2}}\|\eta_i(0)\|_{L^2}$$

$$\le Mh^{k+1-\frac{d}{2}}\|C_i(0)\|_{H^{k+1}} \le M. \tag{4.29}$$

Assume that (4.28) holds for any $t \in [0, T^*]$, $T^* < T$. Use Young's inequality, we have

$$H_3 \le M\left(h^{4k+2} + \sum_{j=1}^{2}\|\xi_j\|_{L^2}^2 + \epsilon\|\nabla\xi_i\|_{L^2}^2\right).$$

Hence (4.27) reads,

$$\frac{1}{2}\partial_t\|\xi_i\|_{L^2}^2 + \|\nabla\xi_i\|_{L^2}^2 \le M\left(h^{4k+2} + h^{2k+2} + h^{2k} + \sum_{j=1}^{2}\|\xi_j\|_{L^2}^2 + \epsilon\|\nabla\xi_i\|_{L^2}^2\right).$$

Take integral with respect to t,

$$\|\xi_i\|_{L^2}^2 + \int_0^t \|\nabla\xi_i\|_{L^2}^2 \le M\left(h^{2k} + \sum_{j=1}^{2}\int_0^t \|\xi_j\|_{L^2}^2\right),$$

therefore,

$$\sum_{i=1}^{2}\left(\|\xi_i\|_{L^2}^2 + \int_0^t \|\nabla\xi_i\|_{L^2}^2\right) \le M\left(h^{2k} + \sum_{j=1}^{2}\int_0^t \|\xi_j\|_{L^2}^2\right),$$

then use Grönwall's inequality, we have for $0 \le t \le T^*$,

$$\sum_{i=1}^{2}\left(\|\xi_i\|_{L^\infty(L^2)} + \|\nabla\xi_i\|_{L^2(L^2)}\right) \le Mh^k,$$

thus for $i = 1, 2$,

$$\|\xi_i\|_{L^\infty(L^2)} + \|\nabla\xi_i\|_{L^2(L^2)} \le Mh^k. \tag{4.30}$$

This implies that for $k \geq d-1$,

$$h^{-\frac{d}{2}}\|\xi_i\|_{L^2} \leq Mh^{k-\frac{d}{2}} \leq M.$$

On the other hand, since $h^{-\frac{d}{2}}\|\xi_i\|_{L^2}$ is a continuous function with respect to $t \in [0,T]$, thus due to the uniform continuity with time, there exists δ such that for any $t \in [0, T^* + \delta]$, we have $h^{-\frac{d}{2}}\|\xi_i\|_{L^2} \leq M$. Because $[0,T]$ is a finite interval, so the induction hypothesis (4.28) holds true for all $t \in [0,T]$.

Therefore, for any $t \in [0,T]$,

$$\|C_i - C_{i,h}\|_{L^\infty(L^2)} + \|\nabla(C_i - C_{i,h})\|_{L^2(L^2)} \leq Mh^k. \tag{4.31}$$

Use (4.31) in (4.15) and (4.16), we can get

$$\|\Phi - \Phi_h\|_{L^\infty(L^2)} + \|\nabla(\Phi - \Phi_h)\|_{L^\infty(L^2)} \leq Mh^k. \tag{4.32}$$

Lastly, we use a similar approach as above to obtain the error estimate $\|\nabla(C_i - C_{i,h})\|_{L^\infty(L^2)}$. Choose $v_h = \partial_t \xi_i \in S_h$ in (4.26), thus

$$(\nabla\xi_i, \partial_t \nabla\xi_i) + (\partial_t\xi_i, \partial_t\xi_i) = \sum_{i=1}^{4} \hat{H}_i \tag{4.33}$$

where $\hat{H}_i$, $i = 1,2,3,4$, are defined as

$$\begin{aligned}
\hat{H}_1 &:= -(\partial_t\eta_i, \partial_t\xi_i), \\
\hat{H}_2 &:= -q_i((\tilde{C}_i - C_{i,h})\nabla\Phi, \partial_t\nabla\xi_i), \\
\hat{H}_3 &:= q_i((C_i - C_{i,h})\nabla(\Phi - \Phi_h), \partial_t\nabla\xi_i), \\
\hat{H}_4 &:= -q_i(C_i\nabla(\Phi - \Phi_h), \partial_t\nabla\xi_i).
\end{aligned}$$

We estimate $\hat{H}_i$ respectively below:

$$
\begin{aligned}
\hat{H}_1 &\le \|\partial_t \eta_i\|_{L^2}\|\partial_t \xi_i\|_{L^2} \le M\left(h^{2k+2} + \epsilon\|\partial_t\xi_i\|_{L^2}^2\right), && \text{(by (4.21))}\\
\hat{H}_2 &= q_i\left(\partial_t\xi_i\nabla\Phi, \nabla\left(\tilde{C}_i - C_{i,h}\right)\right) + q_i\left(\left(\tilde{C}_i - C_{i,h}\right)\partial_t\nabla\Phi, \nabla\xi_i\right) - q_i\partial_t\left(\xi_i\nabla\Phi,\nabla\xi_i\right)\\
&\le \|\nabla\Phi\|_{L^\infty}\|\partial_t\xi_i\|_{L^2}\|\nabla\xi_i\|_{L^2} + \|\partial_t\nabla\Phi\|_{L^\infty}\|\xi_i\|_{L^2}\|\nabla\xi_i\|_{L^2} - q_i\partial_t\left(\xi_i\nabla\Phi,\nabla\xi_i\right)\\
&\le M\left(h^{2k} + \epsilon\|\partial_t\xi_i\|_{L^2}^2 + \|\nabla\xi_i\|_{L^2}^2\right) - q_i\partial_t\left(\xi_i\nabla\Phi,\nabla\xi_i\right), && \text{(by (4.30))}\\
\hat{H}_3 &= -\, q_i\left(\partial_t\left(C_i - C_{i,h}\right)\nabla\left(\Phi-\Phi_h\right), \nabla\xi_i\right) - q_i\left(\left(C_i - C_{i,h}\right)\partial_t\nabla\left(\Phi-\Phi_h\right),\nabla\xi_i\right)\\
&\quad + q_i\partial_t\left(\left(C_i - C_{i,h}\right)\nabla\left(\Phi-\Phi_h\right),\nabla\xi_i\right)\\
&\le \|\partial_t\left(C_i - C_{i,h}\right)\|_{L^2}\|\nabla\left(\Phi-\Phi_h\right)\|_{L^\infty}\|\nabla\xi_i\|_{L^2}\\
&\quad + \|C_i - C_{i,h}\|_{L^2}\|\partial_t\nabla(\Phi-\Phi_h)\|_{L^\infty}\|\nabla\xi_i\|_{L^2}\\
&\quad + q_i\partial_t\left(\left(C_i - C_{i,h}\right)\nabla\left(\Phi-\Phi_h\right),\nabla\xi_i\right)\\
&\le M\left(h^{2k} + \|\partial_t\xi_j\|_{L^2}^2 + \|\nabla\xi_i\|_{L^2}^2\right) + \ q_i\partial_t\left(\left(C_i - C_{i,h}\right)\nabla\left(\Phi-\Phi_h\right),\nabla\xi_i\right)\\
& && \text{(by (4.12), (4.14), (4.21), (4.28), (4.31))}\\
\hat{H}_4 &= q_i\left(\partial_t C_i\nabla\left(\Phi-\Phi_h\right),\nabla\xi_i\right) + q_i\left(C_i\partial_t\nabla\left(\Phi-\Phi_h\right),\nabla\xi_i\right)\\
&\quad - q_i\partial_t\left(C_i\nabla\left(\Phi-\Phi_h\right),\nabla\xi_i\right)\\
&\le \|\partial_t C_i\|_{L^\infty}\|\nabla(\Phi-\Phi_h)\|_{L^2}\|\nabla\xi_i\|_{L^2} + \|C_i\|_{L^\infty}\|\partial_t\nabla(\Phi-\Phi_h)\|_{L^2}\|\nabla\xi_i\|_{L^2}\\
&\quad - q_i\partial_t\left(C_i\nabla\left(\Phi-\Phi_h\right),\nabla\xi_i\right)\\
&\le M\left(h^{2k} + \epsilon\|\partial_t\xi_i\|_{L^2}^2 + \|\nabla\xi_i\|_{L^2}^2\right) - q_i\partial_t\left(C_i\nabla\left(\Phi-\Phi_h\right),\nabla\xi_i\right).\\
& && \text{(by (4.16), (4.18),(4.21), (4.25))}
\end{aligned}
$$

Thus (4.33) becomes

$$
\frac{1}{2}\frac{\partial}{\partial t}\|\nabla\xi_i\|_{L^2}^2 + \|\partial_t\xi_i\|_{L^2}^2 \le M\left(h^{2k} + \epsilon\|\partial_t\xi_i\|_{L^2}^2 + \|\nabla\xi_i\|_{L^2}^2\right) - q_i\partial_t(\xi_i\nabla\Phi,\nabla\xi_i)
$$

$$+ \; q_i\partial_t((C_i - C_{i,h})\nabla(\Phi - \Phi_h), \nabla\xi_i) - q_i\partial_t\left(C_i\nabla\left(\Phi - \Phi_h\right), \nabla\xi_i\right).$$

Since $C_i = C_{i,h}$ and $\Phi = \Phi_h$ when $t = 0$, take integral with respect to t, and use Grönwall's inequality, we have

$$\begin{aligned}
\|\nabla\xi_i\|_{L^2}^2 + \int_0^t \|\partial_t\xi_i\|_{L^2}^2 \;\; \leq \;\; & Mh^{2k} + \|\xi_i\|_{L^2}\|\nabla\Phi\|_{L^\infty}\|\nabla\xi_i\|_{L^2} \\
& + \|C_i - C_{i,h}\|_{L^2}\|\nabla(\Phi - \Phi_h)\|_{L^\infty}\|\nabla\xi_i\|_{L^2} \\
& + \|C_i\|_{L^\infty}\|\nabla(\Phi - \Phi_h)\|_{L^2}\|\nabla\xi_i\|_{L^2}.
\end{aligned}$$

Thus by (4.30), (4.25), (4.31) , and the error estimates of previous terms H_1, H_2, H_3 and H_4, we obtain

$$\|\nabla\xi_i\|_{L^2}^2 + \int_0^t \|\partial_t\xi_i\|_{L^2}^2 \leq M\left(h^{2k} + \epsilon\|\nabla\xi_i\|_{L^2}^2\right),$$

that is,

$$\|\nabla\xi_i\|_{L^\infty(L^2)} + \|\partial_t\xi_i\|_{L^2(L^2)} \leq Mh^k,$$

and

$$\|\nabla(C_i - C_{i,h})\|_{L^\infty(L^2)} + \|(C_i - C_{i,h})_t\|_{L^2(L^2)} \leq Mh^k. \tag{4.34}$$

Finally, together with (4.31), we get

$$\|C_i - C_{i,h}\|_{L^\infty(L^2)} + \|\nabla(C_i - C_{i,h})\|_{L^\infty(L^2)} \leq Mh^k, \tag{4.35}$$

then use (4.15) and (4.16), we get (4.25). □

Remark 4.1. Theorem 4.1 requires that $k \geq d - 1$ in order for the error estimates to hold. This is due to the inverse estimate and mathematical induction technique used in (4.28). Therefore, this restriction of the order of the estimate polynomial should only apply to C_i, $i = 1, 2$, but not Φ. In other words, when $d = 3$, it is sufficient to use second order finite element for C_i and linear finite element for Φ in order to get the results proved in Theorem 4.1.

Theorem 4.1 shows that for PNP system with convection terms in divergence form defined in (4.1) and (4.2), when $k \geq d - 1$, its finite element approximation based upon the weak formulation (4.3) and (4.4) has an optimal convergence rate in both $L^\infty(H^1)$ and $L^2(H^1)$ norms but a sub-optimal convergence rate in $L^\infty(L^2)$ norm. Alternatively, if we break the convection terms in divergence form into two parts, then the first part, $q_i \nabla C_i \cdot \nabla \Phi$, turns out to be a convection term in non-divergence form, and the second part, $q_i C_i \Delta \Phi$, can be further transformed using (4.2), inducing an equivalent governing equation of concentrations with convection terms in non-divergence form and an extra nonlinear term on the right hand side as follows

$$\partial_t C_i - \Delta C_i - q_i \nabla C_i \cdot \nabla \Phi = F_i - q_i C_i \left(C_1 - C_2 + F_3\right). \tag{4.36}$$

Thereafter, following an analogous analysis given in [Ewing and Wheeler (1980)] and the proof of Theorem 4.1, we are able to obtain the following convergence theorem for the above reformulated PNP.

Theorem 4.2. *Let* (C_1, C_2, Φ) *be the solution of (4.36) and (4.4) and* $(C_{1,h}, C_{2,h}, \Phi_h)$ *be the solution of the corresponding discretization equations. We define*

$$M_h = \{v \in H^1(\Omega) : v|_{\partial\Omega} = 0 \text{ and } v|_K \in P_r(K), \forall K \in \mathcal{T}_h\} \tag{4.37}$$

and

$$N_h = \{v \in H^1(\Omega) : v|_{\partial\Omega} = 0 \text{ and } v|_K \in P_s(K), \forall K \in \mathcal{T}_h\} \tag{4.38}$$

such that, for $i = 1, 2$, $\|C_i\|_{L^\infty(H^{r+1})}$, $\|\Phi\|_{L^\infty(H^{s+1})}$ *are bounded, also* $C_{i,h} \in M_h$ *and* $\Phi_h \in N_h$. *Then we have the following error estimates,*

$$\|\Phi - \Phi_h\|_{L^\infty(L^2)} + h\|\nabla(\Phi - \Phi_h)\|_{L^\infty(L^2)} + \|C_i - C_{i,h}\|_{L^\infty(L^2)} + h\|\nabla(C_i - C_{i,h})\|_{L^\infty(L^2)} \leq M\left(h^{s+1} + h^{r+1} + h^{s+r-1}\right), \quad (4.39)$$

where M *is a constant depending only on the regularity of* C_i *and* Φ.

Remark 4.2. Theorem 4.2 shows that, the optimal convergence rate for $C_i - C_{i,h}$ in both L^2 and H^1 norms could be reached if $s = 2$ and $r = 1$, or $s + r \geq 4$. The optimal convergence rate for $\Phi - \Phi_h$ in both L^2 and H^1 norms could be reached if $s = 1$ and $r = 2$, or $s + r \geq 4$.

Remark 4.3. (4.36) shows that, to achieve a fully optimal a priori error estimates given in Theorem 4.2, one has to force an extra nonlinear term into the right hand side of concentration equation, which is, however, not natural for PNP system from the physical background perspective, moreover, the original concentration equation is changed to be a more strongly nonlinear PDE, and may need an advanced linearization scheme and more nonlinear iterations in order to reach a convergent result, which is a tradeoff of such approach.

4.2.5 Error analysis for the full discretization

In this section we give the error estimate of the Galerkin procedure (4.7)-(4.8) in $L^\infty(H^1)$, $L^2(H^1)$ and $L^\infty(L^2)$ norms.

First we give regularity assumptions for C_i, $i = 1, 2$, and Φ in the full discretization analysis:

$$C_i \in W^{3,\infty}(0,T;H^{k+1}\cap W^{1,\infty}(\Omega)) \text{ and } \Phi \in W^{2,\infty}(0,T;W^{k+1,\infty}(\Omega)). \tag{4.40}$$

We also assume that for $i=1,2$,

$$F_i \in W^{2,\infty}(0,T;L^2(\Omega)).$$

Next, using the similar analysis for Lemma 4.3 and 4.4, we can prove the following results.

Lemma 4.6. *Let (C_1, C_2, Φ) be the solution of (4.3)-(4.4) satisfying the regularity assumptions (4.40), let $(C_{1,h}, C_{2,h}, \Phi_h)$ be the solution of (4.5)-(4.6) and let $\tilde{C}_i$ be defined in (4.19). For any $n = 0, 1, ..., N$, we have the following error estimates:*

$$\|\Phi^n - \Phi_h^n\|_{L^2} \leq Mh^{k+1} + M\sum_{i=1}^{2}\|C_i^n - C_{i,h}^n\|_{L^2}, \tag{4.41}$$

$$\|\nabla(\Phi^n - \Phi_h^n)\|_{L^2} \leq Mh^{k} + M\sum_{i=1}^{2}\|C_i^n - C_{i,h}^n\|_{L^2}, \tag{4.42}$$

and

$$\left\|\partial_t^\alpha\left(C_i^n - \tilde{C}_i^n\right)\right\|_{L^2} + h\left\|\partial_t^\alpha\nabla\left(C_i^n - \tilde{C}_i^n\right)\right\|_{L^2} \leq Mh^{k+1}, \tag{4.43}$$

where $\alpha = 0, 1, 2, 3$.

Theorem 4.3. *Let (C_1, C_2, Φ) be the solution of (4.3) and (4.4) satisfying the regularity assumptions (4.40), and $(C_{1,h}, C_{2,h}, \Phi_h)$ be the solution of (4.5) and (4.6). Then there exists a constant M depending only on the regularity of C_i and Φ, such that, when $k \geq d-1$, for $i = 1, 2$,*

$$\|C_i^N - C_{i,h}^N\|_{L^2} + \|\nabla(C_i^N - C_{i,h}^N)\|_{L^2} \leq M\left((\Delta t)^2 + h^k\right), \tag{4.44}$$

and

$$\|\Phi^N - \Phi_h^N\|_{L^2} + \|\nabla(\Phi^N - \Phi_h^N)\|_{L^2} \le M\left((\Delta t)^2 + h^k\right). \tag{4.45}$$

Proof. Let (4.3) and (4.19) take values at $t^{n+1/2}$, $0 \le n \le N-1$. For any $v \in H_0^1$, we get

$$\left(\partial_t C_i(t^{n+\frac{1}{2}}), v\right) + \left(\nabla \tilde{C}_i(t^{n+\frac{1}{2}}), \nabla v\right) + q_i\left(\tilde{C}_i(t^{n+\frac{1}{2}})\nabla\Phi(t^{n+\frac{1}{2}}), \nabla v\right) = \left(F_i(t^{n+\frac{1}{2}}), v\right). \tag{4.46}$$

Subtract (4.7) from (4.46), let $\xi_i^n = \tilde{C}_i^n - C_{i,h}^n$ and $\eta_i^n = C_i^n - \tilde{C}_i^n$, and choose $v_h = \xi_i^{n+\frac{1}{2}} \in S_h$, we have

$$\left(\partial_t C_i(t^{n+\frac{1}{2}}) - d_t C_{i,h}^n, \xi_i^{n+\frac{1}{2}}\right) + \left(\nabla \tilde{C}_i(t^{n+\frac{1}{2}}) - \nabla C_{i,h}^{n+\frac{1}{2}}, \nabla \xi_i^{n+\frac{1}{2}}\right) + q_i\left(\tilde{C}_i(t^{n+\frac{1}{2}})\nabla\Phi(t^{n+\frac{1}{2}}) - C_{i,h}^{n+\frac{1}{2}}\nabla\Phi_h^{n+\frac{1}{2}}, \nabla\xi_i^{n+\frac{1}{2}}\right) = \left(F_i(t^{n+\frac{1}{2}}) - F_i^{n+\frac{1}{2}}, \xi_i^{n+\frac{1}{2}}\right), \tag{4.47}$$

that is

$$\left(d_t\xi_i^n, \xi_i^{n+\frac{1}{2}}\right) + \left(\nabla\xi_i^{n+\frac{1}{2}}, \nabla\xi_i^{n+\frac{1}{2}}\right) = \sum_{k=1}^{7} G_k^n. \tag{4.48}$$

where

$$\begin{aligned}
G_1^n &:= -\left(\partial_t C_i(t^{n+\frac{1}{2}}) - d_t C_i^n, \xi_i^{n+\frac{1}{2}}\right) \\
G_2^n &:= -\left(d_t C_i^n - d_t \tilde{C}_i^n, \xi_i^{n+\frac{1}{2}}\right) \\
G_3^n &:= -\left(\nabla\left(\tilde{C}_i(t^{n+\frac{1}{2}}) - \tilde{C}_i^{n+\frac{1}{2}}\right), \nabla\xi_i^{n+\frac{1}{2}}\right) \\
G_4^n &:= -q_i\left(\tilde{C}_i(t^{n+\frac{1}{2}})\nabla\left(\Phi(t^{n+\frac{1}{2}}) - \Phi_h^{n+\frac{1}{2}}\right), \nabla\xi_i^{n+\frac{1}{2}}\right) \\
G_5^n &:= -q_i\left(\left(\tilde{C}_i(t^{n+\frac{1}{2}}) - \tilde{C}_i^{n+\frac{1}{2}}\right)\nabla\Phi_h^{n+\frac{1}{2}}, \nabla\xi_i^{n+\frac{1}{2}}\right) \\
G_6^n &:= -q_i\left(\xi_i^{n+\frac{1}{2}}\nabla\Phi_h^{n+\frac{1}{2}}, \nabla\xi_i^{n+\frac{1}{2}}\right) \\
G_7^n &:= \left(F_i(t^{n+\frac{1}{2}}) - F_i^{n+\frac{1}{2}}, \xi_i^{n+\frac{1}{2}}\right)
\end{aligned}$$

