



Mixed Finite Element Method for Modified Poisson–Nernst–Planck/Navier–Stokes Equations

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Abstract

In this paper, a complete mixed finite element method is developed for a modified Poisson–Nernst–Planck/Navier–Stokes (PNP/NS) coupling system, where the original Poisson equation in PNP system is replaced by a fourth-order elliptic equation to more precisely account for electrostatic correlations in a simplified form of the Landau–Ginzburg-type continuum model. A stabilized mixed weak form is defined for each equation of the modified PNP/NS model in terms of primary variables and their corresponding vector-valued gradient variables, based on which a stable Stokes-pair mixed finite element is thus able to be utilized to discretize all solutions to the entire modified PNP/NS model in the framework of Stokes-type mixed finite element approximation. Semi- and fully discrete mixed finite element schemes are developed and are analyzed for the presented modified PNP/NS equations, and optimal convergence rates in energy norms are obtained for both schemes. Numerical experiments are carried out to validate all attained theoretical results.

Keywords Modified Poisson–Nernst–Planck/Navier–Stokes (PNP/NS) coupling system · Fourth-order elliptic equation · A stabilized mixed finite element · Taylor–Hood mixed element · Optimal convergence

Mathematics Subject Classification 65M12 · 65M22 · 65M60

1 Introduction

The classical theory of the electric double layer and electrokinetic flow near a charged surface is over a century old and still remains extremely powerful in a number of diverse fields such as colloidal science, biophysics, micro- and nanofluidics, and electrochemistry. The classical

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theory of electrokinetics leads to the popular model of Poisson–Nernst–Planck/Navier–Stokes (PNP/NS) coupling system, which is used to describe the electrohydrodynamic phenomenon, also known as the electro-fluid-dynamics. PNP/NS equations are adopted to study the dynamics of electrically charged fluids, the motions of ionized particles or molecules and their interactions with electric fields and the surrounding fluid. In this model, the convection-diffusion-reaction equations, also particularly called Nernst–Planck equations, are used to model the ionic concentrations, while the Poisson equation is adopted to demonstrate the diffusive behavior of the electrostatic potential, and the fluid flow is generally modeled by Navier–Stokes equations. So, the coupling between PNP equations and Navier–Stokes equations is capable of describing electro-chemical and fluid-mechanical transport throughout the cellular environment. This includes a range of spatial and temporal scales [1]. For extensive applications, we refer to [2–5].

While the usefulness of the classical electrokinetic theory is not in question, there is a long history of recognizing the limitations and offering new formulations for new applications [6,7]. In particular, extensions of the classical electrokinetic theory are required for room-temperature ionic liquids (RTILs). RTILs typically have large organic cations and similar organic or smaller inorganic anions and hold promise as solvent-free electrolytes for supercapacitors, batteries, solar cells, and electroactuators [8–10]. Recently, Bazant, Storey and Kornyshev (BSK) [11–13] derive a Landau–Ginzburg-type continuum model for RTILs to account for the nonlocal dielectric permittivity of ionic liquids resulting from ion-ion correlations, which leads to the following fourth-order modified Poisson equation for a new definition of the electrostatic potential equation:

$$\epsilon (\ell_c^2 \Delta^2 \phi - \Delta \phi) = \rho, \quad (1.1)$$

with a fourth-order modified electrostatic boundary condition

$$\nabla (\Delta \phi) \cdot \mathbf{n} = 0, \quad (1.2)$$

where, ϕ is the electrostatic potential, ρ is the charge density, ℓ_c is an electrostatic correlation length, and ϵ is a constant permittivity to describe the polarizability of the ions. The BSK theory and the fourth-order modified Poisson equation (1.1) are first applied to predict double-layer structure and capacitance (RTIL) by using the ion size as the correlation length scale, and a high agreement to experimental results is achieved [12].