Use Taylor's expansion, Young's inequality and (4.42), we determine the estimates for G_1^n to G_4^n as follows,

$$
\begin{aligned}
|G_1^n| &\le (\Delta t)^2\|\partial_{ttt}C_i\|_{L^\infty(L^2)}\|\xi_i^{n+\frac{1}{2}}\|_{L^2} \le \frac{1}{2}(\Delta t)^4\|\partial_{ttt}C_i\|^2_{L^\infty(L^2)} + \frac{1}{2}\|\xi_i^{n+\frac{1}{2}}\|^2_{L^2},\\
|G_2^n| &= \left|\left(d_t\eta_i^n, \xi_i^{n+\frac{1}{2}}\right)\right| \le (\Delta t)^2\|\partial_{ttt}\eta_i\|_{L^\infty(L^2)}\|\xi_i^{n+\frac{1}{2}}\|_{L^2} + \|\partial_t\eta_i\|_{L^\infty(L^2)}\|\xi_i^{n+\frac{1}{2}}\|_{L^2}\\
&\le \frac{1}{2}(\Delta t)^4\|\partial_{ttt}\eta_i\|^2_{L^\infty(L^2)} + \frac{1}{2}\|\partial_t\eta_i\|^2_{L^\infty(L^2)} + \|\xi_i^{n+\frac{1}{2}}\|^2_{L^2}\\
|G_3^n| &\le (\Delta t)^2\|\partial_{tt}\nabla\tilde{C}_i\|_{L^\infty(L^2)}\|\xi_i^{n+\frac{1}{2}}\|_{L^2} \le \frac{1}{2}(\Delta t)^4\|\partial_{tt}\nabla\tilde{C}_i\|^2_{L^\infty(L^2)} + \frac{1}{2}\|\xi_i^{n+\frac{1}{2}}\|^2_{L^2}\\
|G_4^n| &\le \left|\left(\tilde{C}_i(t^{n+\frac{1}{2}})\nabla\left(\Phi(t^{n+\frac{1}{2}}) - \Phi^{n+\frac{1}{2}}\right), \nabla\xi_i^{n+\frac{1}{2}}\right)\right|\\
&\quad + \left|\left(\tilde{C}_i(t^{n+\frac{1}{2}})\nabla\left(\Phi^{n+\frac{1}{2}} - \Phi_h^{n+\frac{1}{2}}\right), \nabla\xi_i^{n+\frac{1}{2}}\right)\right|\\
&\le (\Delta t)^2\|\partial_{tt}\nabla\Phi\|_{L^\infty(L^2)}\|\tilde{C}_i\|_{L^\infty(L^\infty)}\|\nabla\xi_i^{n+\frac{1}{2}}\|_{L^2} + Mh^k\|\tilde{C}_i\|_{L^\infty(L^\infty)}\|\nabla\xi_i^{n+\frac{1}{2}}\|_{L^2}\\
&\quad + M\sum_{j=1}^{2}\|\xi_j^{n+\frac{1}{2}}\|_{L^2}\|\tilde{C}_i\|_{L^\infty(L^\infty)}\|\nabla\xi_i^{n+\frac{1}{2}}\|_{L^2} + Mh^{k+1}\|\tilde{C}_i\|_{L^\infty(L^\infty)}\|\nabla\xi_i^{n+\frac{1}{2}}\|_{L^2}\\
&\le \frac{M}{4\epsilon}\|\tilde{C}_i\|^2_{L^\infty(L^\infty)}\left((\Delta t)^4\|\partial_{tt}\nabla\Phi\|^2_{L^\infty(L^2)} + \sum_{j=1}^{2}\|\xi_j^{n+\frac{1}{2}}\|^2_{L^2} + h^{2k}\right)\\
&\quad + 2\epsilon\|\nabla\xi_i^{n+\frac{1}{2}}\|^2_{L^2},\\
|G_7^n| &\le (\Delta t)^2\|\partial_{tt}F_i\|_{L^\infty(L^2)}\|\xi_i^{n+\frac{1}{2}}\|_{L^2} \le \frac{1}{2}(\Delta t)^4\|\partial_{tt}F_i\|^2_{L^\infty(L^2)} + \frac{1}{2}\|\xi_i^{n+\frac{1}{2}}\|^2_{L^2}
\end{aligned}
$$

In G_5^n and G_6^n, we shall use mathematical induction again. Since

$$
\begin{aligned}
|G_5^n| &\le (\Delta t)^2\|\partial_{tt}\tilde{C}_i\|_{L^\infty(L^2)}\left\|\nabla\left(\tilde{\Phi}^{n+\frac{1}{2}} - \Phi_h^{n+\frac{1}{2}}\right)\right\|_{L^\infty}\|\nabla\xi_i^{n+\frac{1}{2}}\|_{L^2}\\
&\quad + (\Delta t)^2\|\partial_{tt}\tilde{C}_i\|_{L^\infty(L^2)}\|\nabla\tilde{\Phi}\|_{L^\infty(L^\infty)}\|\nabla\xi_i^{n+\frac{1}{2}}\|_{L^2}\\
|G_6^n| &\le \left\|\nabla\left(\tilde{\Phi}^{n+\frac{1}{2}} - \Phi_h^{n+\frac{1}{2}}\right)\right\|_{L^\infty}\|\xi_i^{n+\frac{1}{2}}\|_{L^2}\|\nabla\xi_i^{n+\frac{1}{2}}\|_{L^2}\\
&\quad + \|\nabla\tilde{\Phi}\|_{L^\infty(L^\infty)}\|\xi_i^{n+\frac{1}{2}}\|_{L^2}\|\nabla\xi_i^{n+\frac{1}{2}}\|_{L^2},
\end{aligned}
$$

and by inverse estimate and (4.42),

$$\left\|\nabla\left(\tilde{\Phi}^{n+\frac{1}{2}}-\Phi_h^{n+\frac{1}{2}}\right)\right\|_{L^\infty} \le h^{-\frac{d}{2}}\left\|\nabla\left(\tilde{\Phi}^{n+\frac{1}{2}}-\Phi_h^{n+\frac{1}{2}}\right)\right\|_{L^2}$$
$$\le h^{-\frac{d}{2}}\sum_{i=1}^{2}\left(\|\xi_i^{n+\frac{1}{2}}\|_{L^2}+\|\eta_i^{n+\frac{1}{2}}\|_{L^2}\right) \le Mh^k + h^{-\frac{d}{2}}\sum_{i=1}^{2}\|\xi_i^{n+\frac{1}{2}}\|_{L^2},$$

we give the following mathematical induction hypothesis to estimate G_5^n and G_6^n, for any $n = 0, 1, ..., N$,

$$h^{-\frac{d}{2}}\|\xi_i^n\|_{L^2} \le M. \tag{4.49}$$

When h is sufficiently small, by the given initial conditions, we have

$$h^{-\frac{d}{2}}\|\xi_i^0\|_{L^2} \le h^{-\frac{d}{2}}\left(\|\eta_i^0\|_{L^2}+\|C_i^0-C_{i,h}^0\|_{L^2}\right) \le Mh^{k+1-\frac{d}{2}} \le M.$$

Assume (4.49) holds for any $n = 0, 1, ..., J$, $0 \le J \le N-2$, then

$$\begin{aligned}
|G_5^n| &\le M(\Delta t)^4\|\partial_{tt}\tilde{C}_i\|^2_{L^\infty(L^2)}\left(1+\|\nabla\tilde{\Phi}\|^2_{L^\infty(L^\infty)}\right)+2\epsilon\|\nabla\xi_i^{n+\frac{1}{2}}\|^2_{L^2},\\
|G_6^n| &\le \frac{1}{4\epsilon}\left(1+\|\nabla\tilde{\Phi}\|^2_{L^\infty(L^\infty)}\right)\|\xi_i^{n+\frac{1}{2}}\|^2_{L^2}+\epsilon\|\nabla\xi_i^{n+\frac{1}{2}}\|^2_{L^2}.
\end{aligned}$$

Note the fact that $\|\nabla\tilde{\Phi}\|_{L^\infty(L^2)}$, $\|\nabla\tilde{\Phi}\|_{L^\infty(L^\infty)}$, $\|\tilde{C}_i\|_{L^\infty(L^\infty)}$, $\|\partial_{tt}\nabla\tilde{C}_i\|_{L^\infty(L^2)}$ and $\|\partial_{ttt}\tilde{C}_i\|_{L^\infty(L^2)}$ are bounded following (4.11), (4.12), (4.24) and (4.43), respectively. Use the regularity of C_i and Φ given in (4.40), and apply a summation of time step n from 0 to J on both side of (4.48), where $0 \le J \le N-1$, we are then able to obtain the following inequality by means of the telescoping technique

$$\frac{1}{2\Delta t}\left(\|\xi_i^{J+1}\|^2_{L^2}-\|\xi_i^0\|^2_{L^2}\right)+\sum_{n=0}^{J}\|\nabla\xi_i^{n+\frac{1}{2}}\|^2_{L^2}$$
$$\le M\sum_{n=0}^{J}\left((\Delta t)^4+h^{2k}+\sum_{j=1}^{2}\|\xi_j^{n+\frac{1}{2}}\|^2_{L^2}+\epsilon\|\nabla\xi_i^{n+\frac{1}{2}}\|^2_{L^2}\right),$$

then apply Grönwall's inequality,

$$\|\xi_i^{J+1}\|^2_{L^2}+\Delta t\sum_{n=0}^{J}\|\nabla\xi_i^{n+\frac{1}{2}}\|^2_{L^2} \le M\left((\Delta t)^4+h^{2k}+\|\xi_i^0\|^2_{L^2}\right).$$

Since

$$\left\|\sum_{n=0}^{J}\nabla\xi_i^n\right\|_{L^2} \le \sum_{n=0}^{J-1}\|\nabla\xi_i^{n+\frac{1}{2}}\|_{L^2} + \frac{1}{2}\|\nabla\xi_i^0\|_{L^2} + \frac{1}{2}\|\nabla\xi_i^J\|_{L^2}$$
$$\le \sum_{n=0}^{J}\|\nabla\xi_i^{n+\frac{1}{2}}\|_{L^2} + \frac{1}{2}\|\nabla\xi_i^0\|_{L^2},$$

we have

$$\|\xi_i^{J+1}\|_{L^2} + \left(\Delta t\left\|\sum_{n=0}^{J}\nabla\xi^n\right\|_{L^2}^2\right)^{\frac{1}{2}} \le M\left((\Delta t)^2 + h^k + \|\nabla\xi_i^0\|_{L^2} + \|\xi_i^0\|_{L^2}\right).$$

Because $\tilde{C}_i^0$ and $C_{i,h}^0$ are both defined in their approximation forms, appropriately, one can pick up an appropriate initial values for both such that $\|\nabla\xi_i^0\|_{L^2} + \|\xi_i^0\|_{L^2} \le M((\Delta t)^2 + h^k)$. Thus

$$\|\xi_i^{J+1}\|_{L^2} + \left(\Delta t\left\|\sum_{n=0}^{J}\nabla\xi^n\right\|_{L^2}^2\right)^{\frac{1}{2}} \le M\left((\Delta t)^2 + h^k\right).$$

This implies that when h and Δt are sufficiently small, for $k \ge d-1$,

$$h^{-\frac{d}{2}}\|\xi_i^{J+1}\|_{L^2} \le M,$$

which proves the mathematical induction hypothesis (4.49) holds uniformly for any $n = 1, 2, ..., N-1$.

Finally, we have

$$\begin{aligned}
&\|C_i^{J+1} - C_{i,h}^{J+1}\|_{L^2} + \left(\Delta t\|\sum_{n=0}^{J}\nabla\left(C_i^n - C_{i,h}^n\right)\|_{L^2}^2\right)^{\frac{1}{2}} \\
\le\ & M\left((\Delta t)^2 + h^k\right) + \|\eta_i^{J+1}\|_{L^2} + \left(\Delta t\left\|\sum_{n=0}^{J}\nabla\eta^n\right\|_{L^2}^2\right)^{\frac{1}{2}} \\
\le\ & M\left((\Delta t)^2 + h^k + (\Delta t)^{\frac{1}{2}}h^k\right).
\end{aligned}$$

Since $\Delta t < 1$, we can get

$$\|C_i^{J+1} - C_{i,h}^{J+1}\|_{L^2} + \left(\Delta t\left\|\sum_{n=0}^{J}\nabla\left(C_i^n - C_{i,h}^n\right)\right\|_{L^2}^2\right)^{\frac{1}{2}} \le M\left((\Delta t)^2 + h^k\right).$$

Let $J = N-1$, we get

$$\|C_i^N - C_{i,h}^N\|_{L^2} \leq M\left((\Delta t)^2 + h^k\right). \tag{4.50}$$

Choosing $v_h = d_t\xi_i^{n+\frac{1}{2}}$ in (4.47) instead of $\xi_i^{n+\frac{1}{2}}$ and follow an analogous proof for $\|\nabla(C_i - C_{i,h})\|_{L^\infty(L^2)}$ in Theorem 4.1, we can prove the error estimate in $L^\infty(H^1)$ norm, i.e.,

$$\|\nabla(C_i^N - C_{i,h}^N)\|_{L^2} \leq M\left((\Delta t)^2 + h^k\right). \tag{4.51}$$

Finally, (4.44) follows from (4.50) and (4.51), and (4.45) follows from (4.41), (4.42) and (4.44). □

Having Theorem 4.3, the following corollary can be easily obtained.

Corollary 4.1. *Let (C_1, C_2, Φ) be the solution of (4.3) and (4.4) satisfying the regularity assumptions (4.40), and $(C_{1,h}, C_{2,h}, \Phi_h)$ be the solution of (4.5) and (4.6). Then there exists a constant M depending only on the regularity of C_i and Φ, such that for $i = 1, 2$,*

$$\left(\Delta t \sum_{n=0}^{N-1} \|\nabla\left(C_i^n - C_{i,h}^n\right)\|_{L^2}^2\right)^{\frac{1}{2}} + \left(\Delta t \sum_{n=0}^{N-1} \|\nabla\left(\Phi^n - \Phi_h^n\right)\|_{L^2}^2\right)^{\frac{1}{2}} \leq M\left((\Delta t)^2 + h^k\right). \tag{4.52}$$

4.2.6 Numerical Experiments

Let $\Omega = [0,1]\times[0,1]$ and choose the right hand side functions such that the exact solutions of (4.1) and (4.2) are given by

$$\left\{\begin{array}{rl} \Phi(x_1,x_2,t) & = \sin(\pi x_1)\sin(\pi x_2)(1-e^{-t}), \\ C_1(x_1,x_2,t) & = \sin(2\pi x_1)\sin(2\pi x_2)\sin(t), \\ C_2(x_1,x_2,t) & = \sin(3\pi x_1)\sin(3\pi x_2)\sin(2t), \end{array}\right. \tag{4.53}$$

The boundary conditions and initial conditions are homogeneous.

In the following, we use Algorithm 4.1 to find the approximate solution and compute the error in $L^\infty(L^2)$, $L^\infty(H^1)$, and $L^2(H^1)$ norm using both bilinear elements and biquadratic elements. We choose the nonlinear iteration tolerance $\varepsilon = 10^{-8}$ in Algorithm 4.1.

We first use bilinear element on uniform rectangular mesh, and choose $\Delta t = h$ and $T = 0.5$. From Tables 4.1-4.3, we can see that the convergence order in $L^2(H^1)$ norm and $L^\infty(H^1)$ norm for both C_i and Φ coincide with the convergence theory shown in Theorem 4.3 and Corollary 4.1. The errors in $L^\infty(L^2)$ norm is second order, which indicates our theoretical estimate is sub-optimal, however, the numerical solution presents an optimal convergence phenomenon in $L^\infty(L^2)$ norm.

Mesh Size	1/4	1/8	1/16	1/32
$\lVert C_1 - C_{1,h} \rVert_{L^\infty(L^2)}$	$4.72E-02$	$1.18E-02$	$2.94E-03$	$7.40E-04$
Order	-	$2.00E+00$	$2.00E+00$	$1.99E+00$
$\lVert C_1 - C_{1,h} \rVert_{L^\infty(H^1)}$	$9.43E-01$	$4.79E-01$	$2.41E-01$	$1.21E-01$
Order	-	$9.77E-01$	$9.92E-01$	$9.98E-01$
$\lVert C_1 - C_{1,h} \rVert_{L^2(H^1)}$	$5.31E-01$	$2.35E-01$	$1.09E-01$	$5.24E-02$
Order	-	$1.18E+00$	$1.10E+00$	$1.06E+00$

Table 4.1. C_1, bilinear element

Next we use biquadratic element on the same rectangular mesh and choose $\Delta t = h^2$ and $T = 0.125$. Tables 4.4-4.6 show that the convergence order is optimal in $L^\infty(L^2)$ norm which also coincide with the error estimates shown in Theorem 4.3. The convergence order in $L^\infty(H^1)$ norm and $L^2(H^1)$ norm for both C_i and Φ are third order, presenting a superconvergence phenomenon. Same to the case of bilinear element

Mesh Size	1/4	1/8	1/16	1/32
$\|C_2 - C_{2,h}\|_{L^\infty(L^2)}$	$1.92E-01$	$4.51E-02$	$1.12E-02$	$2.79E-03$
Order	-	$2.09E+00$	$2.01E+00$	$2.00E+00$
$\|C_2 - C_{2,h}\|_{L^\infty(H^1)}$	$3.72E+00$	$1.88E+00$	$9.49E-01$	$4.76E-01$
Order	-	$9.86E-01$	$9.84E-01$	$9.95E-01$
$\|C_2 - C_{2,h}\|_{L^2(H^1)}$	$2.14E+00$	$9.54E-01$	$4.50E-01$	$2.17E-01$
Order	-	$1.17E+00$	$1.08E+00$	$1.05E+00$

Table 4.2. C_2, bilinear element

Mesh Size	1/4	1/8	1/16	1/32
$\|\Phi - \Phi_h\|_{L^\infty(L^2)}$	$1.19E-02$	$3.01E-03$	$7.55E-04$	$1.89E-04$
Order	-	$1.98E+00$	$2.00E+00$	$2.00E+00$
$\|\Phi - \Phi_h\|_{L^\infty(H^1)}$	$1.97E-01$	$9.90E-02$	$4.95E-02$	$2.48E-02$
Order	-	$9.93E-01$	$9.99E-01$	$1.00E+00$
$\|\Phi - \Phi_h\|_{L^2(H^1)}$	$1.14E-01$	$5.01E-02$	$2.33E-02$	$1.12E-02$
Order	-	$1.19E+00$	$1.11E+00$	$1.06E+00$

Table 4.3. Φ, bilinear element

which produces a numerically optimal but theoretically sub-optimal order convergence rate, such superconvergence for biquadratic element may be caused by the use of uniform meshes and tensor product elements which requires further investigation.

Mesh Size	1/4	1/8	1/16	1/32
$\|C_1 - C_{1,h}\|_{L^\infty(L^2)}$	$2.16E-03$	$3.25E-04$	$4.23E-05$	$5.43E-06$
Order	-	$2.73E+00$	$2.94E+00$	$2.96E+00$
$\|C_1 - C_{1,h}\|_{L^\infty(H^1)}$	$2.37E-02$	$3.07E-03$	$3.87E-04$	$5.05E-05$
Order	-	$2.95E+00$	$2.99E+00$	$2.94E+00$
$\|C_1 - C_{1,h}\|_{L^2(H^1)}$	$6.68E-03$	$6.87E-04$	$8.06E-05$	$1.03E-05$
Order	-	$3.28E+00$	$3.09E+00$	$2.98E+00$

Table 4.4. C_1, biquadratic element

Mesh Size	1/4	1/8	1/16	1/32
$\|C_2 - C_{2,h}\|_{L^\infty(L^2)}$	$1.08E-02$	$2.04E-03$	$2.79E-04$	$3.57E-05$
Order	-	$2.40E+00$	$2.87E+00$	$2.97E+00$
$\|C_2 - C_{2,h}\|_{L^\infty(H^1)}$	$2.12E-01$	$2.98E-02$	$3.78E-03$	$4.75E-04$
Order	-	$2.83E+00$	$2.98E+00$	$2.99E+00$
$\|C_2 - C_{2,h}\|_{L^2(H^1)}$	$5.96E-02$	$6.70E-03$	$7.95E-04$	$9.81E-05$
Order	-	$3.15E+00$	$3.08E+00$	$3.02E+00$

Table 4.5. C_2, biquadratic element

Mesh Size	1/4	1/8	1/16	1/32
$\|\Phi - \Phi_h\|_{L^\infty(L^2)}$	$3.19E-04$	$4.03E-05$	$5.04E-06$	$6.31E-07$
Order	-	$2.99E+00$	$3.00E+00$	$3.00E+00$
$\|\Phi - \Phi_h\|_{L^\infty(H^1)}$	$1.60E-03$	$1.87E-04$	$2.26E-05$	$2.81E-06$
Order	-	$3.10E+00$	$3.04E+00$	$3.01E+00$
$\|\Phi - \Phi_h\|_{L^2(H^1)}$	$6.76E-04$	$5.27E-05$	$5.19E-06$	$6.11E-07$
Order	-	$3.68E+00$	$3.34E+00$	$3.09E+00$

Table 4.6. Φ, biquadratic element

4.3 Error analysis of PNP equations using mixed finite element method

4.3.1 Introduction

This section continues our effort in Section 4.2 and [Sun et al.] where the error estimates of standard finite element method for a time dependent PNP model was conducted. The goal of this section is to accurately analyze the error estimates using Taylor-Hood mixed finite element of the semi-discrete finite element scheme and fully discrete finite element method with Crank-Nicolson scheme for a time dependent PNP model. We obtain the optimal error estimate in $L^\infty(L^2)$ norm and $L^\infty(H^1)$ norm for both finite element schemes in spatial discretization, and second order approximation in temporal discretization for the fully discrete scheme.

In order to improve the convergence rate in $L^\infty(L^2)$ norm from the sub-optimal to optimal when the linear finite element is used for both ionic concentrations and electrostatic potential, we propose the mixed finite element method in this section to discretize the electrostatic potential equation, where, if the Taylor-Hood-type $P2P1$ element is employed, the electrostatic potential is still approximated by linear element, while its gradient, termed as the electric current flux, is approximated by quadratic element. Both of them are approximated within the mixed finite element spaces. At the same time, we still use the standard finite element method to discretize the time-dependent ionic concentrations equations. We can further prove that the convergence rates of both electrostatic potential and ionic concentrations are optimal in both $L^\infty(H^1)$ and $L^\infty(L^2)$ norms, simultaneously, as a byproduct, the electric current flux can also achieve a higher approximation order in contrast with the standard finite element method for PNP system.

Mixed method is applied to a variety of finite element methods which have more than one approximation space. Typically one or more of the spaces play the role of Lagrange multipliers which enforce constraints. One characteristic of mixed methods is that not all choices of finite element spaces will lead to convergent approximations. Standard approximability alone is insufficient to guarantee success [Pettini (2000); Ciarlet (1978)]. The mathematical analysis and applications of mixed finite element methods have been widely developed since 1970s. A general analysis for this kind of methods was first developed by Brezzi [Brezzi (1974)]. We also have to mention the papers by Babuska Babuska (1973) and by Crouzeix and Raviart [Crouzeix and Raviart (1973)] which, although for particular problems, introduced some of the fundamental ideas for the analysis of mixed methods. Mixed finite element method is usually used to solve Stokes equations, Navier-Stokes equations and mixed Poisson equations such as Darcy's system [Arnold et al. (1984); Douglas et al. (1983); Verfurth (1984); Layton et al. (2003)]. So far, we have not seen an error analysis of mixed finite element method was studied for PNP equations in any form.

In this section, we propose to use Taylor-Hood mixed element [Taylor and Hood (1973); Stenberg (1990); Boffi et al. (2012)] instead of Raviart-Thomas element [Raviart and Thomas (1977); Douglas et al. (1983)] or Brezzi-Douglas-Marini element [Arnold et al. (1984)] to tackle the Poisson-type electrostatic potential equation, in view of the convenience of implementation of Taylor-Hood element that is defined by Lagrange-type piecewise interpolating polynomials, and the induced continuity of vector field variable such as the electric current flux in PNP system. It is well known that, however, Taylor-Hood element without any additional stabilization can not be applied to the mixed form of Poisson equation due to the absence of one of two discrete inf-sup conditions of Brezzi's theorem [Brezzi et al. (1993); Correa and Loula; Mardal et al. (2002)]. In order to stabilize the originally unstable Galerkin approximation due to the use of Taylor-Hood element, we can add the residual form of the governing equations to the discretization. Thus both the stability and the convergence are attained at the same time, though, the convergence rate of such discretization for vector field variable is sub-optimal in $[L^2(\Omega)]^2$ [Brezzi et al. (1993); Correa and Loula]. However, the loose of one order of convergence is affordable in those cases where one has to work with continuous vector field variables, as what we require for the electric current flux in PNP system, i.e., a continuous electric current field is crucial in the Nernst-Planck equation to describe the transport of ionic concentrations. In particular, in our case for PNP system, the very interesting fact is that, in order to obtain the optimal convergence rates for both electrostatic potential and ionic concentrations, what we only need is the sub-optimal convergence rate for the electric current field (see our error analysis in Section 4.3.3). Thus, Taylor-Hood element with additional stabilization overcomes the previous difficulty occurring to the standard fintie element method for PNP equations [Sun et al.], and produce the optimal convergence rates for all variables. In addition, since the mixed Taylor-Hood approximation is naturally stable for Stokes/Navier-Stokes equations, it implies that the mixed Taylor-Hood approximation method shall be the most natural way to deal with the coupled system of PNP and Navier-Stokes equations, which is actually a popular model of the electrohydrodynamics problems. Based on the results of this section, we will continue our study on the error analysis of mixed finite element method for the coupled system of PNP and Navier-Stokes equations in the future.

This section is organized as follows. Section 4.3.2 introduces the PNP system and its mixed weak forms, and the error analysis for the semi-discretization scheme with the mixed finite element method is given in Section 4.3.3. Section 4.3.4 conducts the full discretization scheme. Numerical experiments and validations are illustrated in Section 4.3.5.

In the following sections, for the sake of simplicity, we sometimes drop the time dependence in $\boldsymbol{u}(t), \Phi(t)$ and $C_i(t)$ or drop the domain Ω in $W^{l,p}(\Omega), H^1(\Omega), L^2(\Omega)$.

We use M to denote generic constant throughout the section.

4.3.2 PNP system and its modified formulations

Let $\Omega \in \mathbb{R}^d$, $(d = 2, 3)$ be a bounded Lipschitz domain and $J = [0, T]$. Then the PNP system describes the electrostatic potential $\Phi : \Omega \times (0, T] \to \mathcal{R}$, and the mass concentration of ions $C_1, C_2 : \Omega \times (0, T] \to \mathbb{R}_0^+$, satisfying the following governing equations

$$
\begin{aligned}
\partial_t C_i + \nabla \cdot E_i &= F_i, \quad i = 1, 2, &(4.54)\\
-\nabla \cdot (\nabla \Phi) &= \sum_{i=1}^{2} q_i C_i + F_3, &(4.55)
\end{aligned}
$$

and the ionic concentration flux (current density) is defined as

$$E_i = -D_i[\nabla C_i + q_i C_i \nabla \Phi],$$

where $\partial_t = \partial/\partial t$. For $i = 1, 2$, C_i are the concentration of an ion species carrying charge q_i (For example $q_{K^+} = 1, q_{Cl^-} = -1$), and D_i are the spatially dependent diffusion coefficients. F_i $(i = 1, 2, 3)$ denote the reaction source terms.

For the simplicity, we choose $q_1 = 1,\ q_2 = -1$ without loss of generality and restrict the diffusion coefficients D_i $(i = 1, 2)$ as constants, i.e., $D_1 = D_2 = 1$. We impose the following homogeneous boundary conditions and initial conditions, for Φ and C_i $(i = 1, 2)$,

$$C_i = \Phi = 0, \qquad on\ \ \partial\Omega,\ t \in (0, T], \tag{4.56}$$

$$C_i = C_i^0,\ \ \Phi = \Phi^0, \qquad in\ \ \Omega,\ t = 0. \tag{4.57}$$

If we introduce the electric current field

$$\boldsymbol{u} = \nabla\Phi, \tag{4.58}$$

then the Poisson equation (4.55) is reformulated as

$$-\nabla \cdot \boldsymbol{u} = r(C_1, C_2), \tag{4.59}$$

where

$$r(C_1, C_2) = \sum_{i=1}^{2} q_i C_i + F_3. \tag{4.60}$$

Thus the concentration equation (4.54) can be rewritten as

$$\partial_t C_i - \nabla \cdot (\nabla C_i + q_i \boldsymbol{u} C_i) = F_i, \qquad i = 1, 2. \tag{4.61}$$

Define

$$V := H(div; \Omega) = \{\boldsymbol{v} \in [L^2(\Omega)]^d | \nabla \cdot \boldsymbol{v} \in L^2(\Omega)\},$$

and

$$\|\boldsymbol{v}\|_V^2 = \|\boldsymbol{v}\|_{L^2}^2 + \|\nabla \cdot \boldsymbol{v}\|_{L^2}^2,$$

where $\| \cdot \|_{L^2}$ is the usual $L^2(\Omega)$ norm for scalar variables or $[L^2(\Omega)]^d$ norm for the vector variables. From (4.58), we know that without reinforcing Φ with any boundary conditions, its numerical solution is determined only up to an arbitrary additive constant, we shall avoid this trivial difficulty by considering

$$W = L^2(\Omega)/\{\phi \equiv \text{ constant on } \Omega\}.$$

Then, the mixed form of weak formulation of the potential equation (4.55) is given as, find $(\boldsymbol{u}, \Phi) \in V \times W$ such that,

$$\bar{A}(\boldsymbol{u}, \boldsymbol{v}) + B(\boldsymbol{v}, \Phi) = 0, \quad \forall \boldsymbol{v} \in V, \tag{4.62}$$

$$B(\boldsymbol{u}, \phi) = -(r(C_1, C_2), \phi), \quad \forall \phi \in W, \tag{4.63}$$

where

$$\bar{A}(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{u}, \boldsymbol{v}), \tag{4.64}$$

$$B(\boldsymbol{u}, \phi) = (\nabla \cdot \boldsymbol{u}, \phi). \tag{4.65}$$

Based on Brezzi's theory, for the continuous linear and bilinear forms, the existence and uniqueness of solutions of the mixed formulation are assured by the following Ladyzenskaja-Babuška-Brezzi (LBB) or inf-sup conditions,

(1) $\exists \alpha > 0$ such that

$$\bar{A}(\boldsymbol{v}, \boldsymbol{v}) \geq \alpha \|\boldsymbol{v}\|_V^2, \quad \forall \boldsymbol{v} \in Z_0, \tag{4.66}$$

with

$$Z_0 = \{v \in V : B(\boldsymbol{v}, \phi) = 0, \forall \phi \in W\};$$

(2) $\exists \beta > 0$ such that

$$\sup_{\boldsymbol{v} \in V/\{0\}} \frac{B(\boldsymbol{v}, \phi)}{\|\boldsymbol{v}\|_V} \geq \beta \|\phi\|_{L^2}, \forall \phi \in W. \tag{4.67}$$

It is well known that these compatibility conditions impose very severe limitations in the choice of stable finite element approximations for mixed method in general. For instance, if discretizing in the Taylor-Hood-type $P^{k+1}P^k$ mixed finite element space, it satisfies the discrete form of condition (4.67) for $v \in V_h/0$ and $\phi \in W_h$ where $V_h \subset V$, $W_h \subset W$, but it does not satisfy the discrete form of condition (4.66) for $v \in Z_h = \{v \in V_h : B(v, \phi) = 0, \forall \phi \in W_h\}$, which is associated with the coercivity of the bilinear form $\bar{A}(\boldsymbol{v}, \boldsymbol{v})$ in $H(div; \Omega)$ norm restricted to the subspace Z_0 [Brezzi et al. (1993); Correa and Loula; Mardal et al. (2002)]. Therefore, Taylor-Hood approximation is unstable for the mixed Poisson problem, and can not be applied to Poisson equation or its variants without any additional stabilization. To overcome these limitations, some stabilized mixed formulations have been proposed, such as Galerkin-Least-Square (GLS) scheme [Brezzi (1974); Correa and Loula; Loula et al. (1987); Franca et al. (1988)].

We shall address that, there are other mixed elements, such as Raviart-Thomas element [Raviart and Thomas (1977); Douglas et al. (1983)] and Brezzi-Douglas-Marini element [Arnold et al. (1984)], satisfying the compatibility condition (4.66) and thus being naturally stable for the mixed Poisson problem, however, comparing to these mixed element, Taylor-Hood approximation with additional stabilization can produce a continuous electric current field [Brezzi et al. (1993)], which is crucial in the elecctrohydrodynamics problem. In addition, the Lagrange-type interpolating polynomials, which are used to construct Taylor-Hood element, are more convenient to be defined as the nodal basis piecewise function in the local element, and easier to be implemented in the computation in contrast to Raviart-Thomas element and Brezzi-Douglas-Marini element in which only the normal components of the vector variable are required to be continuous across element edges but not on the nodes. On the other hand, as one of the popular Stokes elements, Taylor-Hood element is a natural choice for the mixed finite element approximation of Stokes/Navier-Stokes equations. Hence, if we are able to successfully apply Taylor-Hood mixed approximation to PNP equations as shown in this section, then in our future numerical study on the model of electrohydrodynamics, we can employ the same Taylor-Hood element for both PNP equations and Navier-Stokes equations without the need to introduce different mixed elements, more convenient and more efficient to analyze and implement the mixed finite element approximation for the coupled system of PNP and Navier-Stokes equations of electrohydrodynamics model.

In the following, based on the stabilization scheme given in [Brezzi (1974); Correa and Loula], we introduce a modified weak formulation for the mixed Poisson problem of the electrostatic potential equation when the stable Stokes element such as Taylor-Hood element is adopted in the discretization.

It is clear that, using (4.59), one can consider, in place of (4.58), the alternative setting

$$\boldsymbol{u} - \nabla(\nabla \cdot \boldsymbol{u}) = \nabla\Phi + \nabla r(C_1, C_2), \tag{4.68}$$

then the modified weak formulation of the mixed form of the electrostatic potential equation (4.55) is given as, find $(\boldsymbol{u}, \Phi) \in V \times W$ such that,

$$\begin{aligned} A(\boldsymbol{u}, \boldsymbol{v}) + B(\boldsymbol{v}, \Phi) &= -(r(C_1, C_2), \nabla \cdot \boldsymbol{v}), \quad \forall \boldsymbol{v} \in V, & (4.69)\\ B(\boldsymbol{u}, \phi) &= -(r(C_1, C_2), \phi), \qquad \forall \phi \in W, & (4.70) \end{aligned}$$

where

$$A(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{u}, \boldsymbol{v}) + (\nabla \cdot \boldsymbol{u}, \nabla \cdot \boldsymbol{v}),$$

$$B(\boldsymbol{u}, \phi) = (\nabla \cdot \boldsymbol{u}, \phi).$$

Then the LBB condition (14) can be rewritten as, $\exists \alpha > 0$ such that

$$A(\boldsymbol{v}, \boldsymbol{v}) \geq \alpha \|\boldsymbol{v}\|_V^2, \quad \forall \boldsymbol{v} \in V, \tag{4.71}$$

which can be easily satisfied when discretizing (4.69) and (4.70) in the Taylor-Hood $P^{k+1}P^k$ mixed finite element space.

The weak formulation of the ionic concentration equations (4.61) are defined as, find $C_i \in H_0^1(\Omega)$ such that

$$(\partial_t C_i, c_i) + (\nabla C_i, \nabla c_i) + q_i(\boldsymbol{u} C_i, \nabla c_i) = (F_i, c_i) \quad \forall c_i \in H_0^1(\Omega). \tag{4.72}$$

with the above regularity assumptions, the existence and uniqueness of the solution $(\boldsymbol{u}, \Phi, C_1, C_2)$ of (4.69)-(4.72) can be achieved by an analogous well-posedness analysis which have been detailed in refs. [Gajewski and Gröger (1986); Ciarlet (1978); Brezzi (1974); Brezzi et al. (1993)] and thus is omitted here. In this section, we primarily focus on the error analysis of the mixed finite element method in the following sections.

4.3.3 Error analysis of the semi-discretization

Let S_h^k be the classical C^0 Lagrangian finite element space of degree $k \geq 1$, which is associated with a quasi-regular polygonalization of Ω. In the Taylor-Hood mixed finite element spaces $V_h = [S_h^{k+1}]^d \cap V$ and $W_h = S_h^k \cap W$, the approximation of $V \times W$ by $V_h \times W_h$ is described by the following relations for the mixed Poisson system (4.69) and (4.70). If $\boldsymbol{v} \in V$ and $w \in W$, then the following error estimates of interpolation hold [Pettini (2000); Quarteroni and Valli (2008); Brezzi and Fortin (1991); Loula and Toledo (1988)]

$$
\begin{aligned}
\inf_{\boldsymbol{v}_h \in V_h} \|\boldsymbol{v} - \boldsymbol{v}_h\|_{[L^2]^d} &\leq M\|\boldsymbol{v}\|_{[H^{k+1}]^d} h^{k+1}, && (4.73)\\
\inf_{\boldsymbol{v}_h \in V_h} \|\boldsymbol{v} - \boldsymbol{v}_h\|_{V} &\leq M\left(\|\boldsymbol{v}\|_{[H^{k+1}]^d} + \|\nabla \cdot \boldsymbol{v}\|_{H^{k+1}}\right) h^{k+1}, && (4.74)\\
\inf_{w_h \in W_h} \|w - w_h\|_{L^2} &\leq M\|w\|_{H^{k+1}} h^{k+1}. && (4.75)
\end{aligned}
$$

Let $M_h = S_h^k \cap H_0^1(\Omega)$ be a standard finite element space for Galerkin methods. Then the following error estimate of the interpolation for $c \in H_0^{k+1}$ hold [Ciarlet (1978); Wheeler (1973)]

$$
\inf_{c_h \in M_h} (\|c - c_h\|_{L^2} + h\|c - c_h\|_{H^1}) \leq M\|c\|_{H_0^{k+1}} h^{k+1}. \tag{4.76}
$$

Discretizing (4.69)-(4.70) in $V_h \times M_h$, the corresponding discrete compatibility conditions are now [Brezzi (1974); Brezzi and Fortin (1991)],

(1) $\exists \alpha > 0$ such that

$$
A(\boldsymbol{v}, \boldsymbol{v}) \geq \alpha \|\boldsymbol{v}\|_V^2, \quad \forall \boldsymbol{v} \in V_h, \tag{4.77}
$$

(2) $\exists \beta > 0$ such that

$$
\sup_{\boldsymbol{v} \in V_h/\{0\}} \frac{B(\boldsymbol{v}, \phi)}{\|\boldsymbol{v}\|_V} \geq \beta \|\phi\|_{L^2}, \forall \phi \in W_h, \tag{4.78}
$$

where α and β in (4.77) and (4.78) respectively have to be independent of h. The conditions (4.77) and (4.78) are now easily satisfied in Taylor-Hood spaces.

We define the semi-discrete mixed finite element approximation for the problem (4.55)-(4.57) as follows by finding the map

$$
(\boldsymbol{u}_h, \Phi_h, C_{1,h}, C_{2,h}) : J \to V_h \times W_h \times M_h \times M_h
$$

such that, for $i = 1, 2$ and $t \in (0, T]$,

$$A(\boldsymbol{u}_h, \boldsymbol{v}) + B(\boldsymbol{v}, \Phi_h) = -\left(r(C_{1,h}, C_{2,h}), \nabla \cdot \boldsymbol{v}\right), \quad \forall \boldsymbol{v} \in V_h, \tag{4.79}$$

$$B(\boldsymbol{u}_h, \phi) = -\left(r(C_{1,h}, C_{2,h}), \phi\right), \quad \forall \phi \in W_h, \tag{4.80}$$

$$(\partial_t C_{i,h}, c_i) + (\nabla C_{i,h}, \nabla c_i) + q_i(\boldsymbol{u}_h C_{i,h}, \nabla c_i) = (F_i, c_i), \quad \forall c_i \in M_h, \tag{4.81}$$

with the Dirtichlet boundary condition $\Phi_h = C_{i,h} = 0$, and the initial condition $(\boldsymbol{u}_h^0, \Phi_h^0, C_{1,h}^0, C_{2,h}^0)$ given by the interpolation of $(\boldsymbol{u}^0, \Phi^0, C_1^0, C_2^0)$ in $V_h \times W_h \times M_h \times M_h$, where $\boldsymbol{u}^0 = \nabla \Phi^0$.

In the following, we give the a priori error estimates for the approximation of the solutions $(\boldsymbol{u}_h, \Phi_h, C_{1,h}, C_{2,h})$ of the semi-discrete system (4.79)-(4.81) to the analytic solutions (u, Φ, C_1, C_2) of (4.55)-(4.57).

First of all, we assume the following regularity properties hold for $\boldsymbol{u}$, Φ and C_i ($i = 1, 2$),

$$\begin{aligned} &\boldsymbol{u} \in W^{1,\infty}(J; [W^{k+1,\infty}]^d), \\ &\Phi \in W^{1,\infty}(J; H^{k+3} \cap W^{k+2,\infty}), \\ &C_i \in W^{1,\infty}(J; W^{k+1,\infty}) \end{aligned} \tag{4.82}$$

Because of the nonlinearity of the finite element approximation equations (4.79) and (4.80), it is always necessary to decompose the approximation error of finite element solution by introducing a linear projection of the solution of the differential problem (4.59) and (4.68) into the finite element space. Consider the projection of $(u, \Phi) \in V \times W$, i.e., $(\tilde{\boldsymbol{u}}, \tilde{\Phi}) : J \to V_h \times W_h$, defined as

$$A(\tilde{\boldsymbol{u}}, \boldsymbol{v}) + B(\boldsymbol{v}, \tilde{\Phi}) = -\left(r(C_1, C_2), \nabla \cdot \boldsymbol{v}\right), \quad \forall \boldsymbol{v} \in V_h, \tag{4.83}$$

$$B(\tilde{\boldsymbol{u}}, \phi) = -\left(r(C_1, C_2), \phi\right), \quad \forall \phi \in W_h. \tag{4.84}$$

Since $A(\tilde{\boldsymbol{u}}, \tilde{\boldsymbol{u}})$ and $B(\boldsymbol{v}, \tilde{\Phi})$ satisfy the compatibility conditions (4.77) and (4.78), and C_1 and C_2 are the continuous functions in $H_0^1(\Omega)$, then by Breezi's theory, we have the following Lemma [Pettini (2000); Ciarlet (1978); Brezzi and Fortin (1991)].

Lemma 4.7. *Let $(\boldsymbol{u}, \Phi, C_1, C_2)$ be the solution of (4.69)-(4.72) satisfying the regularity assumptions (4.82), and $(\tilde{\boldsymbol{u}}, \tilde{\Phi})$ be the solution of (4.83)-(4.84), then for any $t \in J$, we have the following error estimates,*

$$\|\boldsymbol{u} - \tilde{\boldsymbol{u}}\|_V + \|\Phi - \tilde{\Phi}\|_{L^2} \leq M\{\inf_{\boldsymbol{v} \in V_h} \|\boldsymbol{u} - \boldsymbol{v}\|_V + \inf_{\phi \in W_h} \|\Phi - \phi\|_{L^2}\},$$

then based on (4.74) and (4.75), it follows that

$$\|\boldsymbol{u} - \tilde{\boldsymbol{u}}\|_V + \|\Phi - \tilde{\Phi}\|_{L^2} \leq M\|\Phi\|_{H^{k+3}} h^{k+1},$$

where M is independent of h.

In the following lemma, we shall derive the error bounds of $\boldsymbol{u}_h - \tilde{\boldsymbol{u}}$ and $\Phi_h - \tilde{\Phi}$ before we eventually get to the error estimates of $\boldsymbol{u} - \boldsymbol{u}_h$ and $\Phi - \Phi_h$.