Although “The BSK theory provides reasonable agreement to simulation and experimental results for ionic liquids and multivalent electrolytes”, however, Souza and Bazant [13] point out that “the boundary conditions have not yet been proved or validated systematically”. Therefore, our goal in this paper is to mathematically and numerically investigate the rationality of (1.1) and (1.2) while they substitute the original Poisson equation in PNP/NS coupling system, as well as study the numerical performance of the entire PNP/NS model in a more comprehensive way, i.e., not only the primary variables of PNP/NS coupling system, but also their gradient variables which all represent corresponding physical significance, will be analyzed and approximated in an efficient and accurate fashion. Note that the vector-valued gradient of primary variables of PNP equations are crucial for obtaining an accurate electric current field which is remarkable for the validation with experimental data, since the electric current seems the easiest physical quantity to be measured in the experiment. For instance, the electric current across the biological membrane channel can be calculated by the following expression [14]

$$I = \sum_{i=1}^2 q_i \int_{\text{MEM}} D_i \left(\nabla C_i + \frac{q_i}{\kappa_B T} C_i \nabla \phi \right) \cdot \mathbf{n} \, dx, \quad (1.3)$$

where C_i ($i = 1, 2$) represent the ionic concentrations. Equation (1.3) clearly shows that the gradients of ionic concentrations and of electrostatic potential are important to produce an accurate electric current everywhere inside the membrane channel. Moreover, another important electrokinetic phenomena existing in ion channels of electrophysiology, the electrical double layer (Debye layer) [15], is formed near the surface of a charged object (membrane) due to the exponential decreases of the electrostatic potential, further, of the ionic concentrations, away from the surface, featuring a distance called Debye length [16]. Such exponential decrease induces a large gradient, so an accurate computation of gradient for the electrostatic potential and ionic concentrations are crucial to determine the location of Debye layer, which has a significant influence on the behavior of surfaces of the charged objects in contact with solutions or solid-state fast ion conductors. Therefore in the PNP system, it is highly necessary to numerically resolve the gradients ∇C_1 , ∇C_2 and $\nabla \phi$ in an accurate and efficient fashion.

To achieve the above goal, the mixed finite element method (FEM) shall be the best candidate for stably approximating the fourth-order modified PNP/NS coupling system with the optimal convergence to both primary variables and their gradients, comparing with conventional Lagrange-type finite element methods which need to use certain numerical differentiation for computing the gradient and then lead to a loss in accuracy. In this paper we will employ the Stokes-type mixed FEM by means of a stable Stokes-pair mixed element, e.g., Taylor–Hood element, to tackle each equation in PNP/NS coupling system. To that end, we will need to first reformulate the fourth-order modified Poisson equation and two parabolic-type ionic concentration equations to obtain their $\mathbf{H}(\text{div})$ -type mixed formulations in terms of both primary variables and their corresponding vector-valued gradient variables, then stabilize them by appropriately introducing stabilization terms in order to apply the Stokes-type mixed FEM to both modified PNP equations and Navier–Stokes equations, simultaneously. Thus, we avoid to introduce different types of mixed finite elements for Stokes-type and $\mathbf{H}(\text{div})$ -type mixed problem, respectively, which shall be more convenient and more efficient for us to analyze and implement the mixed finite element approximation for the modified PNP/NS coupling in one unified finite element space, simultaneously, bearing with the benefit of optimal convergence rates for all primary variables as well as their gradient variables in respectively proper norms.

Numerical study and analysis for PNP equations [17–19] and PNP/NS coupling system [20–23] have been extensively studied, where the standard FEM is most popularly adopted in recent years. Prohl and Schmuck [19] propose two nonlinear schemes with a linear FEM which preserve electric energy decay and entropy decay properties, respectively. Later, numerical methods for PNP/NS coupling are investigated in [20]. Sun et al. [24] develop a fully nonlinear Crank–Nicolson FEM for PNP equations, where a Picard linearization is used in the inner iteration, an optimal error estimate in H^1 norm and a suboptimal error estimate in L^2 norm are obtained. Then, Gao and He [25] propose a linearized finite element discretization and establish unconditionally optimal error estimates for all variables in both L^2 and H^1 norms. To overcome the convergence order reduction and to accurately resolve the electric current that is the gradient of the electrostatic potential as well, He and Sun [26] propose a nonlinear mixed FEM for Poisson equation and still apply the standard FEM to Nernst–Planck equations, which provides optimal error estimates for the electrostatic potential and ionic concentrations in both H^1 and L^2 norms, moreover, for electric current in $\mathbf{H}(\text{div})$ norm as well. Later, Gao and Sun [27] develop a linearized mixed finite element discretization for both Poisson equation and Nernst–Planck equations by using Raviart–Thomas element. Considering that the Lagrange-type Taylor–Hood mixed finite element is naturally stable for Stokes equations and easily implementable, it inspires the authors of this paper to

employ Taylor–Hood element as a unique mixed finite element to discretize both the mixed Poisson equations and Stokes equations in [28], and obtain optimal convergence rates for all variables of PNP equations and Stokes equations in their energy norms, respectively. In this paper, we will consider to apply the stable Stokes-pair mixed finite element to discretize all solutions to the entire fourth-order modified PNP/NS coupling system, develop its Stokes-type mixed FEM and analyze optimal convergence behaviors of primary variables and of all vector-valued gradient variables of modified PNP equations in both semi- and full discretizations.

This paper is organized as follows. In Sect. 2 we introduce the model of fourth-order modified PNP/NS coupling system. The semi-discrete scheme of the mixed FEM and its error analysis are given in Sect. 3. Section 4 contributes to the definition and analysis of the full discretization. Numerical experiments and validations are illustrated in Sect. 5. Finally, the paper ends with a conclusion in Sect. 6.

In what follows, we adopt the standard notation for Sobolev spaces $W^{l,p}(\Omega)$ and their associated norms and seminorms. For $p = 2$, $W^{l,2}(\Omega) = H^l(\Omega)$ and $\mathbf{H}^l(\Omega) = H^l(\Omega)^d$. The standard L^2 inner product is adopted, as $(\psi, \tilde{\psi}) = \int_{\Omega} \psi \tilde{\psi} dx$, $\langle \psi, \tilde{\psi} \rangle_{\partial\Omega} = \int_{\partial\Omega} \psi \tilde{\psi} ds$. Some norm notations are given as $\|\cdot\|_l = \|\cdot\|_{H^l(\Omega)}$, $\|\cdot\|_0 = \|\cdot\|_{L^2(\Omega)}$, and $\|\cdot\|_{W^{l,m}(W^{p,q})} = \|\cdot\|_{W^{l,m}(0,T;W^{p,q}(\Omega))}$. For the sake of simplicity, we sometimes drop the time dependence in variables, such as $\psi = \psi(t)$, drop $i = 1, 2$ for explaining C_i , and use M to denote a generic constant independent of any discretization parameter (h and Δt) throughout the paper.

2 Model Description and Weak Formulations

In this section, we first present the model of fourth-order modified Poisson–Nernst–Planck/Navier–Stokes coupling system, then reformulate it to a fully mixed form in terms of primary variables and extra vector-valued gradient variables, finally define its stabilized weak formulation in the sense that a stable Stokes-pair mixed finite element defined in a subspace of $\mathbf{H}^1(\Omega) \times L^2(\Omega)$ [26,28], instead of a $\mathbf{H}(\text{div})$ -type mixed finite element space belonging to $\mathbf{H}(\text{div};\Omega) \times L^2(\Omega)$ [27], can be adopted to discretize the fully mixed modified Poisson–Nernst–Planck system.

2.1 The Fourth-Order Modified PNP/NS Coupling System

Let $\Omega \in \mathbb{R}^d$ ($d = 2, 3$) be a bounded Lipschitz domain and $T > 0$. We introduce the following governing equations to describe the fourth-order modified PNP/NS coupling system in $\Omega \times [0, T]$ [11–13]:

$$\begin{cases} \Delta^2 \phi - \Delta \phi = C_1 - C_2, \\ \partial_t C_i - \nabla \cdot (\nabla C_i + z_i \nabla \phi C_i - \mathbf{u} C_i) = 0, \quad i = 1, 2, \\ \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} - \Delta \mathbf{u} + \nabla p = - (C_1 - C_2) \nabla \phi, \\ \nabla \cdot \mathbf{u} = 0, \end{cases} \tag{2.1}$$