Lemma 4.8. *Let $(\boldsymbol{u}, \Phi, C_1, C_2)$ be the solution of (4.69)-(4.72) satisfying the regularity assumptions (4.82), $(\boldsymbol{u}_h, \Phi_h, C_{1,h}, C_{2,h})$ be the solution of (4.79)-(4.81) and $(\tilde{\boldsymbol{u}}, \tilde{\Phi})$ be the solution of (4.83)-(4.84), then for any $t \in J$, we have the following error estimates,*

$$\|\boldsymbol{u_h} - \tilde{\boldsymbol{u}}\|_V + \|\Phi_h - \tilde{\Phi}\|_{L^2} \leq M \sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2}. \tag{4.85}$$

Proof. Substract (4.83) from (4.79) and (4.84) from (4.80), we have the following equations,

$$\begin{aligned} A(\boldsymbol{u}_h - \tilde{\boldsymbol{u}}, \boldsymbol{v}) + B(\boldsymbol{v}, \Phi_h - \tilde{\Phi}) &= (r(C_1, C_2) - r(C_{1,h}, C_{2,h}), \nabla \cdot \boldsymbol{v}), \quad \forall \boldsymbol{v} \in V_h, \\ B(\boldsymbol{u}_h - \tilde{\boldsymbol{u}}, \phi) &= (r(C_1, C_2) - r(C_{1,h}, C_{2,h}), \phi), \qquad \forall \phi \in W_h. \end{aligned}$$

Let $\boldsymbol{v} = \boldsymbol{u}_h - \tilde{\boldsymbol{u}} \in V_h$, $\phi = \Phi_h - \tilde{\Phi} \in W_h$, then

$$\begin{aligned} &(\boldsymbol{u}_h - \tilde{\boldsymbol{u}}, \boldsymbol{u}_h - \tilde{\boldsymbol{u}}) + (\nabla \cdot (\boldsymbol{u}_h - \tilde{\boldsymbol{u}}), \nabla \cdot (\boldsymbol{u}_h - \tilde{\boldsymbol{u}})) + (\nabla \cdot (\boldsymbol{u}_h - \tilde{\boldsymbol{u}}), \Phi_h - \tilde{\Phi}) \\ &\qquad = (r(C_1, C_2) - r(C_{1,h}, C_{2,h}), \nabla \cdot (\boldsymbol{u}_h - \tilde{\boldsymbol{u}})) \end{aligned} \tag{4.86}$$

$$(\nabla \cdot (\boldsymbol{u}_h - \tilde{\boldsymbol{u}}), \Phi_h - \tilde{\Phi}) = (r(C_1, C_2) - r(C_{1,h}, C_{2,h}), \Phi_h - \tilde{\Phi}). \tag{4.87}$$

Considering (4.60) in (4.86), we have

$$\|\boldsymbol{u_h} - \tilde{\boldsymbol{u}}\|_V^2 + (\nabla \cdot (\boldsymbol{u}_h - \tilde{\boldsymbol{u}}), \Phi_h - \tilde{\Phi}) \leq M \sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2} \|\nabla \cdot (\boldsymbol{u_h} - \tilde{\boldsymbol{u}})\|_{L^2}, \tag{4.88}$$

then

$$(\nabla \cdot (\boldsymbol{u}_h - \tilde{\boldsymbol{u}}), \Phi_h - \tilde{\Phi}) \leq M \sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2} \|\nabla \cdot (\boldsymbol{u_h} - \tilde{\boldsymbol{u}})\|_{L^2}. \tag{4.89}$$

Applying the LBB condition (4.78) to (4.89), we attain

$$\begin{aligned} \|\Phi_h - \tilde{\Phi}\|_{L^2} &\leq \frac{1}{\beta} \sup_{\boldsymbol{u}_h - \tilde{\boldsymbol{u}} \in V_h/\{0\}} \frac{B(\boldsymbol{u}_h - \tilde{\boldsymbol{u}}, \Phi_h - \tilde{\Phi})}{\|\boldsymbol{u}_h - \tilde{\boldsymbol{u}}\|_V} \\ &\leq M \frac{\sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2} \|\nabla \cdot (\boldsymbol{u_h} - \tilde{\boldsymbol{u}})\|_{L^2}}{\|\boldsymbol{u}_h - \tilde{\boldsymbol{u}}\|_V} \\ &\leq M \sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2}. \end{aligned} \tag{4.90}$$

On the other hand, we can get the following estimate with the help of (4.88) and (4.90)

$$
\begin{aligned}
&\|\boldsymbol{u_h} - \tilde{\boldsymbol{u}}\|_V^2 \\
\leq\ & M\left(\|\nabla\cdot(\boldsymbol{u_h} - \tilde{\boldsymbol{u}})\|_{L^2}\|\Phi_h - \tilde{\Phi}\|_{L^2} + \sum_{i=1}^{2}\|C_i - C_{i,h}\|_{L^2}\|\nabla\cdot(\boldsymbol{u_h} - \tilde{\boldsymbol{u}})\|_{L^2}\right), \\
\leq\ & M\sum_{i=1}^{2}\|C_i - C_{i,h}\|_{L^2}\|\boldsymbol{u_h} - \tilde{\boldsymbol{u}}\|_V,
\end{aligned}
$$

then

$$\|\boldsymbol{u_h} - \tilde{\boldsymbol{u}}\|_V \leq M\sum_{i=1}^{2}\|C_i - C_{i,h}\|_{L^2}. \tag{4.91}$$

□

Using the triangular inequality, Lemma 4.7 and Lemma 4.8, we have the following Theorem.

Theorem 4.4. *Let* $(\boldsymbol{u}, \Phi, C_1, C_2)$ *be the solution of(4.69)-(4.72) satisfying the regularity assumptions (4.82),* $(\boldsymbol{u}_h, \Phi_h, C_{1,h}, C_{2,h})$ *be the solution of (4.79)-(4.81), then for any* $t \in J$*, we have the following error estimates,*

$$\|\boldsymbol{u} - \boldsymbol{u_h}\|_V + \|\Phi - \Phi_h\|_{L^2} \leq M\left(\|\Phi\|_{H^{k+3}}h^{k+1} + \sum_{i=1}^{2}\|C_i - C_{i,h}\|_{L^2}\right). \tag{4.92}$$

Remark 4.4. Since $\|\boldsymbol{u} - \boldsymbol{u_h}\|_{[L^2]^d} \leq \|\boldsymbol{u} - \boldsymbol{u_h}\|_V$, we also hold the following error estimates,

$$\|\boldsymbol{u} - \boldsymbol{u_h}\|_{[L^2]^d} \leq M\left(\|\Phi\|_{H^{k+3}}h^{k+1} + \sum_{i=1}^{2}\|C_i - C_{i,h}\|_{L^2}\right). \tag{4.93}$$

Next we move our focus to C_i and introduce its H^1-projection first. Define $\tilde{C}_i$ be the projection of C_i on M_h given by, for any $t \in (0, T]$,

$$(\nabla(C_i - \tilde{C}_i), \nabla c_i) + q_i(\boldsymbol{u}(C_i - \tilde{C}_i), \nabla c_i) = 0 \quad \forall c_i \in M_h, \tag{4.94}$$

then we have the following Lemma.

Lemma 4.9. *Let $(\boldsymbol{u}, \Phi, C_1, C_2)$ be the solution of (4.69)-(4.72) satisfying the regularity assumptions (4.82), $\tilde{C}_i$ be the solution of (4.94), then we hold the following error estimates for $\tilde{C}_i$ and their temporal derivatives,*

$$\|C_i - \tilde{C}_i\|_{L^2} + h\|C_i - \tilde{C}_i\|_{H^1} \leq M\|C_i\|_{H^{k+1}} h^{k+1}, \tag{4.95}$$

$$\|\partial_t(C_i - \tilde{C}_i)\|_{L^2} + h\|\partial_t(C_i - \tilde{C}_i)\|_{H^1} \leq M\left(\|C_i\|_{H^{k+1}} + \|\partial_t C_i\|_{H^{k+1}}\right) h^{k+1}. \tag{4.96}$$

Proof. Let $C_i - \tilde{C}_i = C_i - \Pi_h C_i + \Pi_h C_i - \tilde{C}_i$, where $\Pi_h C_i \in M_h$ is the finite element nodal interpolation of C_i and consider (4.94), we get

$$\begin{aligned}
&(\nabla(C_i - \tilde{C}_i), \nabla(C_i - \tilde{C}_i)) + q_i(\boldsymbol{u}(C_i - \tilde{C}_i), \nabla(C_i - \tilde{C}_i)) \\
&\qquad = (\nabla(C_i - \tilde{C}_i), \nabla(C_i - \Pi_h C_i)) + q_i(\boldsymbol{u}(C_i - \tilde{C}_i), \nabla(C_i - \Pi_h C_i)).
\end{aligned} \tag{4.97}$$

Use Cauchy-Schwarz inequality and Young's inequality,

$$\begin{aligned}
&\|\nabla(C_i - \tilde{C}_i)\|_{L^2}^2 \\
\leq\ & \|\nabla(C_i - \tilde{C}_i)\|_{L^2}\|\nabla(C_i - \Pi_h C_i)\|_{L^2} + \|\boldsymbol{u}\|_{[L^\infty]^d}\|C_i - \tilde{C}_i\|_{L^2}\|\nabla(C_i - \Pi_h C_i)\|_{L^2} \\
&+\|\boldsymbol{u}\|_{[L^\infty]^d}\|C_i - \tilde{C}_i\|_{L^2}\|\nabla(C_i - \tilde{C}_i)\|_{L^2} \\
\leq\ & \left(\frac{1}{4\epsilon} + \frac{1}{2}\right)\left(\|\nabla(C_i - \Pi_h C_i)\|_{L^2}^2 + \|\boldsymbol{u}\|_{[L^\infty]^d}^2\|C_i - \tilde{C}_i\|_{L^2}^2\right) \\
+\ & 2\epsilon\|\nabla(C_i - \tilde{C}_i)\|_{L^2}^2,
\end{aligned} \tag{4.98}$$

where $\epsilon > 0$ is sufficiently small. Since $\|\boldsymbol{u}\|_{[L^\infty]^d}$ is bounded by the regularity assumption, and use the interpolation error estimates (4.76), we have

$$\|\nabla(C_i - \tilde{C}_i)\|_{L^2} \le M(\|\nabla(C_i - \Pi_h C_i)\|_{L^2} + \|C_i - \tilde{C}_i\|_{L^2})$$
$$\le M(h^k\|C_i\|_{H^{k+1}} + \|C_i - \tilde{C}_i\|_{L^2}).$$

By the commonly used Aubin-Nitsche duality argument for the error estimate in L^2 norm [Sun et al.; Pettini (2000); Ciarlet (1978)], we can derive

$$\|C_i - \tilde{C}_i\|_{L^2} \le Mh\|\nabla(C_i - \tilde{C}_i)\|_{L^2}. \tag{4.99}$$

Thus when h is small enough, (4.95) is obtained.

Take the derivative with respect to t for each term in (4.94), we have the temporal derivative H^1 projection,

$$(\nabla\partial_t(C_i - \tilde{C}_i), \nabla c_i) + q_i(\boldsymbol{u}\partial_t(C_i - \tilde{C}_i) + \partial_t\boldsymbol{u}(C_i - \tilde{C}_i), \nabla c_i) = 0$$

take $c_i = \partial_t(C_i - \tilde{C}_i)$, then do the error analysis which is analogous to the derivation of (4.97)-(4.99), we can get the additional error estimate of (4.96). □

Take the derivative with respect to t for each term in (4.97), we have,

$$(\nabla\partial_t(C_i - \tilde{C}_i), \nabla(C_i - \tilde{C}_i)) + q_i(\boldsymbol{u}\partial_t(C_i - \tilde{C}_i) + \partial_t\boldsymbol{u}(C_i - \tilde{C}_i), \nabla(C_i - \tilde{C}_i))$$
$$= (\nabla\partial_t(C_i - \tilde{C}_i), \nabla(C_i - \Pi_h C_i)) + q_i(\boldsymbol{u}\partial_t(C_i - \tilde{C}_i) + \partial_t\boldsymbol{u}(C_i - \tilde{C}_i), \nabla(C_i - \Pi_h C_i)). \tag{4.100}$$

Then being analogous to the derivation of (4.98)-(4.99), we can get the additional error estimate of (4.96).

Similarly, we shall have the following classic maximum norm error estimates [Ciarlet (1978); Girault et al. (2004); Shen and Deng (1993)].

Lemma 4.10. *Let* $(\boldsymbol{u}, \Phi, C_1, C_2)$ *be the solution of (4.69)-(4.72) satisfying the regularity assumptions (4.82), and* $(\tilde{\boldsymbol{u}}, \tilde{\Phi}, \tilde{C}_1, \tilde{C}_2)$ *be the solution of (4.83), (4.84) and (4.94), then for any* $t \in J$, *we have the following error estimates,*

$$
\begin{aligned}
\|\boldsymbol{u} - \tilde{\boldsymbol{u}}\|_{[L^\infty]^d} &\leq M\|\Phi\|_{W^{k+2,\infty}}|\ln h| h^{k+2-\frac{d}{2}} \\
\|C_i - \tilde{C}_i\|_{L^\infty} &\leq \begin{cases} M\|C_i\|_{W^{k+1,\infty}}|\ln h| h^{k+1-\frac{d}{2}}, & k=1, \\ M\|C_i\|_{W^{k+1,\infty}} h^{k+1-\frac{d}{2}}, & k>1, \end{cases}
\end{aligned}
$$

which indicates that both $\|\tilde{\boldsymbol{u}}\|_{[L^\infty]^d}$ *and* $\|\tilde{C}_i\|_{L^\infty}$ *are bounded.*

Finally, we give the error estimates for $\boldsymbol{u} - \boldsymbol{u_h}$, $\Phi - \Phi_h$ and $C_i - C_{i,h}$ in the following Theorem.

Theorem 4.5. *Let* $(\boldsymbol{u}, \Phi, C_1, C_2)$ *be the solution of (4.69)-(4.72) satisfying the regularity assumptions (4.82), and* $(\boldsymbol{u}_h, \Phi_h, C_{1,h}, C_{2,h})$ *be the finite element solution of (4.79)-(4.81), we have the following error estimates,*

$$\|\boldsymbol{u} - \boldsymbol{u_h}\|_{L^\infty(J;V)} + \|\Phi - \Phi_h\|_{L^\infty(J;L^2(\Omega))} \leq Mh^{k+1}, \tag{4.101}$$

$$\|C_i - C_{i,h}\|_{L^\infty(J;L^2(\Omega))} + h\|\nabla(C_i - C_{i,h})\|_{L^\infty(J;L^2(\Omega))} \leq Mh^{k+1}, \tag{4.102}$$

where M *is a constant independent of* h *and dependent of the regularity of* $\boldsymbol{u}$, Φ *and* C_i.

Proof. Subtract (4.81) from (4.72), for any given $c_i \in M_h$ we have,

$$(\partial_t(C_i - C_{i,h}), c_i) + (\nabla(C_i - C_{i,h}), \nabla c_i) + q_i(\boldsymbol{u}C_i - \boldsymbol{u}_h C_{i,h}, \nabla c_i) = 0. \tag{4.103}$$

Since

$$
\begin{aligned}
&q_i(\boldsymbol{u}C_i - \boldsymbol{u}_h C_{i,h}, \nabla c_i) \\
&\qquad = q_i(\boldsymbol{u}(C_i - \tilde{C}_i), \nabla c_i) + q_i((\boldsymbol{u} - \boldsymbol{u}_h)\tilde{C}_i, \nabla c_i) + q_i(\boldsymbol{u}_h(\tilde{C}_i - C_{i,h}), \nabla c_i),
\end{aligned}
$$

(4.103) can be written as

$$(\partial_t \xi_i, c_i) + (\partial_t \eta_i, c_i) + (\nabla \xi_i, \nabla c_i) + (\nabla \eta_i, \nabla c_i) + q_i(\boldsymbol{u}\eta_i, \nabla c_i) \\ + q_i\left((\boldsymbol{u} - \boldsymbol{u}_h)\tilde{C}_i, \nabla c_i\right) + q_i(\boldsymbol{u}_h \xi_i, \nabla c_i) = 0, \quad (4.104)$$

where $\xi_i = \tilde{C}_i - C_{i,h}$, $\eta_i = C_i - \tilde{C}_i$. Let $c_i = \xi_i$ and consider (4.94), we obtain

$$(\partial_t \xi_i, \xi_i) + (\nabla \xi_i, \nabla \xi_i) = -(\partial_t \eta_i, \xi_i) - q_i\left((\boldsymbol{u} - \boldsymbol{u}_h)\tilde{C}_i, \nabla \xi_i\right) - q_i(\boldsymbol{u}_h \xi_i, \nabla \xi_i). \quad (4.105)$$

In the following, we shall estimate the terms on the right hand side of (4.105), respectively, by means of Lemma 3.1-3.4.

$$\begin{aligned} (\partial_t \eta_i, \xi_i) &\leq \|\partial_t \eta_i\|_{L^2} \|\xi_i\|_{L^2} \\ &\leq Mh^{k+1} \left(\|C_i\|_{H^{k+1}} + \|\partial_t C_i\|_{H^{k+1}}\right) \|\xi_i\|_{L^2} \\ &\leq Mh^{2k+2} + \epsilon \|\xi_i\|_{L^2}^2, \end{aligned} \quad (4.106)$$

$$\begin{aligned} &\left((\boldsymbol{u} - \boldsymbol{u}_h)\tilde{C}_i, \nabla \xi_i\right) \\ \leq\ & \|\tilde{C}_i\|_{L^\infty} \|\boldsymbol{u} - \boldsymbol{u}_h\|_{[L^2]^d} \|\nabla \xi_i\|_{L^2} \\ \leq\ & M\left(\|\Phi\|_{H^{k+3}} h^{k+1} + \sum_{j=1}^{2} \|C_j - C_{j,h}\|_{L^2}\right) \|\nabla \xi_i\|_{L^2} \\ \leq\ & M\left(\|\Phi\|_{H^{k+3}} h^{k+1} + \sum_{j=1}^{2} \|C_j\|_{H^{k+1}} h^{k+1} + \sum_{j=1}^{2} \|\xi_j\|_{L^2}\right) \|\nabla \xi_i\|_{L^2} \\ \leq\ & M\left(h^{2k+2} + \sum_{j=1}^{2} \|\xi_j\|_{L^2}^2\right) + \epsilon \|\nabla \xi_i\|_{L^2}^2, \end{aligned}$$

$$(\boldsymbol{u}_h \xi_i, \nabla \xi_i) \leq \left(\|\boldsymbol{u}_h - \tilde{\boldsymbol{u}}\|_{[L^\infty]^d} + \|\tilde{\boldsymbol{u}}\|_{[L^\infty]^d}\right) \|\xi_i\|_{L^2} \|\nabla \xi_i\|_{L^2}.$$

By the inverse inequality and Lemma 4.8, we have

$$\|\boldsymbol{u}_h - \tilde{\boldsymbol{u}}\|_{[L^\infty]^d} \leq M h^{-\frac{d}{2}} \|\boldsymbol{u}_h - \tilde{\boldsymbol{u}}\|_{[L^2]^d} \leq M h^{-\frac{d}{2}} \sum_{j=1}^{2} \|C_j - C_{j,h}\|_{L^2}$$
$$\leq M h^{-\frac{d}{2}} \sum_{j=1}^{2} \left(\|\xi_j\|_{L^2} + \|\eta_j\|_{L^2}\right),$$

then by Lemma 4.9,

$$\begin{aligned}
& (\boldsymbol{u}_h \xi_i, \nabla \xi_i) \\
\leq \;& M h^{-\frac{d}{2}} \sum_{j=1}^{2} \left(\|\xi_j\|_{L^2} + \|C_j\|_{H^{k+1}} h^{k+1}\right) \|\xi_i\|_{L^2} \|\nabla \xi_i\|_{L^2} + M \|\xi_i\|_{L^2} \|\nabla \xi_i\|_{L^2} \\
\leq \;& M \left(h^{-\frac{d}{2}} \|\xi_i\|_{L^2} \|\nabla \xi_i\|_{L^2} \sum_{j=1}^{2} \|\xi_j\|_{L^2} + \|\xi_i\|_{L^2}^2 + \epsilon \|\nabla \xi_i\|_{L^2}^2 \right). \qquad (4.107)
\end{aligned}$$

Now we make an induction hypothesis as

$$h^{-\frac{d}{2}} \|\xi_i(t)\|_{L^2} \leq M, \quad \forall t \in [0, T^*]. \qquad (4.108)$$

Certainly, for any reasonable choice of the initial condition (4.108) holds for $t = 0$. Let (4.108) hold for $t \leq T^* < T$ for some $T^* > 0$. Thus, then

$$(\boldsymbol{u}_h \xi_i, \nabla \xi_i) \leq M \left(\sum_{j=1}^{2} \|\xi_j\|_{L^2}^2 + \epsilon \|\nabla \xi_i\|_{L^2}^2 \right).$$

So, (4.105) reads,

$$\frac{1}{2} \partial_t (\xi_i, \xi_i) + (\nabla \xi_i, \nabla \xi_i) \leq M \left(h^{2k+2} + \sum_{j=1}^{2} \|\xi_j\|_{L^2}^2 + \epsilon \|\nabla \xi_i\|_{L^2}^2 \right). \qquad (4.109)$$

Take integral with respect to t in (4.109), we have

$$\|\xi_i\|_0^2 + \int_0^t \|\nabla \xi_i(\tau)\|_0^2 d\tau \leq M \left(\sum_{j=1}^{2} \int_0^t \|\xi_j(\tau)\|_0^2 d\tau + h^{2k+2} \right),$$

and further,

$$\sum_{i=1}^{2} \left(\|\xi_i\|_0^2 + \int_0^t \|\nabla \xi_i(\tau)\|_0^2 d\tau \right) \leq M \left(\sum_{j=1}^{2} \int_0^t \|\xi_j(\tau)\|_0^2 d\tau + h^{2k+2} \right).$$

By Grönwall's inequality, for any $t \in [0, T^*]$, we attain

$$\sum_{i=1}^{2} \left(\|\xi_i\|^2_{L^\infty(J;L^2(\Omega))} + \|\nabla \xi_i\|^2_{L^2(J;L^2(\Omega))} \right) \leq M h^{2k+2},$$

thus for $i = 1, 2$,

$$\|\xi_i\|_{L^\infty(J;L^2(\Omega))} + \|\nabla \xi_i\|_{L^2(J;L^2(\Omega))} \leq M h^{k+1}, \tag{4.110}$$

where M depends on T and the regularity of $\boldsymbol{u}, \Phi$ and C_i $(i = 1, 2)$, but does not depend on h.