where, $\partial_t = \partial/\partial t$, ϕ is the electrostatic potential, C_i ($i = 1, 2$) are the mass concentration of ions carrying charge z_i , (such as $z_1 = 1$, $z_2 = -1$), \mathbf{u} and p are the fluid velocity and pressure, respectively. Since in this paper we do not really consider the intrinsic physical feature of the modified PNP/NS coupling system, but put our full efforts on developing numerical discretizations and error analyses of the mixed FEM for the presented model in mathematical and numerical sense, only. So, without loss of generality in this paper, we

simply treat all involved physical coefficients as the unit constant “1”, which actually does not really matter in the following error analyses since the value of physical coefficients which are involved in the presented model are all positive constants. In addition, we impose the following boundary conditions and initial conditions for (2.1):

$$\begin{cases} \phi = f_1, \nabla(\Delta\phi) \cdot \mathbf{n} = f_2, & \text{on } \partial\Omega, t \in (0, T], \\ C_i = g_i, \mathbf{u} = 0, & \text{on } \partial\Omega, t \in (0, T], \\ C_i = C_i^0, \mathbf{u} = \mathbf{u}^0, & \text{in } \Omega, t = 0, \end{cases} \tag{2.2}$$

where $f_1, f_2, g_1, g_2, C_1^0, C_2^0$ and \mathbf{u}^0 are all given functions properly defined on $\partial\Omega$ and in Ω , respectively.

2.2 Reformulation of Mixed Weak Forms

We first reformulate (2.1) in terms of the following three extra vector-valued variables:

$$\mathbf{q} = -\nabla\phi, \quad z = \nabla \cdot \mathbf{q}, \quad \mathbf{J}_i = \nabla C_i - z_i \mathbf{q} C_i - \mathbf{u} C_i. \tag{2.3}$$

Here one can see that \mathbf{J}_1 and \mathbf{J}_2 are the mass flux of positively and negatively charged particles, respectively, while \mathbf{q} denotes the potential flux. With the above variables, we can reformulate the original modified PNP/NS system (2.1) to the following three new systems regarding the fourth-order elliptic equation, Nernst–Planck equations and Navier–Stokes equations, respectively:

$$\begin{cases} \mathbf{q} = -\nabla\phi, \\ z = \nabla \cdot \mathbf{q}, \\ -\Delta z + z = C_1 - C_2, \\ \mathbf{J}_i = \nabla C_i - z_i \mathbf{q} C_i - \mathbf{u} C_i, \\ \partial_t C_i - \nabla \cdot \mathbf{J}_i = 0, \\ \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} - \Delta \mathbf{u} + \nabla p = (C_1 - C_2) \mathbf{q}, \\ \nabla \cdot \mathbf{u} = 0, \end{cases} \tag{2.4}$$

with boundary conditions

$$\phi = f_1, \nabla z \cdot \mathbf{n} = -f_2, \quad C_i = g_i, \quad \mathbf{u} = 0, \quad \text{on } \partial\Omega, t \in (0, T], \tag{2.5}$$

and initial conditions

$$C_i = C_i^0, \quad \mathbf{u} = \mathbf{u}^0, \quad \text{in } \Omega. \tag{2.6}$$

Define $\mathbf{V} := \mathbf{H}(\text{div}; \Omega) = \{\mathbf{v} \in \mathbf{L}^2(\Omega), \nabla \cdot \mathbf{v} \in L^2(\Omega)\}$, and $\|\mathbf{v}\|_{\mathbf{V}}^2 = \|\mathbf{v}\|_0^2 + \|\nabla \cdot \mathbf{v}\|_0^2$, where $\|\cdot\|_0$ is the usual $L^2(\Omega)$ -norm for vector-valued variables or $L^2(\Omega)$ -norm for scalar-valued variables. Particularly, for the trial functional spaces of ϕ, C_i, \mathbf{u} and p , we introduce $L^2_{f_1}(\Omega) := \{\phi \in L^2(\Omega) | \phi = f_1 \text{ on } \partial\Omega\}$, $L^2_{g_i}(\Omega) := \{C_i \in L^2(\Omega) | C_i = g_i \text{ on } \partial\Omega\}$ ($i = 1, 2$), $\mathbf{H}^1_0(\Omega) := \{\mathbf{u} \in \mathbf{H}^1(\Omega) | \mathbf{u} = 0 \text{ on } \partial\Omega\}$, and $L^2_0(\Omega) := \{p \in L^2(\Omega) | \int_{\Omega} p dx = 0\}$, respectively.