Note that since we require $k \geq 1$ in Taylor-Hood space, (4.110) implies that the induction hypothesis (4.108) holds for $t \in [0, T]$ in dimension $d = 2$ and 3, considering that $\|\xi_i(t)\|_{L^2}$ is a continuous function of t.

Therefore, combining with Lemma 4.9, we obtain the following error estimate, for any $t \in [0, T]$,

$$\|C_i - C_{i,h}\|_{L^\infty(J;L^2(\Omega))} + h\|\nabla(C_i - C_{i,h})\|_{L^2(J;L^2(\Omega))} \leq M h^{k+1}. \tag{4.111}$$

Then the combination of (4.92) and (4.111) leads to (4.101).

Finally, we give the error estimate of $\|\nabla(C_i - C_{i,h})\|_{L^\infty(J;L^2(\Omega))}$. Choose $c_i = \partial_t \xi_i$ in (4.104) and use (4.94), we obtain

$$\begin{aligned} &(\nabla \xi_i, \partial_t \nabla \xi_i) + (\partial_t \xi_i, \partial_t \xi_i) \\ &\qquad = -(\partial_t \eta_i, \partial_t \xi_i) - q_i \left((\boldsymbol{u} - \boldsymbol{u}_h)\tilde{C}_i, \partial_t \nabla \xi_i \right) - q_i(\boldsymbol{u}_h \xi_i, \nabla \partial_t \nabla \xi_i). \end{aligned} \tag{4.112}$$

By doing an analogous error analysis as above, we shall obtain

$$\|\nabla(C_i - C_{i,h})\|_{L^\infty(J;L^2(\Omega))} + \|\partial_t(C_i - C_{i,h})\|_{L^2(J;L^2(\Omega))} \leq M h^{k+1}.$$

Together with (4.111), we get (4.102).

□

4.3.4 Error analysis of the fully discrete scheme

In order to give the full discretiation of the system (4.69)-(4.72), we first define a uniform partition $0 = t_0 < t_1 < \cdots < t_N = T$ with time-step size $\Delta t = T/N$, then set $t^\kappa = \kappa\Delta t$ ($\kappa \in \mathcal{R}$). Let $\varphi^n = \varphi(t^n)$, $\varphi^{n+\frac{1}{2}} = \frac{\varphi^{n+1}+\varphi^n}{2}$, and $d_t\varphi^{n+\frac{1}{2}} = \frac{\varphi^{n+1}-\varphi^n}{\Delta t}$.

In the following, we employ Crank-Nicolson scheme to define the full discretization of finite element approximation for the system (4.69)-(4.72). For $n = 0, 1, \cdots$, suppose $(\boldsymbol{u}_h^n, \Phi_h^n, C_{1,h}^n, C_{2,h}^n)$ are given, find $(\boldsymbol{u}_h^{n+1}, \Phi_h^{n+1}, C_{1,h}^{n+1}, C_{2,h}^{n+1}) \in V_h \times W_h \times M_h \times M_h$ such that

$$A(\boldsymbol{u}_h^{n+\frac{1}{2}}, \boldsymbol{v}) + B(\boldsymbol{v}, \Phi_h^{n+\frac{1}{2}}) = -\left(r^{n+\frac{1}{2}}(C_{1,h}, C_{2,h}), \nabla\cdot\boldsymbol{v}\right), \forall \boldsymbol{v} \in V_h, \quad (4.113)$$

$$B(\boldsymbol{u}_h^{n+\frac{1}{2}}, \phi) = -\left(r^{n+\frac{1}{2}}(C_{1,h}, C_{2,h}), \phi\right), \forall \phi \in W_h, \quad (4.114)$$

$$(d_t C_{i,h}^{n+\frac{1}{2}}, c_i) + (\nabla C_{i,h}^{n+\frac{1}{2}}, \nabla c_i) + q_i(\boldsymbol{u}_h^{n+\frac{1}{2}} C_{i,h}^{n+\frac{1}{2}}, \nabla c_i) = (F_i^{n+\frac{1}{2}}, c_i), \forall c_i \in M_h, \quad (4.115)$$

where $r^{n+\frac{1}{2}}(C_{1,h}, C_{2,h}) = \sum_{i=1}^{2} q_i C_{i,h}^{n+\frac{1}{2}} + F_3^{n+\frac{1}{2}}$. We use Picard's method to linearize the nonlinear term in (4.115), and implement the following numerical algorithm to carry out the finite element computation for the proposed PNP system.

Algorithm 4.2. *1. Initialization for the time marching: set time step* $n = 0$ *and set* $(\boldsymbol{u}_h^0, \Phi_h^0, C_{1,h}^0, C_{2,h}^0)$ *as the initial values.*

2. Initialization for the nonlinear iteration: let $(\boldsymbol{u}_h^{n+1,0}, \Phi_h^{n+1,0}, C_{1,h}^{n+1,0}, C_{2,h}^{n+1,0}) = (u_h^n, \Phi_h^n, C_{1,h}^n, C_{2,h}^n)$ *as* $n \geq 0$.

3. Mixed finite element computation on each nonlinear iteration: For $m \geq 0$, *find* $(\boldsymbol{u}_h^{n+1,m+1}, \Phi_h^{n+1,m+1}, C_{1,h}^{n+1,m+1}, C_{2,h}^{n+1,m+1}) \in V_h \times W_h \times M_h \times M_h$ *such that*

$$A(\boldsymbol{u}_h^{n+\frac{1}{2},m+1}, \boldsymbol{v}) + B(\boldsymbol{v}, \Phi_h^{n+\frac{1}{2},m+1}) = -\left(r^{n+\frac{1}{2},m}(C_{1,h}, C_{2,h}), \nabla\cdot\boldsymbol{v}\right), \forall \boldsymbol{v} \in V_h,$$

$$B(\boldsymbol{u}_h^{n+\frac{1}{2},m+1}, \phi) = -\left(r^{n+\frac{1}{2},m}(C_{1,h}, C_{2,h}), \phi\right), \forall \phi \in W_h,$$

$$\left(\frac{C_{i,h}^{n+1,m+1} - C_{i,h}^{n}}{\Delta t}, c_i\right) + \left(\nabla C_{i,h}^{n+\frac{1}{2},m+1}, \nabla c_i\right) + q_i \left(\boldsymbol{u}_h^{n+\frac{1}{2},m} C_{i,h}^{n+\frac{1}{2},m+1}, \nabla c_i\right) = \left(F_i^{n+\frac{1}{2}}, c_i\right), \forall c_i \in M_h.$$

4. Checking the stopping criteria for the nonlinear iteration: For a given tolerance ϵ, *stop the iteration if*

$$\|\boldsymbol{u}_{i,h}^{n+1,m+1} - \boldsymbol{u}_{i,h}^{n+1,m}\|_{[L^2]^d} + \|\Phi_{i,h}^{n+1,m+1} - \Phi_{i,h}^{n+1,m}\|_{L^2} + \sum_{i=1}^{2} \|C_{i,h}^{n+1,m+1} - C_{i,h}^{n+1,m}\|_{L^2} \leq \epsilon, \quad (4.116)$$

and set $(\boldsymbol{u}_h^{n+1}, \Phi_h^{n+1}, C_{1,h}^{n+1}, C_{2,h}^{n+1}) = (\boldsymbol{u}_h^{n+1,m+1}, \Phi_h^{n+1,m+1}, C_{1,h}^{n+1,m+1}, C_{2,h}^{n+1,m+1})$ *. Otherwise, set* m *to* $m+1$ *and go to Step 3 to continue.*

5. Time marching: stop if $n+1 = N$. *Otherwise set* n *to* $n+1$ *and go to Step 2 to continue.*

Based on our semi-discrete analysis, we derive the analogous results for the fully discrete scheme in the following.

First of all, we assume the following regularity properties hold for $\boldsymbol{u}, \Phi$ and C_i $(i = 1, 2)$ in the full discretization analysis,

$$\begin{aligned} \boldsymbol{u} &\in W^{2,\infty}(J; [W^{k+1,\infty}]^d), \\ \Phi &\in W^{2,\infty}(J; H^{k+3} \cap W^{k+2,\infty}), \\ C_i &\in W^{3,\infty}(J; W^{k+1,\infty}). \end{aligned} \quad (4.117)$$

Similar to the analyses of Theorem 4.4 and Lemma 4.9, we have the following results.

Lemma 4.11. *Let $(\boldsymbol{u}, \Phi, C_1, C_2)$ be the solution of (4.69)-(4.72) satisfying the regularity assumptions (4.117), $(\boldsymbol{u}_h, \Phi_h, C_{1,h}, C_{2,h})$ be the solution of (4.113)-(4.115), and $\tilde{C}_i$ be defined in (4.94), for any $n = 0, 1, 2, ..., N$, we have the following error estimates*

$$\|\boldsymbol{u}^n - \boldsymbol{u}_h^n\|_V + \|\Phi^n - \Phi_h^n\|_{L^2} \leq M \left(h^{k+1} + \sum_{i=1}^{2} \|C_i^n - C_{i,h}^n\|_{L^2} \right), \tag{4.118}$$

$$\left\|\partial_t^\alpha \left(C_i^n - \tilde{C}_i^n\right)\right\|_{L^2} + h \left\|\partial_t^\alpha \left(C_i^n - \tilde{C}_i^n\right)\right\|_{H^1} \leq M h^{k+1}, \tag{4.119}$$

where where M is a constant independent of h and dependent of the regularity of $\boldsymbol{u}$, Φ and C_i, $\alpha = 0, 1, 2, 3$.

Next we give the error analysis of the fully discrete scheme based on Crank-Nicolson scheme (4.113)-(4.115) in the theorem below.

Theorem 4.6. *Let $(\boldsymbol{u}^R, \Phi^R, C_1^R, C_2^R)$, $1 \leq R \leq N$, be the solution of (4.69)-(4.72) at $t = R\Delta t$ satisfying the regularity assumptions (4.117), and $(\boldsymbol{u}_h^R, \Phi_h^R, C_{1,h}^R, C_{2,h}^R)$ be the solution of (4.113)-(4.115). We have the following error estimates,*

$$\|\boldsymbol{u}^R - \boldsymbol{u}_{\boldsymbol{h}}^R\|_V + \|\Phi^R - \Phi_h^R\|_{L^2} \leq M((\Delta t)^2 + h^{k+1}), \tag{4.120}$$

$$\|C_i^R - C_{i,h}^R\|_{L^2} + h\|\nabla(C_i^R - C_{i,h}^R)\|_{L^2} \leq M((\Delta t)^2 + h^{k+1}). \tag{4.121}$$

Proof. First, let each term in (4.94) take value at $t^{n+\frac{1}{2}} = (n + \frac{1}{2})\Delta t,\ 0 \leq n \leq N - 1$, then we have the following equation for the projection $\tilde{C}_i$,

$$\begin{aligned}&\left(\nabla(C_i(t^{n+\frac{1}{2}}) - \tilde{C}_i(t^{n+\frac{1}{2}})), \nabla c_i\right) \\ &\qquad + q_i \left(\boldsymbol{u}(t^{n+\frac{1}{2}}) \left(C_i(t^{n+\frac{1}{2}}) - \tilde{C}_i(t^{n+\frac{1}{2}})\right), \nabla c_i\right) = 0, \quad \forall c_i \in M_h,\end{aligned} \tag{4.122}$$

Let $\xi_i^n = \tilde{C}_i^n - C_{i,h}^n$, $\eta_i = C_i^n - \tilde{C}_i^n$, subtract (4.115) from (4.72), combine the projection equation (4.122) and choose $c_i = \xi_i^{n+\frac{1}{2}}$, we have

$$\left(\partial_t C_i(t^{n+\frac{1}{2}}) - d_t C_{i,h}^{n+\frac{1}{2}}, \xi_i^{n+\frac{1}{2}}\right) + \left(\nabla \tilde{C}_i(t^{n+\frac{1}{2}}) - \nabla C_{i,h}^{n+\frac{1}{2}}, \nabla \xi_i^{n+\frac{1}{2}}\right)$$
$$+ q_i \left(\boldsymbol{u}(t^{n+\frac{1}{2}})\tilde{C}_i(t^{n+\frac{1}{2}}) - \boldsymbol{u}_h^{n+\frac{1}{2}} C_{i,h}^{n+\frac{1}{2}}, \nabla \xi_i^{n+\frac{1}{2}}\right) = (F_i(t^{n+\frac{1}{2}}) - F_i^{n+\frac{1}{2}}, \xi_i^{n+\frac{1}{2}}). \quad (4.123)$$

Each term on the left hand side of (4.123) can be further derived as

$$\begin{aligned}
& \left(\partial_t C_i(t^{n+\frac{1}{2}}) - d_t C_{i,h}^{n+\frac{1}{2}}, \xi_i^{n+\frac{1}{2}}\right) \\
= \; & \left(\partial_t C_i(t^{n+\frac{1}{2}}) - d_t C_i^{n+\frac{1}{2}}, \xi_i^{n+\frac{1}{2}}\right) + \left(d_t \eta_i^{n+\frac{1}{2}}, \xi_i^{n+\frac{1}{2}}\right) + \left(d_t \xi_i^{n+\frac{1}{2}}, \xi_i^{n+\frac{1}{2}}\right) \\
= \; & \left(\partial_t C_i(t^{n+\frac{1}{2}}) - d_t C_i^{n+\frac{1}{2}}, \xi_i^{n+\frac{1}{2}}\right) + \left(\partial_t \eta_i(t^{n+\frac{1}{2}}), \xi_i^{n+\frac{1}{2}}\right) \\
& + \left(d_t \eta_i^{n+\frac{1}{2}} - \partial_t \eta_i(t^{n+\frac{1}{2}}), \xi_i^{n+\frac{1}{2}}\right) + \left(d_t \xi_i^{n+\frac{1}{2}}, \xi_i^{n+\frac{1}{2}}\right) \\
:= \; & G_1^n + G_2^n + G_3^n + G_4^n. \\
& \left(\nabla \tilde{C}_i(t^{n+\frac{1}{2}}) - \nabla C_{i,h}^{n+\frac{1}{2}}, \nabla \xi_i^{n+\frac{1}{2}}\right) \\
= \; & \left(\nabla(\tilde{C}_i(t^{n+\frac{1}{2}}) - \tilde{C}_i^{n+\frac{1}{2}}), \nabla \xi_i^{n+\frac{1}{2}}\right) + \left(\nabla \xi_i^{n+\frac{1}{2}}, \nabla \xi_i^{n+\frac{1}{2}}\right) \\
:= \; & G_5^n + G_6^n. \\
& q_i \left(\boldsymbol{u}(t^{n+\frac{1}{2}})\tilde{C}_i(t^{n+\frac{1}{2}}) - \boldsymbol{u}_h^{n+\frac{1}{2}} C_{i,h}^{n+\frac{1}{2}}, \nabla \xi_i^{n+\frac{1}{2}}\right) \\
= \; & q_i \left((\boldsymbol{u}(t^{n+\frac{1}{2}}) - \boldsymbol{u}_h^{n+\frac{1}{2}})\tilde{C}_i(t^{n+\frac{1}{2}}), \nabla \xi_i^{n+\frac{1}{2}}\right) + q_i \left(\boldsymbol{u}_h^{n+\frac{1}{2}}(\tilde{C}_i(t^{n+\frac{1}{2}}) - \tilde{C}_i^{n+\frac{1}{2}}), \nabla \xi_i^{n+\frac{1}{2}}\right) \\
& + q_i \left(\boldsymbol{u}_h^{n+\frac{1}{2}} \xi_i^{n+\frac{1}{2}}, \nabla \xi_i^{n+\frac{1}{2}}\right) \\
:= \; & G_7^n + G_8^n + G_9^n.
\end{aligned}$$

By Taylor's expansion, we have

$$\begin{aligned}
\partial_t \varphi(t^{n+\frac{1}{2}}) - d_t \varphi^{n+\frac{1}{2}} &= O(\Delta t)^2 |\partial_t^3 \varphi|, \\
\varphi(t^{n+\frac{1}{2}}) - \varphi^{n+\frac{1}{2}} &= O(\Delta t)^2 |\partial_t^2 \varphi|.
\end{aligned}$$

So by using Cauchy-Schwarz inequality and Young's inequality with ϵ, we have the following estimates

$$
\begin{aligned}
G_1^n &\leq M(\Delta t)^2\|C_i\|_{W^{3,\infty}(J;L^2)}\|\xi_i^{n+\frac{1}{2}}\|_{L^2} \leq M\left((\Delta t)^4\|C_i\|^2_{W^{3,\infty}(J;L^2)} + \|\xi_i^{n+\frac{1}{2}}\|^2_{L^2}\right),\\
G_2^n &\leq Mh^{k+1}\|\xi_i^{n+\frac{1}{2}}\|_{L^2} \leq M\left(h^{2k+2} + \|\xi_i^{n+\frac{1}{2}}\|^2_{L^2}\right),\\
G_3^n &\leq M(\Delta t)^2\|\eta_i\|_{W^{3,\infty}(J;L^2)}\|\xi_i^{n+\frac{1}{2}}\|_{L^2} \leq M\left((\Delta t)^4\|\eta_i\|^2_{W^{3,\infty}(J;L^2)} + \|\xi_i^{n+\frac{1}{2}}\|^2_{L^2}\right),\\
G_5^n &\leq M(\Delta t)^2\|\nabla\tilde{C}_i\|_{W^{2,\infty}(J;L^2)}\|\nabla\xi_i^{n+\frac{1}{2}}\|_{L^2}\\
&\leq M\left((\Delta t)^4\|\nabla\tilde{C}_i\|^2_{W^{2,\infty}(J;L^2)} + \epsilon\|\nabla\xi_i^{n+\frac{1}{2}}\|^2_{L^2}\right),\\
G_{10}^n &:= (F_i(t^{n+\frac{1}{2}}) - F_i^{n+\frac{1}{2}}, \xi_i^{n+\frac{1}{2}}) \leq M\left((\Delta t)^4\|F_i\|^2_{W^{2,\infty}(J;L^2)} + \epsilon\|\xi_i^{n+\frac{1}{2}}\|^2_0\right).
\end{aligned}
$$

Using the error estimate (4.93), we have

$$
\begin{aligned}
G_7^n &= q_i\left((\boldsymbol{u}(t^{n+\frac{1}{2}}) - \boldsymbol{u}^{n+\frac{1}{2}})\tilde{C}_i^{n+\frac{1}{2}}, \nabla\xi_i^{n+\frac{1}{2}}\right) + q_i\left((\boldsymbol{u}^{n+\frac{1}{2}} - \boldsymbol{u}_h^{n+\frac{1}{2}})\tilde{C}_i^{n+\frac{1}{2}}, \nabla\xi_i^{n+\frac{1}{2}}\right)\\
&\leq M(\Delta t)^2\|\boldsymbol{u}\|_{W^{2,\infty}(J;[L^2]^d)}\|\tilde{C}_i^{n+\frac{1}{2}}\|_{L^\infty}\|\nabla\xi_i^{n+\frac{1}{2}}\|_{L^2}\\
&+ M\left(h^{k+1} + \sum_{j=1}^{2}\left(\|\xi_j^{n+\frac{1}{2}}\|_{L^2} + \|\eta_j^{n+\frac{1}{2}}\|_{L^2}\right)\right)\|\tilde{C}_i^{n+\frac{1}{2}}\|_{L^\infty}\|\nabla\xi_i^{n+\frac{1}{2}}\|_{L^2}\\
&\leq M\left((\Delta t)^2\|\boldsymbol{u}\|_{W^{2,\infty}(J;[L^2]^d)} + h^{k+1} + \sum_{j=1}^{2}\|\xi_j^{n+\frac{1}{2}}\|_{L^2}\right)\|\tilde{C}_i^{n+\frac{1}{2}}\|_{L^\infty}\|\nabla\xi_i^{n+\frac{1}{2}}\|_{L^2}\\
&\leq M\left((\Delta t)^4\|\boldsymbol{u}\|^2_{W^{2,\infty}(J;[L^2]^d)} + h^{2k+2} + \sum_{j=0}^{2}\|\xi_j^{n+\frac{1}{2}}\|^2_{L^2}\right) + \epsilon\|\nabla\xi_i^{n+\frac{1}{2}}\|^2_{L^2},
\end{aligned}
$$

where where M is a constant independent of h and dependent of the regularity of $\boldsymbol{u}$, Φ and C_i,