Then, the mixed weak formulation of (2.4) can be defined as follows: find $(\phi, \mathbf{q}, z) \in L^2_{f_1}(\Omega) \times \mathbf{V} \times H^1(\Omega)$, $(C_i, \mathbf{J}_i) \in L^2_{g_i}(\Omega) \times \mathbf{V}$, $(\mathbf{u}, p) \in \mathbf{H}^1_0(\Omega) \times L^2_0(\Omega)$ such that

$$\begin{cases} (\mathbf{q}, \tilde{\mathbf{q}}) - (\phi, \nabla \cdot \tilde{\mathbf{q}}) = - \langle f_1, \tilde{\mathbf{q}} \cdot \mathbf{n} \rangle_{\partial\Omega}, & \forall \tilde{\mathbf{q}} \in \mathbf{V}, & (2.7a) \\ (\nabla \cdot \mathbf{q}, \tilde{\phi}) = (z, \tilde{\phi}), & \forall \tilde{\phi} \in L^2(\Omega), & (2.7b) \\ (\nabla z, \nabla \tilde{z}) + (z, \tilde{z}) = (C_1 - C_2, \tilde{z}) - \langle f_2, \tilde{z} \rangle_{\partial\Omega}, & \forall \tilde{z} \in H^1(\Omega), & (2.7c) \end{cases}$$

where, $a_q(\mathbf{q}, \tilde{\mathbf{q}})$ is redefined as $a_q(\mathbf{q}, \tilde{\mathbf{q}}) = (\mathbf{q}, \tilde{\mathbf{q}}) + (\nabla \cdot \mathbf{q}, \nabla \cdot \tilde{\mathbf{q}})$ that is definitely coercive in \mathbf{V} .

As to the mixed parabolic form of the concentration equations (2.8a)-(2.8b), we differentiate (2.8a) in time and take $\tilde{C}_i = \nabla \cdot \tilde{\mathbf{J}}_i$ in (2.8b), leading to

$$\begin{cases} (\partial_t \tilde{\mathbf{J}}_i, \tilde{\mathbf{J}}_i) + (\partial_t C_i, \nabla \cdot \tilde{\mathbf{J}}_i) + (z_i \partial_t (q C_i), \tilde{\mathbf{J}}_i) + (\partial_t (u C_i), \tilde{\mathbf{J}}_i) = \langle \partial_t g_i, \tilde{\mathbf{J}}_i \cdot \mathbf{n} \rangle_{\partial\Omega}, & (2.11a) \\ (\partial_t C_i, \nabla \cdot \tilde{\mathbf{J}}_i) - (\nabla \cdot \tilde{\mathbf{J}}_i, \nabla \cdot \tilde{\mathbf{J}}_i) = 0. & (2.11b) \end{cases}$$

Subtract (2.11b) from (2.11a), then add to (2.8a), yield a stabilized mixed weak formulation for the concentration equations [37]

$$\begin{cases} (\partial_t \tilde{\mathbf{J}}_i, \tilde{\mathbf{J}}_i) + (\tilde{\mathbf{J}}_i, \tilde{\mathbf{J}}_i) + (\nabla \cdot \tilde{\mathbf{J}}_i, \nabla \cdot \tilde{\mathbf{J}}_i) + (C_i, \nabla \cdot \tilde{\mathbf{J}}_i) + (z_i q C_i, \tilde{\mathbf{J}}_i) + (u C_i, \tilde{\mathbf{J}}_i) \\ + (z_i \partial_t (q C_i), \tilde{\mathbf{J}}_i) + (\partial_t (u C_i), \tilde{\mathbf{J}}_i) = \langle g_i, \tilde{\mathbf{J}}_i \cdot \mathbf{n} \rangle_{\partial\Omega} + \langle \partial_t g_i, \tilde{\mathbf{J}}_i \cdot \mathbf{n} \rangle_{\partial\Omega}, & \forall \tilde{\mathbf{J}}_i \in \mathbf{V}, & (2.12) \\ (\partial_t C_i, \tilde{C}_i) - (\nabla \cdot \tilde{\mathbf{J}}_i, \tilde{C}_i) = 0, & \forall \tilde{C}_i \in L^2(\Omega), \end{cases}$$

where, we can rewrite the bilinear form $a_{\mathbf{J}}(\tilde{\mathbf{J}}_i, \tilde{\mathbf{J}}_i) = (\tilde{\mathbf{J}}_i, \tilde{\mathbf{J}}_i) + (\nabla \cdot \tilde{\mathbf{J}}_i, \nabla \cdot \tilde{\mathbf{J}}_i)$ that is certainly coercive in \mathbf{V} as well.

On the other hand, the bilinear form $b_q(\tilde{\mathbf{q}}, \tilde{\phi})$ in (2.10), $b_{\mathbf{J}}(\tilde{\mathbf{J}}_i, \tilde{C}_i)$ in (2.12) and $b_u(\tilde{u}, \tilde{p})$ in (2.9) all satisfy the *inf-sup* condition in their respective spaces [33,35,38], so by Brezzi’s theory, the above mixed weak formulations (2.10), (2.12) and (2.9) are all well-posed in their own spaces.

In addition, we assume the following regularity properties hold for the real solutions ϕ, \mathbf{u}, p and C_i ($i = 1, 2$) to (2.1)

$$\phi \in \left(H^1 \cap L^\infty \right) \left(0, T; H^{k+3}(\Omega) \cap W^{k+2,\infty}(\Omega) \right) \cap H^2 \left(0, T; H^1(\Omega) \right), \tag{2.13}$$

$$C_i \in \left(H^1 \cap L^\infty \right) \left(0, T; H^{k+3}(\Omega) \cap L^\infty(\Omega) \right) \cap H^2 \left(0, T; H^1(\Omega) \right), \quad i = 1, 2, \tag{2.14}$$

$$\begin{cases} \mathbf{u} \in \left(H^1 \cap L^\infty \right) \left(0, T; \mathbf{H}^{k+2}(\Omega) \cap \mathbf{H}_0^1(\Omega) \cap W^{k+2,\infty}(\Omega) \right) \cap H^2 \left(0, T; L^2(\Omega) \right), \\ p \in L^2 \left(0, T; H^{k+1}(\Omega) \cap L_0^2(\Omega) \cap W^{k+1,\infty}(\Omega) \right). \end{cases} \tag{2.15}$$

3 Semi-discrete Mixed Finite Element Approximation

Let \mathcal{T}_h be a shape-regular simplicial triangulation of Ω on which we introduce the following finite element spaces for $k \geq 1$:

$$\begin{aligned} \mathbf{V}_h &:= \left\{ \mathbf{v} \in \mathbf{H}^1(\Omega) \subset \mathbf{V} : \mathbf{v}|_K \in \left[P^{k+1}(K) \right]^d, \forall K \in \mathcal{T}_h \right\}, \\ W_h &:= \left\{ w \in L^2(\Omega) : w|_K \in P^k(K), \forall K \in \mathcal{T}_h \right\}, \\ W_{h,f_1} &:= \left\{ w \in L^2(\Omega) : w|_{\partial\Omega} = f_1, w|_K \in P^k(K), \forall K \in \mathcal{T}_h \right\}, \\ W_{h,g_i} &:= \left\{ w \in L^2(\Omega) : w|_{\partial\Omega} = g_i, w|_K \in P^k(K), \forall K \in \mathcal{T}_h \right\} \quad (i = 1, 2), \\ Z_h &:= \left\{ z \in H^1(\Omega) : z|_K \in P^k(K), \forall K \in \mathcal{T}_h \right\}, \\ U_{h,0} &:= \left\{ \mathbf{u} \in \mathbf{H}_0^1(\Omega) : \mathbf{u}|_K \in \left[P^{k+1}(K) \right]^d, \forall K \in \mathcal{T}_h \right\}, \end{aligned} \tag{3.1}$$