In G_8^n and G_9^n, we shall apply mathematical induction again, since

$$
G_8^n = q_i\left((\boldsymbol{u}_h^{n+\frac{1}{2}} - \tilde{\boldsymbol{u}}^{n+\frac{1}{2}} + \tilde{\boldsymbol{u}}^{n+\frac{1}{2}})(\tilde{C}_i(t^{n+\frac{1}{2}}) - \tilde{C}_i^{n+\frac{1}{2}}), \nabla\xi_i^{n+\frac{1}{2}}\right)
$$

$$
\begin{aligned}
&\leq && M(\Delta t)^2 \left(\|\boldsymbol{u}_h^{n+\frac{1}{2}} - \tilde{\boldsymbol{u}}^{n+\frac{1}{2}}\|_{[L^\infty]^2} + \|\tilde{\boldsymbol{u}}^{n+\frac{1}{2}}\|_{[L^\infty]^d} \right) \|\tilde{C}_i\|_{W^{2,\infty}(J,L^2)} \|\nabla \xi_i^{n+\frac{1}{2}}\|_{L^2} \\
G_9^n &= && q_i \left((\boldsymbol{u}_h^{n+\frac{1}{2}} - \tilde{\boldsymbol{u}}^{n+\frac{1}{2}} + \tilde{\boldsymbol{u}}^{n+\frac{1}{2}}) \xi_i^{n+\frac{1}{2}}, \nabla \xi_i^{n+\frac{1}{2}} \right) \\
&\leq && \left(\|\boldsymbol{u}_h^{n+\frac{1}{2}} - \tilde{\boldsymbol{u}}^{n+\frac{1}{2}}\|_{[L^\infty]^d} + \|\tilde{\boldsymbol{u}}^{n+\frac{1}{2}}\|_{[L^\infty]^d} \right) \|\xi_i^{n+\frac{1}{2}}\|_{L^2} \|\nabla \xi_i^{n+\frac{1}{2}}\|_{L^2},
\end{aligned}
$$

then by inverse inequality and Lemma 4.8, we have

$$
\begin{aligned}
\|\boldsymbol{u}_h^{n+\frac{1}{2}} - \tilde{\boldsymbol{u}}^{n+\frac{1}{2}}\|_{[L^\infty]^d} &\leq Mh^{-\frac{d}{2}} \|\boldsymbol{u}_h^{n+\frac{1}{2}} - \tilde{\boldsymbol{u}}^{n+\frac{1}{2}}\|_{[L^2]^d} \\
&\leq Mh^{-\frac{d}{2}} \sum_{j=1}^{2} \left(\|\xi_j^{n+\frac{1}{2}}\|_{L^2} + \|\eta_j^{n+\frac{1}{2}}\|_{L^2} \right) \\
&\leq Mh^{k+1-\frac{d}{2}} + h^{-\frac{d}{2}} \sum_{j=1}^{2} \|\xi_j^{n+\frac{1}{2}}\|_{L^2}.
\end{aligned}
$$

Make the mathematical induction hypothesis as

$$
h^{-\frac{d}{2}} \|\xi_i^r\|_{L^2} \leq M, \quad 0 \leq r \leq R. \tag{4.124}
$$

Assume (4.124) holds for any $n = 0, 1, 2, ..., R$, $0 \leq R \leq N-2$, then

$$
\begin{aligned}
G_8^n &\leq M(\Delta t)^4 \|\tilde{C}_i\|_{W^{2,\infty}(J,L^2)} \left(1 + \|\tilde{\boldsymbol{u}}\|_{L^\infty(J;[L^\infty]^d)}\right) + 2\epsilon \|\nabla \xi_i^{n+\frac{1}{2}}\|_{L^2}^2 \\
G_9^n &\leq M \left(1 + \|\tilde{\boldsymbol{u}}\|_{L^\infty(J;[L^\infty]^d)}\right) \|\xi_i^{n+\frac{1}{2}}\|_{L^2}^2 + \epsilon \|\nabla \xi_i^{n+\frac{1}{2}}\|_{L^2}^2.
\end{aligned}
$$

Note the fact that $\|\tilde{\boldsymbol{u}}\|_{L^\infty(J;[L^\infty]^d)}$, $\|\partial_t^\alpha \tilde{C}_i\|_{L^\infty(J;L^2)}$, $(\alpha = 0, 1, 2, 3)$ are bounded following Lemma 4.10 and Lemma 4.11. Use the regularity of (4.117), we apply a summation of the time step n from 0 to R on both sides of (4.123), then

$$
\sum_{n=0}^{R} (G_4^n + G_6^n) = -\sum_{n=0}^{R} (G_1^n + G_2^n + G_3^n + G_5^n + G_7^n + G_8^n + G_9^n - G_{10}^n). \tag{4.125}
$$

Using the telescoping technique, and take ϵ sufficiently small, we thus obtain

$$
\frac{1}{2\Delta t} (\|\xi_i^{R+1}\|_0^2 - \|\xi_i^0\|_0^2) + \sum_{n=0}^{R} \|\nabla \xi_i^{n+\frac{1}{2}}\|_0^2 \;\leq\; M \left((\Delta t)^4 + h^{2k+2} + \sum_{n=0}^{R+1} \sum_{j=1}^{2} \|\xi_j^n\|_0^2 \right).
$$

Then by the discrete Grönwall's inequality, we have

$$\sum_{i=1}^{2} \|\xi_i^{R+1}\|_0^2 + \Delta t \sum_{n=0}^{R} \|\nabla \xi_i^{n+\frac{1}{2}}\|_0^2 \;\; \leq \;\; M((\Delta t)^4 + h^{2k+2} + \|\xi_i^0\|_0^2),$$

then we have

$$\|\xi_i^{R+1}\|_{L^2} + \left(\Delta t \sum_{n=0}^{R} \|\nabla \xi_i^{n+\frac{1}{2}}\|_{L^2}^2 \right)^{\frac{1}{2}} \;\; \leq \;\; M((\Delta t)^2 + h^{k+1} + \|\xi_i^0\|_{L^2}).$$

Since the initial value of C_i, C_i^0, are originally given, we can always properly prescribe the initial value for $C_{i,h}$, named as $C_{i,h}^0$, to approximate C_0 such that $\|\xi_i^0\|_{L^2} \leq M((\Delta t)^2 + h^{k+1})$, so that we have the following estimate

$$\|\xi_i^{R+1}\|_{L^2} + \left(\Delta t \sum_{n=0}^{R} \|\nabla \xi_i^{n+\frac{1}{2}}\|_{L^2}^2 \right)^{\frac{1}{2}} \;\; \leq \;\; M((\Delta t)^2 + h^{k+1}).$$

Finally, combining with (4.119), we obtain the following error estimate holding for any $R \in [0, N]$

$$\|C_i^R - C_{i,h}^R\|_{L^2} + \left(\Delta t \sum_{n=0}^{R} \|\nabla (C_i^{n+\frac{1}{2}} - C_{i,h}^{n+\frac{1}{2}})\|_{L^2}^2 \right)^{\frac{1}{2}} \leq M((\Delta t)^2 + h^{k+1}). \quad (4.126)$$

On the other hand, if choosing $c_i = d_t \xi_i^{n+\frac{1}{2}}$ in (4.123) instead of $\xi_i^{n+\frac{1}{2}}$ and proceeding the similar procedure shown as above, we can prove the error estimate of $C_i - C_{i,h}$ in $L^\infty(J, H^1)$ norm, that is, for $0 \leq R \leq N$

$$\|\nabla (C_i^R - C_{i,h}^R)\|_{L^2} \;\; \leq \;\; M((\Delta t)^2 + h^k). \quad (4.127)$$

Finally, (4.126) and (4.127) give us (4.121), and (4.118) gives us (4.120). □

Remark 4.5. The term

$$\left(\Delta t \sum_{n=0}^{R} \|\nabla (C_i^{n+\frac{1}{2}} - C_{i,h}^{n+\frac{1}{2}})\|_{L^2}^2 \right)^{\frac{1}{2}}$$

in (4.126) actually could be considered as the corresponding term to the $L^2(H^1)$ norm in semi-discretization. This is because

$$\begin{aligned}
&\int_0^{t_{R+1}} \|u(\tau)\|_{L^2}^2 d\tau = \sum_{n=0}^{R} \int_{t_n}^{t_{n+1}} \|u(\tau)\|_{L^2}^2 d\tau = \frac{\Delta t}{2} \sum_{n=0}^{R} \left(\|u^n\|_{L^2}^2 + \|u^{n+1}\|_{L^2}^2\right) \\
= \ & \frac{\Delta t}{2} \sum_{n=0}^{R} \int_\Omega \left((u^n)^2 + (u^{n+1})^2\right) dx \\
\geq \ & \Delta t \sum_{n=0}^{R} \int_\Omega \left(\frac{u^n + u^{n+1}}{2}\right)^2 dx = \Delta t \sum_{n=0}^{R} \|u^{n+\frac{1}{2}}\|_{L^2}^2.
\end{aligned}$$

Thus

$$\Delta t \sum_{n=0}^{R} \|\nabla(C_i^{n+\frac{1}{2}} - C_{i,h}^{n+\frac{1}{2}})\|_{L^2}^2 \leq \int_0^{t_{R+1}} \|\nabla(C_i(\tau) - C_{i,h}(\tau))\|_{L^2}^2 d\tau.$$

4.3.5 Numerical Experiments

In this section we will carry out some numerical experiments to test the performance of the mixed finite element method for PNP system.

Let

$$\left\{ \begin{array}{lcl}
\Phi & = & sin(\pi x)sin(\pi y)(1 - e^{-t}), \\
\boldsymbol{u} & = & (\pi cos(\pi x)sin(\pi y)(1 - e^{-t}),\ \pi sin(\pi x)cos(\pi y))\,(1 - e^{-t})), \\
C_1 & = & sin(2\pi x)sin(2\pi y)sin(t), \\
C_2 & = & sin(2\pi x)sin(2\pi y)sin(2t).
\end{array} \right.$$

be the real solutions of the following time-dependent PNP problem, for $t \in J$,

$$\left\{ \begin{array}{lll}
\partial_t C_1 - \nabla \cdot (\nabla C_1) - \nabla \cdot (\boldsymbol{u} C_1) = F_1, & (x, y) \in \Omega, & \\
\partial_t C_2 - \nabla \cdot (\nabla C_2) + \nabla \cdot (\boldsymbol{u} C_2) = F_2, & (x, y) \in \Omega, \boldsymbol{u} = \nabla \Phi, & (x, y) \in \Omega, \\
-\nabla \cdot \boldsymbol{u} = C_1 - C_2 + F_3, & (x, y) \in \Omega, &
\end{array} \right.$$

where $J = [0, 0.5]$ and $\Omega = [0, 1] \times [0, 1]$. F_1, F_2, F_3 are properly calculated using the above real solutions. The boundary conditions and initial conditions are homogeneous, which matches with the adopted real solutions on the boundary and at $t = 0$.

In the following, we use Algorithm 4.2 to find the approximate solution and compute the convergence errors in $L^\infty(J;[L^2]^d)$ and $L^\infty(J;V)$ norm for $\boldsymbol{u}$, and $L^\infty(J;L^2)$ and $L^\infty(J;H^1)$ norm for Φ, C_1 and C_2. The tolerance of nonlinear iteration in Algorithm 4.2 is taken as $\epsilon = 10^{-8}$.

Let $\Delta t = h$, $T = 0.5$. the numerical results of Taylor-Hood P^2P^1 mixed finite element for $(\boldsymbol{u}, \Phi)$ and P^1 finite element for C_1 and C_2 are reported in Table 4.7 - Table 4.9 by using uniform grids with sizes $h = 1/4$, $1/8$, $1/16$ and $1/32$.

Mesh size	$\|\boldsymbol{u} - \boldsymbol{u}_h\|_{L^\infty(J;V)}$	Order	$\|\Phi - \Phi_h\|_{L^\infty(J;L^2)}$	Order
1/4	7.4166E-2	-	8.4328E-3	-
1/8	1.8468E-2	2.00	1.6915E-3	2.32
1/16	4.6217E-3	2.00	4.1450E-4	2.03
1/32	1.1557E-3	2.00	1.0309E-4	2.01
1/64	2.8895E-4	2.00	2.5468E-5	2.02

Table 4.7. Numerical results for $\boldsymbol{u} - \boldsymbol{u}_h$ and $\Phi - \Phi_h$

Mesh size	$\|C_1 - C_{1,h}\|_{L^\infty(J;L^2)}$	Order	$\|C_1 - C_{1,h}\|_{L^\infty(J;H^1)}$	Order
1/4	5.7490E-2	-	9.5555E-1	-
1/8	1.4165E-2	2.02	4.8083E-1	0.99
1/16	3.5187E-3	2.01	2.4117E-1	1.00
1/32	8.7938E-4	2.00	1.2069E-1	1.00
1/64	2.1982E-4	2.00	6.0361E-2	1.00

Table 4.8. Numerical results for $C_1 - C_{1,h}$

Mesh size	$\|C_2 - C_{2,h}\|_{L^\infty(J;L^2)}$	Order	$\|C_2 - C_{2,h}\|_{L^\infty(J;H^1)}$	Order
1/4	1.0433E-1	-	1.6771	-
1/8	2.5835E-2	2.01	8.4381E-1	0.99
1/16	6.4406E-3	2.00	4.2328E-1	1.00
1/32	1.6100E-3	2.00	2.1183E-1	1.00
1/64	4.0250E-4	2.00	1.0594E-1	1.00

Table 4.9. Numerical results for $C_2 - C_{2,h}$

From these tables, we can clearly observe the second-order convergence ('Order' in Tables) in $L^\infty(J;V)$ norm for $\boldsymbol{u}$ and in $L^\infty(J;L^2)$ norm for Φ, C_1, C_2; and the first-order convergence in $L^\infty(J;H^1)$ norm for C_1, C_2, which verify our theories in Theorem 4.6.

CHAPTER 5

NEW FUEL CELL MODEL

5.1 A new fuel cell model based on PNP equations

This chapter is a continuation of the model studies in Chapter 3 and Chapter 4. Here we propose a new fuel cell model that utilize the PNP model to replace the Butler-Volmer equation so the model is no longer limited to the strong assumption of equilibrium condition. The focus the changes of the new model is mainly on the transfer current density, j, which is adopted to define the electrochemical kinetics, and all the source/sink term of the governing equations of the traditional fuel cell model are the functional of j. We know that the transfer current density j is defined by Butler-Volmer equation based on the assumption of local equilibrium or electroneutrality of the electrolyte [Biesheuvel et al. (2009)]. The innovation of the new fuel cell model supposes to substitute the ionic concentrations for the transfer current density j in an appropriate fashion, thus the ionic concentration equations will be introduced, together with the electrostatic potential equation which essentially relates to the protonic and electronic potential equations, therefore, the PNP system is introduced into the new fuel cell model, coupling with Brinkman model, two-phase transport equations of species concentrations, and/or energy equation. The governing equations of the new fuel cell model are attempted to be defined as follows in a heuristic and not very accurate fashion.

$$
\left\{
\begin{array}{ll}
\partial_t C^J - \nabla \cdot (D_g^J \nabla C^J) + \nabla \cdot (\boldsymbol{u} C^J) = 0, & \text{in gas channel} \\
\partial_t C^J - \nabla \cdot (D_g^J \nabla C^J) + \nabla \cdot (\gamma_c \boldsymbol{u} C^J) - G_J = S_J(j) + & \nabla \cdot (\frac{C^J}{\rho_g} \Gamma \nabla C^J), \\
 & \text{in porous media,}
\end{array}
\right. \tag{5.1}
$$

where $J = H_2O,\ O_2,\ H_2$.

$$
\partial_t C_i - \nabla \cdot (\nabla C_i + q_i C_i \nabla(\Phi_s - \Phi_e)) = F_i, \quad i = 1, 2, \tag{5.2}
$$

$$
\partial_t \boldsymbol{u} + \tfrac{1}{\epsilon^2} \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = \nabla \cdot (\mu \nabla \boldsymbol{u}) - \nabla p - \tfrac{\mu}{K} \boldsymbol{u}, \tag{5.3}
$$

$$
\nabla \cdot (\rho \boldsymbol{u}) = S_m(j), \tag{5.4}
$$

$$
\partial_t T + \nabla \cdot (K \nabla T) + \nabla \cdot (\gamma_T \rho c_p \boldsymbol{u} T) = S_T(j), \tag{5.5}
$$

$$
\nabla \cdot (\kappa^{eff} \nabla \Phi_e) = S_{\Phi_e}(j), \tag{5.6}
$$

$$
\nabla \cdot (\sigma_s^{eff} \nabla \Phi_s) = S_{\Phi_s}(j), \tag{5.7}
$$

where, j is the newly developed transfer current density of the reaction, defined as follows in terms of the ionic concentrations which are derived from the Nernst-Planck equations (5.2).

$$
j = \frac{e}{\epsilon_0}(C_1 - C_2),
$$

where, e denotes the electron charge, and ϵ_0 the permittivity of free space.

5.2 Error analysis of PNP-Brinkman coupling system

In this section, we focus on the numerical analysis for the combination of PNP equations and the modified Stokes (Brinkman) equations since these two systems are the core part of the new fuel cell model (5.1)-(5.7), which are also crucial for other electrohydrodynamical problems. We will leave the analysis for a more broader combination of other governing equations in the new fuel cell model (5.1)-(5.7), i.e., the species transports and energy equations, for the future work. The fundamental analysis techniques used in these numerical analyses shall be analogous to those employed in Chapters 3 and 4, but the overall numerical analysis will be in a more sophisticated manner.

Let $\Omega = \Omega_D \cup \Omega_S \in \mathbb{R}^d$ $(d = 2, 3)$, Ω_D denotes the Darcy domain and Ω_S the Stokes domain, $\Gamma = \partial\Omega_D \cap \partial\Omega_S$ represents the interface of Ω_D and Ω_S. The governing equations are defined in Ω given as [Jerome (2011); Brinkman (1949)]:

$$\partial_t C_i - \nabla \cdot (\nabla C_i + q_i \boldsymbol{\Psi} C_i - \boldsymbol{u} C_i) = F_i, \tag{5.8}$$

$$\boldsymbol{\Psi} = \nabla \Phi, \tag{5.9}$$

$$-\nabla \cdot \boldsymbol{\Psi} = (C_1 - C_2) + F_3, \tag{5.10}$$

$$\partial_t \boldsymbol{u} - \Delta \boldsymbol{u} + \nabla p + \tfrac{1}{K} \boldsymbol{u} = -(C_1 - C_2)\boldsymbol{\Psi} + \boldsymbol{F}_4, \tag{5.11}$$

$$-\nabla \cdot \boldsymbol{u} = 0, \tag{5.12}$$

where $\partial_t = \partial/\partial t$. Φ is the electrostatic potential, C_i, $i = 1, 2$, are the mass concentration of ions carrying charge q_i (For example $q_{K+} = 1$, $q_{Cl} = -1$), $\boldsymbol{u}$ is the velocity, p is the pressure. The parameter K is a piecewise constant defined as

$$K = \begin{cases} K_D, & \text{in } \Omega_D, \\ K_S, & \text{in } \Omega_S, \end{cases}$$

where $0 < K_{min} \leq K_D < 1$ and $1 < K_S \leq K_{max} < \infty$. As a consequence, the right hand side $\boldsymbol{F}_4$ turns out to be a piecewise function defined as

$$\boldsymbol{F}_4 = \begin{cases} \boldsymbol{f}_D, & \text{in } \Omega_D, \\ \boldsymbol{f}_S, & \text{in } \Omega_S. \end{cases}$$

(5.8)-(5.12) shall incorporate with some prescribed boundary conditions and initial conditions in order to fulfill the well-posedness property. The existence of a solution to a time dependent Navier-Stokes problem has been proven by Leray [Leray (1934)] and Hopf [Hopf (1951)]. Uniqueness is still an open problem in the three-dimensional case, whereas for $d = 2$ the solution $\boldsymbol{u}$ has been shown to belong to $C^0([0,T]; H_{div})$ and to be unique [Ladyzhenskaya (1958); Lions and Prodi (1959)]. Our problem (5.11)-(5.12) is a time dependent Stokes problem which is the linear counter part of a time dependent Navier-Stokes problem, we can have the wellposedness of the such a solution with nonlinear right hand side of 2 dimensional case achieved from the theories above.

Let $H(div;\Omega)$ be the set of vector functions $\boldsymbol{\Psi} \in [L^2(\Omega)]^d$, such that $\nabla\cdot\boldsymbol{\Psi} \in L^2(\Omega)$. Define

$$V := H(div;\Omega) \tag{5.13}$$

and

$$\|\boldsymbol{\Psi}\|_V^2 = \|\boldsymbol{\Psi}\|_{L^2}^2 + \|\nabla\cdot\boldsymbol{\Psi}\|_{L^2}^2 \tag{5.14}$$

From (5.9), we know that without reinforcing Φ with any boundary conditions, its numerical solution is determined only up to an arbitrary additive constant. We shall define

$$W = L^2(\Omega)/\{\phi \equiv constant\ on\ \Omega\}. \tag{5.15}$$

We also define

$$U = [H_0^1(\Omega)]^d, \quad Q = L_0^2(\Omega) = \{q \in L^2(\Omega), \int q dx = 0\}. \tag{5.16}$$

Let

$$r(C_1, C_2) = \sum_{i=1}^{2} q_i C_i + F_3.$$

It is clear that, using (5.10), one can consider, in place of (5.9), the alternative setting [Brezzi et al. (1993)] is

$$\boldsymbol{\Psi} - \nabla(\nabla \cdot \boldsymbol{\Psi}) = \nabla \Phi + \nabla r(C_1, C_2). \tag{5.17}$$

For $\boldsymbol{\Psi}, \boldsymbol{\psi} \in V$, $\Phi \in W$, $\boldsymbol{u}, \boldsymbol{v} \in U$ and $p \in Q$, define the bilinear forms as follows,

$$\alpha(\boldsymbol{\Psi}, \boldsymbol{\psi}) = (\boldsymbol{\Psi}, \boldsymbol{\psi}) + (\nabla \cdot \boldsymbol{\Psi}, \nabla \cdot \boldsymbol{\psi}), \tag{5.18}$$

$$\beta(\boldsymbol{\psi}, \Phi) = (\nabla \cdot \boldsymbol{\psi}, \Phi), \tag{5.19}$$

$$a(\boldsymbol{u}, \boldsymbol{v}) = \frac{1}{K_D}(\boldsymbol{u}, \boldsymbol{v})_D + \frac{1}{K_S}(\boldsymbol{u}, \boldsymbol{v})_S + (\nabla \boldsymbol{u}, \nabla \boldsymbol{v}), \tag{5.20}$$

$$b(\boldsymbol{v}, p) = -(\nabla \cdot \boldsymbol{v}, p), \tag{5.21}$$

The governing equations (5.8)-(5.12) can be treated by the following weak form by finding $(C_1, C_2, \boldsymbol{\Psi}, \Phi, \boldsymbol{u}, p) \in M \times M \times V \times W \times U \times Q$ such that,

$$(\partial_t C_i, c) + (\nabla C_i, \nabla c) + q_i(\boldsymbol{\Psi} C_i, \nabla c) - (\boldsymbol{u} C_i, \nabla c) = (F_i, c), \qquad \forall c \in H_0^1, \tag{5.22}$$

$$\alpha(\boldsymbol{\Psi}, \boldsymbol{\psi}) + \beta(\boldsymbol{\psi}, \Phi) = -(r(C_1, C_2), \nabla \cdot \boldsymbol{\psi}), \qquad \forall \boldsymbol{\psi} \in V, \tag{5.23}$$

$$\beta(\boldsymbol{\Psi}, \phi) = -(r(C_1, C_2), \phi), \qquad \forall \phi \in W, \tag{5.24}$$

$$(\partial_t \boldsymbol{u}, \boldsymbol{v}) + a(\boldsymbol{u}, \boldsymbol{v}) - b(\boldsymbol{v}, p) = -((C_1 - C_2)\boldsymbol{\Psi}, \boldsymbol{v}) + (\boldsymbol{F}_4, \boldsymbol{v}), \qquad \forall \boldsymbol{v} \in U, \tag{5.25}$$

$$b(\boldsymbol{u}, q) = 0, \qquad \forall q \in Q. \tag{5.26}$$

The semi-discrete mixed finite element approximation for the problem (5.8)-(5.12) is defined by: find $(C_{1,h}, C_{2,h}, \boldsymbol{\Psi}_h, \Phi_h, \boldsymbol{u}_h, p_h) \in M_h \times M_h \times V_h \times W_h \times U_h \times Q_h$ such that, $\forall (c, \boldsymbol{\psi}, \phi, \boldsymbol{v}, q) \in M_h \times V_h \times W_h \times U_h \times Q_h$,

$$(\partial_t C_{i,h}, c) + (\nabla C_{i,h}, \nabla c) + q_i(\boldsymbol{\Psi}_h C_{i,h}, \nabla c) - (\boldsymbol{u}_h C_{i,h}, \nabla c) = (F_i, c), \tag{5.27}$$

$$\alpha(\boldsymbol{\Psi}_h, \boldsymbol{\psi}) + \beta(\boldsymbol{\psi}, \Phi_h) = -(r(C_{1,h}, C_{2,h}), \nabla \cdot \boldsymbol{\psi}), \tag{5.28}$$

$$\beta(\boldsymbol{\Psi}_h, \phi) = -(r(C_{1,h}, C_{2,h}), \phi), \tag{5.29}$$

$$(\partial_t \boldsymbol{u}_h, \boldsymbol{v}) + a(\boldsymbol{u}_h, \boldsymbol{v}) - b(\boldsymbol{v}, p_h) = -((C_{1,h} - C_{2,h})\boldsymbol{\Psi}_h, \boldsymbol{v}) + (\boldsymbol{F}_4, \boldsymbol{v}), \tag{5.30}$$

$$b(\boldsymbol{u}_h, q) = 0. \tag{5.31}$$

In the following, we assume the following regularity properties hold for C_1, C_2, $\boldsymbol{\Psi}$, Φ, $\boldsymbol{u}$, p,

$$C_i \in W^{1,\infty}(0,T; W^{s+1,\infty}) \tag{5.32}$$

$$\boldsymbol{\Psi} \in W^{1,\infty}(0,T; [W^{s+1,\infty}]^d), \tag{5.33}$$

$$\Phi \in W^{1,\infty}(0,T; H^{s+3} \cap W^{s+2,\infty}), \tag{5.34}$$

$$\boldsymbol{u} \in L^2(0,T; [H^{s+2}]^d \cap [L^\infty]^d \cap [H_0^1]^d), \tag{5.35}$$

$$p \in L^2(0,T; H^{s+1} \cap L_0^2), \tag{5.36}$$

We define the projection $(\tilde{\boldsymbol{\Psi}}, \tilde{\Phi}) \in V_h \times W_h$, as follows,

$$\alpha(\tilde{\boldsymbol{\Psi}}, \boldsymbol{\psi}) + \beta(\boldsymbol{\psi}, \tilde{\Phi}) = -(r(C_1, C_2), \nabla \cdot \boldsymbol{\psi}), \tag{5.37}$$

$$\beta(\tilde{\boldsymbol{\Psi}}, \phi) = -(r(C_1, C_2), \phi). \tag{5.38}$$

Then we have the classic result for the max norm given in the following lemma,

Lemma 5.1. *Let $\boldsymbol{\Psi}$ be the solution of (5.23) satisfying the regularity assumption (5.33), and $\boldsymbol{\Psi}_h$ be the finite element solution of (5.28). Suppose that $\tilde{\boldsymbol{\Psi}}$ and $\tilde{\Phi}$ are defined in (5.37) and (5.38), respectively, then we have the following error estimate,*

$$\|\boldsymbol{\Psi} - \tilde{\boldsymbol{\Psi}}\|_{[L^\infty]^d} \le M\|\Phi\|_{W^{s+2,\infty}} |\ln h| h^{s+2-\frac{d}{2}}. \tag{5.39}$$

Remark 5.1. Since $h^2 < h|\ln h| < 1$, we can change (5.39) as follows,

$$\|\boldsymbol{\Psi} - \tilde{\boldsymbol{\Psi}}\|_{[L^\infty]^d} \le M\|\Phi\|_{W^{s+2,\infty}} h^{s+1-\frac{d}{2}}. \tag{5.40}$$

Moreover, this indicates that $\|\boldsymbol{\Psi} - \tilde{\boldsymbol{\Psi}}\|_{[L^\infty]^d}$ and $\|\tilde{\boldsymbol{\Psi}}\|_{[L^\infty]^d}$ are bounded.

By the analysis of PNP equations with mixed finite element method, we know that (5.23)-(5.24) has a unique solution, and moreover, we have the following lemma

Lemma 5.2. *Let $(C_1, C_2, \boldsymbol{\Psi}, \Phi)$ be the solution of (5.22)-(5.24) satisfying the regularity assumptions (5.32)-(5.34), and $(C_{1,h}, C_{2,h}, \boldsymbol{\Psi}_h, \Phi_h)$ be the finite element solution of (5.27)-(5.29), then we have the following error estimate,*

$$\|\boldsymbol{\Psi} - \boldsymbol{\Psi}_h\|_{[L^2]^d} + h\|\boldsymbol{\Psi} - \boldsymbol{\Psi}_h\|_V + \|\Phi - \Phi_h\|_{L^2} \\ \leq M(h^{s+1}\|\Phi\|_{H^{s+3}} + \sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2}). \quad (5.41)$$

Since $a(\boldsymbol{u}, \boldsymbol{v})$ is coercive and continuous, $b(\boldsymbol{v}, p)$ is continuous and also satisfy the LBB condition, by Brezzi's theory, there is a unique solution to (5.25)-(5.26). It is frequently valuable to decompose the analysis of the convergence of finite element methods by passing through a projection of the solution of the differential problem into the finite element space. Consider the projection $(\tilde{\boldsymbol{u}}, \tilde{p}) \in U_h \times Q_h$ given by

$$a(\tilde{\boldsymbol{u}}, \boldsymbol{v}) - b(\boldsymbol{v}, \tilde{p}) = -((C_1 - C_2)\boldsymbol{\Psi}, \boldsymbol{v}) + (\boldsymbol{F}_4, \boldsymbol{v}), \qquad \forall \boldsymbol{v} \in U_h, \quad (5.42)$$

$$b(\tilde{\boldsymbol{u}}, q) = 0, \qquad \forall q \in Q_h. \quad (5.43)$$

By Theorem 4.1 of Brinkman, we have the following lemma.

Lemma 5.3. *Let $(\boldsymbol{u}, p)$ be the solution of (5.25)-(5.26) satisfying the regularity assumptions (5.35)-(5.36). Suppose $\tilde{\boldsymbol{u}}$ and $\tilde{p}$ are defined in (5.42) and (5.43), respectively, then we have the following error estimates,*

$$\|\boldsymbol{u} - \tilde{\boldsymbol{u}}\|_{L^2} + h\|\boldsymbol{u} - \tilde{\boldsymbol{u}}\|_{H^1} \leq Mh^{s+2}\left(\left(\frac{K_S}{K_D} + 1\right)\|\boldsymbol{u}\|_{H^{s+2}} + K_S\|p\|_{H^{s+1}}\right), \quad (5.44)$$

$$\|p - \tilde{p}\|_{L^2} \leq M h^{s+1} \left(\frac{K_S}{K_D} + 1 \right) \left(\frac{1}{K_D} \|\boldsymbol{u}\|_{H^{s+2}} + \|p\|_{H^{s+1}} \right). \tag{5.45}$$

Remark 5.2. For the sake of the simplification of later proofs, we further deduce (5.44)-(5.45) to the following equations,

$$\|\boldsymbol{u} - \tilde{\boldsymbol{u}}\|_{[L^2]^d} + h\|\boldsymbol{u} - \tilde{\boldsymbol{u}}\|_{[H^1]^d} \leq M \frac{K_S}{K_D} h^{s+2} \left(\|\boldsymbol{u}\|_{H^{s+2}} + \|p\|_{H^{s+1}} \right), \tag{5.46}$$

$$\|p - \tilde{p}\|_{L^2} \leq M \frac{K_S}{K_D^2} h^{s+1} \left(\|\boldsymbol{u}\|_{H^{s+2}} + \|p\|_{H^{s+1}} \right). \tag{5.47}$$

Also by the results given in [Girault et al. (2005)], we also have the following results.

Lemma 5.4. *Let* $(\boldsymbol{u}, p)$ *be the solution of (5.25)-(5.26) satisfying the regularity assumptions (5.35)-(5.36), and* p_h *be the finite element solution of (5.31). Suppose that* $\tilde{\boldsymbol{u}}$ *is defined in (5.42), then we have the following error estimate,*

$$\|\nabla(\boldsymbol{u} - \tilde{\boldsymbol{u}})\|_{[L^\infty]^d} + \|p - p_h\|_{L^\infty} \leq M h^{s+1} (\|\boldsymbol{u}\|_{[H^{s+1}]^d} + \|p\|_{H^{s+1}}) \tag{5.48}$$

Next, we consider the error estimates of $\boldsymbol{u} - \boldsymbol{u}_h$ and $p - p_h$.

Theorem 5.1. *Let* $(C_i, \boldsymbol{u}, p)$ *be the solution of (5.22), (5.25) and (5.26), respectively, satisfying the regularity assumptions (5.32), (5.35) and (5.36), and* $(C_{i,h}, \boldsymbol{u}_h, p_h)$ *be the finite element solution of (5.27) (5.25) and (5.31), respectively, then we have the following error estimates,*

$$\|\boldsymbol{u} - \boldsymbol{u}_h\|_{L^2([L^2]^d)} \leq M h^{-\frac{d}{2}} \left(\sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2} \right)^2 + M \sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2} + M \frac{K_S}{K_D} h^{s+2}. \tag{5.49}$$

$$\frac{1}{K_S}\|\boldsymbol{u}-\boldsymbol{u}_h\|_{L^\infty(U)}$$
$$\le Mh^{-\frac{d}{2}}\left(\sum_{i=1}^{2}\|C_i-C_{i,h}\|_{L^2}\right)^2+M\sum_{i=1}^{2}\|C_i-C_{i,h}\|_{L^2}+M\frac{K_S}{K_D}h^{s+1}. \quad (5.50)$$

$$\|p-p_h\|_Q$$
$$\le M\frac{K_S}{K_D}h^{-\frac{d}{2}}\left(\sum_{i=1}^{2}\|C_i-C_{i,h}\|_{L^2}\right)^2+M\frac{K_S}{K_D}\sum_{i=1}^{2}\|C_i-C_{i,h}\|_{L^2}+M\frac{K_S^2}{K_D^2}h^{s+1}. \quad (5.51)$$

Proof. Subtract (5.30) and (5.31) from (5.42) and (5.43), we have

$$(\partial_t\boldsymbol{u}-\partial_t\boldsymbol{u}_h,\boldsymbol{v})+a(\tilde{\boldsymbol{u}}-\boldsymbol{u}_h,\boldsymbol{v})-b(\boldsymbol{v},\tilde{p}-p_h)=-\sum_{i=1}^{2}q_i(C_i\boldsymbol{\Psi}-C_{i,h}\boldsymbol{\Psi}_h,\boldsymbol{v}), \quad (5.52)$$

$$b(\tilde{\boldsymbol{u}}-\boldsymbol{u}_h,q)=0. \quad (5.53)$$

Choose $\boldsymbol{v}=\tilde{\boldsymbol{u}}-\boldsymbol{u}_h$ and $q=\tilde{p}-p_h$, then

$$(\partial_t\boldsymbol{u}-\partial_t\boldsymbol{u}_h,\tilde{\boldsymbol{u}}-\boldsymbol{u}_h)+a(\tilde{\boldsymbol{u}}-\boldsymbol{u}_h,\tilde{\boldsymbol{u}}-\boldsymbol{u}_h)=-\sum_{i=1}^{2}q_i(C_i\boldsymbol{\Psi}-C_{i,h}\boldsymbol{\Psi}_h,\tilde{\boldsymbol{u}}-\boldsymbol{u}_h) \quad (5.54)$$

By Poincaré inequality, we have

$$-\sum_{i=1}^{2}q_i((C_i-C_{i,h})\boldsymbol{\Psi},\tilde{\boldsymbol{u}}-\boldsymbol{u}_h)\le M\sum_{i=1}^{2}\|\boldsymbol{\Psi}\|_{[L^\infty]^d}\|C_i-C_{i,h}\|_{L^2}\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_U, \quad (5.55)$$

then by inverse inequality and (5.41), we have

$$\begin{aligned}
&-\sum_{i=1}^{2}q_i(C_{i,h}(\boldsymbol{\Psi}-\boldsymbol{\Psi}_h),\tilde{\boldsymbol{u}}-\boldsymbol{u}_h)\\
=&\sum_{i=1}^{2}q_i((C_i-C_{i,h})(\boldsymbol{\Psi}-\boldsymbol{\Psi}_h),\tilde{\boldsymbol{u}}-\boldsymbol{u}_h)-\sum_{i=1}^{2}q_i(C_i(\boldsymbol{\Psi}-\boldsymbol{\Psi}_h),\tilde{\boldsymbol{u}}-\boldsymbol{u}_h)\\
\le&\sum_{i=1}^{2}\|C_i-C_{i,h}\|_{L^2}\|\boldsymbol{\Psi}-\boldsymbol{\Psi}_h\|_{[L^2]^d}h^{-\frac{d}{2}}\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_{[L^2]^d}\\
&+\sum_{i=1}^{2}\|C_i\|_{L^\infty}\|\boldsymbol{\Psi}-\boldsymbol{\Psi}_h\|_{[L^2]^d}\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_{[L^2]^d}
\end{aligned}$$

$$\begin{aligned}
&\leq Mh^{-\frac{d}{2}}\sum_{i=1}^{2}\|C_i-C_{i,h}\|_{L^2}\|\boldsymbol{\Psi}-\boldsymbol{\Psi}_h\|_{[L^2]^d}\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_U \\
&\quad +M\sum_{i=1}^{2}\|C_i\|_{L^\infty}\|\boldsymbol{\Psi}-\boldsymbol{\Psi}_h\|_{[L^2]^d}\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_U \\
&\leq Mh^{-\frac{d}{2}}\left(\sum_{i=1}^{2}\|C_i-C_{i,h}\|_{L^2}\right)^2\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_U+M\sum_{i=1}^{2}\|C_i-C_{i,h}\|_{L^2}\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_U.
\end{aligned}$$

So now we have

$$\begin{aligned}
&(\partial_t\tilde{\boldsymbol{u}}-\partial_t\boldsymbol{u}_h,\tilde{\boldsymbol{u}}-\boldsymbol{u}_h)+a(\tilde{\boldsymbol{u}}-\boldsymbol{u}_h,\tilde{\boldsymbol{u}}-\boldsymbol{u}_h) \\
&= -\sum_{i=1}^{2}q_i((C_i-C_{i,h})\boldsymbol{\Psi},\tilde{\boldsymbol{u}}-\boldsymbol{u}_h)-\sum_{i=1}^{2}q_i(C_{i,h}(\boldsymbol{\Psi}-\boldsymbol{\Psi}_h),\tilde{\boldsymbol{u}}-\boldsymbol{u}_h) \\
&\quad -(\partial_t\boldsymbol{u}-\partial_t\tilde{\boldsymbol{u}},\tilde{\boldsymbol{u}}-\boldsymbol{u}_h) \\
&\leq Mh^{-\frac{d}{2}}\left(\sum_{i=1}^{2}\|C_i-C_{i,h}\|_{L^2}\right)^2\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_U+M\sum_{i=1}^{2}\|C_i-C_{i,h}\|_{L^2}\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_U \\
&\quad +M\frac{K_S}{K_D}h^{s+2}\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_U,
\end{aligned}$$

and further by the coercivity of $a(\boldsymbol{u}_h,\boldsymbol{v}_h)$, we have,

$$\begin{aligned}
&\frac{1}{2}\partial_t\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_{[L^2]^d}^2+\frac{1}{K_S}\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_U^2 \\
&\leq Mh^{-\frac{d}{2}}\left(\sum_{i=1}^{2}\|C_i-C_{i,h}\|_{L^2}\right)^2\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_U+M\sum_{i=1}^{2}\|C_i-C_{i,h}\|_{L^2}\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_U \\
&\quad +M\frac{K_S}{K_D}h^{s+2}\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_U.
\end{aligned}$$

Use Young's inequality with ϵ, then take integral on both sides with respect to t, and finally use Grönwall's inequality, we get that

$$\begin{aligned}
&\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_{L^2([L^2]^d)}+\frac{1}{K_S}\|\tilde{\boldsymbol{u}}-\boldsymbol{u}_h\|_{L^\infty(U)} \\
&\qquad \leq Mh^{-\frac{d}{2}}\left(\sum_{i=1}^{2}\|C_i-C_{i,h}\|_{L^2}\right)^2+M\sum_{i=1}^{2}\|C_i-C_{i,h}\|_{L^2}+M\frac{K_S}{K_D}h^{s+2}. \quad (5.56)
\end{aligned}$$

By (5.46), we can get the following error estimate (5.56).

From the LBB condition, for each $\tilde{p} \in Q_h$, we have

$$\|p_h - \tilde{p}\|_Q \leq M \sup_{\boldsymbol{v} \in U_h, \boldsymbol{v} \neq 0} \frac{b(\boldsymbol{v}, p_h - \tilde{p})}{\|\boldsymbol{v}\|_U}.$$

Subtract (5.30) from (5.25), we have

$$b(\boldsymbol{v}, \tilde{p} - p_h) = a(\boldsymbol{u} - \boldsymbol{u}_h, \boldsymbol{v}) - b(\boldsymbol{v}, p - \tilde{p}) + \sum_{i=1}^{2} q_i (C_i(\boldsymbol{\Psi} - \boldsymbol{\Psi}_h), \boldsymbol{v}).$$

By the continuity of $b(\boldsymbol{v}_h, p_h)$ we obtain

$$\begin{aligned}
& \|\tilde{p} - p_h\|_Q \\
\leq\ & M \frac{1}{K_D} \|\boldsymbol{u} - \boldsymbol{u}_h\|_U + M \|p - \tilde{p}\|_Q \\
& + M h^{-\frac{d}{2}} \left(\sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2} \right)^2 + M \sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2} \\
\leq\ & M \frac{K_S}{K_D} h^{-\frac{d}{2}} \left(\sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2} \right)^2 + M \frac{K_S}{K_D} \sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2} + M \frac{K_S^2}{K_D^2} h^{s+1},
\end{aligned}$$

then

$$\begin{aligned}
& \|p - p_h\|_Q \leq \|p - \tilde{p}\|_Q + \|\tilde{p} - p_h\|_Q \\
\leq\ & M \frac{K_S}{K_D} h^{-\frac{d}{2}} \left(\sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2} \right)^2 + M \frac{K_S}{K_D} \sum_{i=1}^{2} \|C_i - C_{i,h}\|_{L^2} + M \frac{K_S^2}{K_D^2} h^{s+1}.
\end{aligned}$$

□

Define the finite element solution $\tilde{C}_i \in S_h$ to satisfy the following variational problem at any given time $\tau \in [0, T]$ as

$$\begin{aligned}
& \left(\nabla \left(C_i - \tilde{C}_i \right), \nabla c \right) + q_i \left(\left(C_i - \tilde{C}_i \right) \boldsymbol{\Psi}, \nabla c \right) \\
& \qquad - \left(\left(C_i - \tilde{C}_i \right) \boldsymbol{u}, \nabla c \right) = 0, \forall c \in M_h. \quad (5.57)
\end{aligned}$$

The well-posedness of (5.57) can be proved by a similar approach for (5.22) [Prohl and Schmuck (2009)], which shall be even simpler since $\mathbf{\Psi}$ is a continuous function in (5.57).

Because $\|\boldsymbol{u}\|_{[L^\infty]^d}$ and $\|\mathbf{\Psi}\|_{[L^\infty]^d}$ are bounded, similar to Lemma 4 in PNP, we have the following lemma.

Lemma 5.5. *Let (C_1, C_2) be the solution of (5.22) satisfying the regularity assumptions (5.32), and $(C_{1,h}, C_{2,h})$ be the finite element solution of (5.27). Suppose that $\tilde{C}_i$, $i = 1, 2$, are defined in (5.57), then we have the following error estimates,*

$$\left\|C_i - \tilde{C}_i\right\|_{L^2} + h\left\|\nabla\left(C_i - \tilde{C}_i\right)\right\|_{L^2} \leq Mh^{s+1}\left\|C_i\right\|_{H^{s+1}}, \tag{5.58}$$

and further,

$$\left\|\partial_t\left(C_i - \tilde{C}_i\right)\right\|_{L^2} + h\left\|\partial_t\nabla\left(C_i - \tilde{C}_i\right)\right\|_{L^2} \leq Mh^{s+1}\left(\left\|C_i\right\|_{H^{s+1}} + \left\|\partial_t C_i\right\|_{H^{s+1}}\right). \tag{5.59}$$

Theorem 5.2. *Let $(C_1, C_2, \mathbf{\Psi}, \Phi, \boldsymbol{u}, p)$ be the solution of (5.22)-(5.26) satisfying the regularity assumptions (5.32)-(5.36), and $(C_{1,h}, C_{2,h}, \mathbf{\Psi}_h, \Phi_h, \boldsymbol{u}_h, p_h)$ be the finite element solution of (5.27)-(5.31), then we have the following error estimate,*

$$\|C_i - C_{i,h}\|_{L^\infty(L^2)} + h\|\nabla(C_i - C_{i,h})\|_{L^\infty(L^2)} \leq M\frac{K_S}{K_D}h^{s+1}, \tag{5.60}$$

where $i = 1, 2$ and M is a constant depending only on the regularities of C_i and Φ.

Proof. Subtract (5.27) from (5.22), and use the Galerkin orthogonality (5.57), we have

$$(\partial_t(C_i - C_{i,h}), c) + (\nabla(\tilde{C}_i - C_{i,h}), \nabla c) + q_i(\tilde{C}_i\mathbf{\Psi} - C_{i,h}\mathbf{\Psi}_h, \nabla c) - (\tilde{C}_i\boldsymbol{u} - C_{i,h}\boldsymbol{u}_h, \nabla c) = 0, \forall c \in M_h.$$

Hence,

$$(\partial_t(\tilde{C}_i - C_{i,h}), c) + (\nabla(\tilde{C}_i - C_{i,h}), \nabla c) = -(\partial_t(C_i - \tilde{C}_i), c) - q_i((\tilde{C}_i - C_{i,h})\boldsymbol{\Psi}, \nabla c)$$
$$+ q_i((C_i - C_{i,h})(\boldsymbol{\Psi} - \boldsymbol{\Psi}_h), \nabla c) - q_i(C_i(\boldsymbol{\Psi} - \boldsymbol{\Psi}_h), \nabla c) + ((\tilde{C}_i - C_{i,h})\boldsymbol{u}, \nabla c)$$
$$- ((C_i - C_{i,h})(\boldsymbol{u} - \boldsymbol{u}_h), \nabla c) + (C_i(\boldsymbol{u} - \boldsymbol{u}_h), \nabla c). \quad (5.61)$$

Let $\eta_i = C_i - \tilde{C}_i$ and $\xi_i = \tilde{C}_i - C_{i,h}$, choose $c = \xi_i \in M_h$, we can write (5.61) as

$$(\partial_t \xi_i, \xi_i) + (\nabla \xi_i, \nabla \xi_i) = \sum_{i=1}^{7} \tilde{H}_i, \quad (5.62)$$

where H_i, $i = 1, ..., 7$, are defined as

$$\begin{aligned}
H_1 &:= -(\partial_t \eta_i, \xi_i), \\
H_2 &:= -q_i(\xi_i \boldsymbol{\Psi}, \nabla \xi_i), \\
H_3 &:= q_i((C_i - C_{i,h})(\boldsymbol{\Psi} - \boldsymbol{\Psi}_h), \nabla \xi_i), \\
H_4 &:= -q_i(C_i(\boldsymbol{\Psi} - \boldsymbol{\Psi}_h), \nabla \xi_i), \\
H_5 &:= (\xi_i \boldsymbol{u}, \nabla \xi_i), \\
H_6 &:= -((C_i - C_{i,h})(\boldsymbol{u} - \boldsymbol{u}_h), \nabla \xi_i), \\
H_7 &:= (C_i(\boldsymbol{u} - \boldsymbol{u}_h), \nabla \xi_i).
\end{aligned}$$

Then we have

$$\begin{aligned}
H_1 &\leq \|\partial_t \eta_i\|_{L^2} \|\xi_i\|_{L^2} \leq M h^{s+1} \|\xi_i\|_{L^2} \leq \frac{M}{2} h^{2s+2} + \frac{1}{2} \|\xi_i\|_{L^2}^2, \\
H_2 &\leq \|\boldsymbol{\Psi}\|_{[L^\infty]^d} \|\xi_i\|_{L^2} \|\nabla \xi_i\|_{L^2} \leq \frac{1}{4\epsilon} \|\boldsymbol{\Psi}\|_{[L^\infty]^d}^2 \|\xi_i\|_{L^2}^2 + \epsilon \|\nabla \xi_i\|_{L^2}^2, \\
H_5 &\leq \|\boldsymbol{u}\|_{[L^\infty]^d} \|\xi_i\|_{L^2} \|\nabla \xi_i\|_{L^2} \leq \frac{1}{4\epsilon} \|\boldsymbol{u}\|_{[L^\infty]^d}^2 \|\xi_i\|_{L^2}^2 + \epsilon \|\nabla \xi_i\|_{L^2}^2, \\
H_4 &\leq \|C_i\|_{L^\infty} \|\boldsymbol{\Psi} - \boldsymbol{\Psi}_h\|_{[L^2]^d} \|\nabla \xi_i\|_{L^2}
\end{aligned}$$

$$
\begin{aligned}
&\leq \|C_i\|_{L^\infty}\left(Mh^{s+1}\|\Phi\|_{H^{s+3}}+\sum_{j=1}^{2}\|C_j-C_{j,h}\|_{L^2}\right)\|\nabla\xi_i\|_{L^2} \\
&\leq Mh^{2s+2}+M\sum_{j=1}^{2}\|\xi_j\|_{L^2}^2+2\epsilon\|\nabla\xi_i\|_{L^2}^2.
\end{aligned}
$$

Use the boundedness of $\|\boldsymbol{\Psi}-\tilde{\boldsymbol{\Psi}}\|_{[L^\infty]^d}$ and $\|\boldsymbol{u}-\tilde{\boldsymbol{u}}\|_{[L^\infty]^d}$

$$
\begin{aligned}
H_3 \leq\ & q_i(\eta_i(\boldsymbol{\Psi}-\boldsymbol{\Psi}_h),\nabla\xi_i)+q_i(\xi_i(\boldsymbol{\Psi}-\boldsymbol{\Psi}_h),\nabla\xi_i) \\
\leq\ & M\|\eta_i\|_{L^2}(\|\boldsymbol{\Psi}-\tilde{\boldsymbol{\Psi}}\|_{[L^\infty]^d}+\|\tilde{\boldsymbol{\Psi}}-\boldsymbol{\Psi}_h)\|_{[L^\infty]^d})\|\nabla\xi_i\|_{L^2} \\
& + M\|\xi_i\|_{L^2}(\|\boldsymbol{\Psi}-\tilde{\boldsymbol{\Psi}}\|_{[L^\infty]^d}+\|\tilde{\boldsymbol{\Psi}}-\boldsymbol{\Psi}_h)\|_{[L^\infty]^d})\|\nabla\xi_i\|_{L^2} \\
\leq\ & Mh^{s+1}(h^{s+1-\frac{d}{2}}+h^{-\frac{d}{2}}\|\tilde{\boldsymbol{\Psi}}-\boldsymbol{\Psi}_h\|_{[L^2]^d})\|\nabla\xi_i\|_{L^2} \\
& + M\|\xi_i\|_{L^2}(h^{s+1-\frac{d}{2}}+h^{-\frac{d}{2}}\|\tilde{\boldsymbol{\Psi}}-\boldsymbol{\Psi}_h\|_{[L^2]^d})\|\nabla\xi_i\|_{L^2} \\
\leq\ & Mh^{2s+2-\frac{d}{2}}\|\nabla\xi_i\|_{L^2}+Mh^{s+1-\frac{d}{2}}\|\xi_i\|_{L^2}\|\nabla\xi_i\|_{L^2} \\
& +Mh^{s+1-\frac{d}{2}}(h^{s+1}+\sum_{j=1}^{2}\|\xi_j\|_{L^2})\|\nabla\xi_i\|_{L^2} \\
& +Mh^{-\frac{d}{2}}(h^{s+1}+\sum_{j=1}^{2}\|\xi_j\|_{L^2})\|\xi_i\|_{L^2}\|\nabla\xi_i\|_{L^2} \\
\leq\ & Mh^{2s+2-\frac{d}{2}}\|\nabla\xi_i\|_{L^2}+Mh^{s+1-\frac{d}{2}}\|\xi_i\|_{L^2}\|\nabla\xi_i\|_{L^2} \\
& +Mh^{s+1-\frac{d}{2}}\sum_{j=1}^{2}\|\xi_j\|_{L^2}\|\nabla\xi_i\|_{L^2}+Mh^{-\frac{d}{2}}\sum_{j=1}^{2}\|\xi_j\|_{L^2}\|\xi_i\|_{L^2}\|\nabla\xi_i\|_{L^2}.
\end{aligned}
$$

Now we conduct a mathematical induction process and propose the following induction hypothesis

$$
h^{-\frac{d}{2}}\|\xi_i(t)\|_{L^2}\leq M,\forall t\in[0,T]. \tag{5.63}
$$

then for any $k\geq 1$,

$$
\begin{aligned}
h^{-\frac{d}{2}}\|\xi_i(0)\|_{L^2}\leq h^{-\frac{d}{2}}\|C_i(0)-C_{i,h}(0)\|_{L^2}+h^{-\frac{d}{2}}\|\eta_i(0)\|_{L^2} \\
\leq Mh^{k+1-\frac{d}{2}}\|C_i(0)\|_{H^{k+1}}\leq M.
\end{aligned} \tag{5.64}
$$

Assume that (5.63) holds for any $t \in [0, T^*]$, $T^* < T$. Use Young's inequality, we have

$$H_3 \le M \left(h^{2s+2} + h^2 \sum_{j=1}^{2} \|\xi_j\|_{L^2}^2 + \epsilon \|\nabla \xi_i\|_{L^2}^2 \right)$$

Apply (5.63) to (5.56), we have that

$$\|\tilde{\boldsymbol{u}} - \boldsymbol{u}_h\|_{[L^2]^d} \le M \sum_{i=1}^{2} \|C_i - C_{i,h}\|_0 + M \frac{K_S}{K_D} h^{s+2}, \tag{5.65}$$

and by (5.48), we also have

$$\|\boldsymbol{u} - \tilde{\boldsymbol{u}}\|_{[L^\infty]^d} \le \|\nabla(\boldsymbol{u} - \tilde{\boldsymbol{u}})\|_{[L^\infty]^d} \le M h^{s+1}, \tag{5.66}$$

then use (5.65), (5.65) and inverse estimate, we have

$$\begin{aligned} H_6 \;\; \le \;\; & M \|\eta_i\|_{L^2} (\|\boldsymbol{u} - \tilde{\boldsymbol{u}}\|_{[L^\infty]^d} + \|\tilde{\boldsymbol{u}} - \boldsymbol{u}_h\|_{[L^\infty]^d}) \|\nabla \xi_i\|_{L^2} \\ & + M \|\xi_i\|_{L^2} (\|\boldsymbol{u} - \tilde{\boldsymbol{u}}\|_{[L^\infty]^d} + \|\tilde{\boldsymbol{u}} - \boldsymbol{u}_h\|_{[L^\infty]^d}) \|\nabla \xi_i\|_{L^2} \\ \le \;\; & M h^{s+1} \left(h^{-\frac{d}{2}} \sum_{j=1}^{2} \|C_j - C_{j,h}\|_{L^2} + \frac{K_S}{K_D} h^{s+2-\frac{d}{2}} \right) \|\nabla \xi_i\|_{L^2} \\ & + M \|\xi_i\|_{L^2} \left(h^{-\frac{d}{2}} \sum_{j=1}^{2} \|C_j - C_{j,h}\|_{L^2} + \frac{K_S}{K_D} h^{s+2-\frac{d}{2}} \right) \|\nabla \xi_i\|_{L^2}. \end{aligned}$$

Use Young's inequality with ϵ and use (5.63) again, we further obtain,

$$\begin{aligned} H_6 \;\; \le \;\; & M h^{s+1} \left(1 + h^{s+1} + \frac{K_S}{K_D} h^{s+2-\frac{d}{2}} \right) \|\nabla \xi_i\|_{L^2} \\ & + M \|\xi_i\|_{L^2} \left(1 + h^{s+1} + \frac{K_S}{K_D} h^{s+2-\frac{d}{2}} \right) \|\nabla \xi_i\|_{L^2}, \\ \le \;\; & M \frac{K_S}{K_D} h^{s+1} \|\nabla \xi_i\|_{L^2} + M \frac{K_S}{K_D} \|\xi_i\|_{L^2} \|\nabla \xi_i\|_{L^2}, \\ \le \;\; & M \frac{K_S^2}{K_D^2} h^{2s+2} + M \frac{K_S^2}{K_D^2} \|\xi_i\|_{L^2}^2 + \epsilon \|\nabla \xi_i\|_{L^2}^2. \end{aligned}$$

Apply (5.63) to (5.56), we have

$$\begin{aligned} H_7 &\leq \|C_i\|_{L^\infty}\|\boldsymbol{u}-\boldsymbol{u}_h\|_{[L^2]^d}\|\nabla\xi_i\|_{L^2} \\ &\leq \|C_i\|_{L^\infty}\left(\sum_{j=1}^{2}\|\xi_j\|_{L^2}+h^{s+1}\frac{K_S}{K_D}\right)\|\nabla\xi_i\|_{L^2} \\ &\leq M\frac{K_S^2}{K_D^2}h^{2s+2}+\sum_{j=1}^{2}\|\xi_j\|_{L^2}^2+\epsilon\|\nabla\xi_i\|_{L^2}^2, \end{aligned}$$

Hence (5.62) reads,

$$\frac{1}{2}\partial_t\|\xi_i\|_{L^2}^2+\|\nabla\xi_i\|_{L^2}^2 \leq M\left(\frac{K_S^2}{K_D^2}h^{2s+2}+\frac{K_S^2}{K_D^2}\sum_{j=1}^{2}\|\xi_j\|_{L^2}^2+\epsilon\|\nabla\xi_i\|_{L^2}^2\right). \tag{5.67}$$

Take the integral of (5.67) with respect to t, take the sum of $i = 1, 2$, and use Grönwall's inequality, then we get, for any $t \in [0, T]$,

$$\sum_{i=1}^{2}(\|\xi_i\|_{L^\infty(L^2)}^2+\|\xi_i\|_{L^2(H^1)}^2) \leq M\frac{K_S^2}{K_D^2}h^{2s+2},$$

thus for $i = 1, 2$,

$$\|\xi_i\|_{L^\infty(L^2)}+\|\xi_i\|_{L^2(H^1)} \leq M\frac{K_S}{K_D}h^{s+1}.$$

This also shows that (5.63) holds when $s \geq 1$ and $d = 2, 3$.

Therefore, by (5.58), we get

$$\|C_i-C_{i,h}\|_{L^\infty(L^2)}+h\|\nabla(C_i-C_{i,h})\|_{L^2(L^2)} \leq M\frac{K_S}{K_D}h^{s+1}, \tag{5.68}$$

and further,

$$\|\nabla(C_i-C_{i,h})\|_{L^\infty(L^2)} \leq M\frac{K_S}{K_D}h^{s}. \tag{5.69}$$

Finally, by (5.68) and (5.69), we arrive at (5.60). □

By Theorem 5.1, Theorem 5.2 and Lemma 5.2, we have

Theorem 5.3. *Let* $(C_1, C_2, \boldsymbol{\Psi}, \Phi, \boldsymbol{u}, p)$ *be the solution of (5.22)-(5.26) satisfying the regularity assumptions (5.32)-(5.36), and* $(C_{1,h}, C_{2,h}, \boldsymbol{\Psi}_h, \Phi_h, \boldsymbol{u}_h, p_h)$ *be the finite element solution of (5.27)-(5.31), then we have the following error estimates,*

$$\|\boldsymbol{u} - \boldsymbol{u}_h\|_{[L^2]^d} + \|\boldsymbol{u} - \boldsymbol{u}_h\|_U \le M \frac{K_S^2}{K_D} h^{s+1}, \tag{5.70}$$

$$\|p - p_h\|_Q \le M \frac{K_S^2}{K_D^2} h^{s+1}, \tag{5.71}$$

$$\|\boldsymbol{\Psi} - \boldsymbol{\Psi}_h\|_{[L^2]^d} + h\|\boldsymbol{\Psi} - \boldsymbol{\Psi}_h\|_V \le M \frac{K_S}{K_D} h^{s+1}. \tag{5.72}$$

$$\|\Phi - \Phi_h\|_{L^2} \le M \frac{K_S}{K_D} h^{s+1}, \tag{5.73}$$

where M *is a constant that is only dependent on* $\|\boldsymbol{u}\|_{[H^{s+2}]^d}$, $\|p\|_{H^{s+1}}$, $\|C_i\|_{H^{s+1}}$, $\|\partial_t C_i\|_{H^{s+1}}$ *and* $\|\Phi\|_{H^{s+3}}$.

CHAPTER 6

CONCLUSION

Electrohydrodynamics (EHD) is the term used for the hydrodynamics coupled with electrostatics, whose governing equations consist of the electrostatic potential (Poisson) equation, the ionic concentration (Nernst-Planck) equations, and Navier-Stokes equations for an incompressible, viscous dielectric liquid. Electrohydrodynamics can be regarded as a branch of fluid mechanics concerned with electrical force effects. It can also be considered as that part of electrodynamics which is involved with the influence of moving media on electric fields. EHD has been applied in many areas, such as EHD enhanced heat transfer, EHD pump, electrospray mass spectrometry, electrospray nanotechnology, EHD printing, ion channel in biophysics and electrophysiology, fuel cell dynamics, etc. Excellent review work on the history, research, and applications of EHD have been published in [Fylladitakis et al. (2014); Chen et al. (2003)].

In this dissertation, we focus on a specific application of EHD - fuel cell dynamics - in the field of renewable and clean energy, study its traditional model and attempt to develop a new fuel cell model based on the EHD model. Meanwhile, we develop a series of efficient and robust numerical methods for these models, and carry out their numerical analyses on the approximation accuracy. In particular, we analyze the error estimates of finite element method for a simplified 2D isothermal steady state two-phase transport model of Proton Exchange Membrane Fuel Cell (PEMFC). With the help of Kirchhoff transformation, we overcome the discontiuous and degenerate water diffusivity and made finite element analysis successful. The optimal convergence orders in H^1 norm and the sub-optimal convergence order in L^2 norm for both pressure and water concentration, are achieved. It is the first time the finite element error estimates are analyzed for a steady state multiphase mixture (M^2) model of FEMFC. The results of numerical experiment verify the accuracy of our presented error estimates on a sequence of nested grids produced by a grid doubling. We also analyze the error estimates of finite element method for a simplified 2D isothermal transient two-phase transport model of PEMFC. The optimal convergence orders in $L^\infty(H^1)$ norm and the sub-optimal convergence order in $L^\infty(L^2)$ norm for both pressure and water concentration, are achieved in semi-dicretization and full dicretization, repectively. It is the first time the finite element error estimates are analyzed for a transient multiphase mixture (M^2) model of FEMFC.

On the aspect of hydrodynamics arising in the fuel cell system, the fluid flow through the open channels and porous media at the same time, both Navier-Stokes equations and Darcy's law are involved in the fluid domains, leading to a Navier-Stokes-Darcy coupling problem. In this dissertation, we study a one-continuum model approach, so-called Brinkman model, to overcome this problem. Specifically, we study the 2D or 3D steady state Brinkman model derived from the traditional form using a parameter re-scaling technique to overcome the difficulties raised from the discontinuous pressure and flux. We analyze the error estimates of mixed finite element method for Brinkman model and Forchheimer model and obtain the optimal convergence rate for both velocity and pressure. On the other hand, we apply an asymptotic analysis on Brinkman model to figure out how accurate the Brinkman model approximates to its corresponding Stokes-Darcy coupling problem, we get the convergence result in quantitative measure with respect to the piecewise constant permeability. Numerical experiments are given to verify the convergence with respect to mesh size for both Brinkman model and Forchheimer model, and with respect to the piecewise permeability as well.

To develop a new fuel cell model based on EHD theory, in addition to the two-phase transport model of fuel cell, we carry out a series of numerical analyses for Poisson-Nernst-Planck (PNP) equations, which are the essential governing equations involved by EHD model. We first develop a standard finite element method for PNP equations, and give a priori error estimates of both semi- and fully discrete finite element approximation schemes. The optimal convergence order in $L^\infty(H^1)$ and $L^2(H^1)$ norms and sub-optimal convergence order in $L^\infty(L^2)$ norm with linear element, and optimal order in $L^\infty(L^2)$ norm with quadratic or higher-order element, for both the ion concentration and the electrostatic potential are achieved. To the best of the authors knowledge, it is the first time a complete a priori error analysis is given for the finite element discretization of the time-dependent PNP equations with convection terms written in the divergence form. The theoretical results are verified by numerical experiments. In addition, we also develop a mixed finite element method to solve the Poisson equation in PNP system for the first time, in correspondence with the mixed finite element method for Navier-Stokes equations. Considering that EHD model consists of both Navier-Stokes equations and PNP equations, it is natural to choose the same numerical method to discretize the coupled system of governing equations.

In particular, we propose to solve the electrostatic potential equation with a mixed finite element method by introducing the gradient of the elecctrostatic potential as a new variable, and solve the time-dependent ionic concentrations equations with the standard finite element method. The optimal convergence orders in $L^\infty(L^2)$ for the electrostatic potential Φ, and, $L^\infty(L^2)$ and $L^\infty(H^1)$ for the concentration of ions C_1 and C_2 are achieved in both the theoretical analysis and numerical experiment.

Finally, we are able to further extend the traditional fuel cell model in view of EHD characteristics, and develop a new fuel cell model by appropriately combining PNP equations with the traditional fuel cell model. In this dissertation, we only carry out a numerical analysis for the coupled Brinkman model and PNP equations, which is the essential spirit of EHD model, and leave the analysis of the rest coupling system for the future work. In particular, we give a priori error estimates of both semi- and fully discrete mixed finite element approximation schemes for the time-dependent Brinkman coupled with PNP model. A sub-optimal convergence order in L^2 norm for velocity and optimal convergence orders in all the other necessary norms for the ion concentration, the electrostatic potential, the velocity and the pressure are achieved.

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