where the pairs, $\mathbf{V}_h \times W_{h,f_1}$, $\mathbf{V}_h \times W_{h,g_i}$ and $U_{h,0} \times W_h$, are chosen as Taylor-Hood (P^{k+1}, P^k) mixed finite element spaces, whereas Z_h is a k -th order standard finite element. In what follows, we will develop and analyze a fully mixed finite element discretization for (2.10), (2.12) and (2.9) in the above finite element spaces.

3.1 Semi-discrete Mixed Finite Element Discretization

According to weak forms (2.10), (2.12) and (2.9), the semi-discrete mixed finite element approximation to the fourth-order modified PNP/NS model (2.1) is then defined as follows: find $(\phi_h, \mathbf{q}_h, z_h) \in W_h, f_1 \times V_h \times Z_h$, $(C_{i,h}, \mathbf{J}_{i,h}) \in W_h, g_i \times V_h$, $(\mathbf{u}_h, p_h) \in U_h, 0 \times W_h$ such that

$$\begin{cases} (\mathbf{q}_h, \tilde{\mathbf{q}}) + (\nabla \cdot \mathbf{q}_h, \nabla \cdot \tilde{\mathbf{q}}) - (\phi_h, \nabla \cdot \tilde{\mathbf{q}}) = (z_h, \nabla \cdot \tilde{\mathbf{q}}) - \langle f_1, \tilde{\mathbf{q}} \cdot \mathbf{n} \rangle_{\partial\Omega}, & \forall \tilde{\mathbf{q}} \in V_h, \\ (\nabla \cdot \mathbf{q}_h, \tilde{\phi}) = (z_h, \tilde{\phi}), & \forall \tilde{\phi} \in W_h, \\ (\nabla z_h, \nabla \tilde{z}) + (z_h, \tilde{z}) = (C_{1,h} - C_{2,h}, \tilde{z}) - \langle f_2, \tilde{z} \rangle_{\partial\Omega}, & \forall \tilde{z} \in Z_h, \end{cases} \quad (3.2)$$

$$\begin{cases} \left(\partial_t \mathbf{J}_{i,h}, \tilde{\mathbf{J}}_i \right) + \left(\mathbf{J}_{i,h}, \tilde{\mathbf{J}}_i \right) + \left(\nabla \cdot \mathbf{J}_{i,h}, \nabla \cdot \tilde{\mathbf{J}}_i \right) + \left(C_{i,h}, \nabla \cdot \tilde{\mathbf{J}}_i \right) + \left(z_i \mathbf{q}_h C_{i,h}, \tilde{\mathbf{J}}_i \right) + \left(\mathbf{u}_h C_{i,h}, \tilde{\mathbf{J}}_i \right) \\ + \left(z_i \partial_t (\mathbf{q}_h C_{i,h}), \tilde{\mathbf{J}}_i \right) + \left(\partial_t (\mathbf{u}_h C_{i,h}), \tilde{\mathbf{J}}_i \right) = \langle g_i, \tilde{\mathbf{J}}_i \cdot \mathbf{n} \rangle_{\partial\Omega} + \langle \partial_t g_i, \tilde{\mathbf{J}}_i \cdot \mathbf{n} \rangle_{\partial\Omega}, & \forall \tilde{\mathbf{J}}_i \in V_h, \\ \left(\partial_t C_{i,h}, \tilde{C}_i \right) - \left(\nabla \cdot \mathbf{J}_{i,h}, \tilde{C}_i \right) = 0, & \forall \tilde{C}_i \in W_h, \end{cases} \quad (3.3)$$

$$\begin{cases} (\partial_t \mathbf{u}_h, \tilde{\mathbf{u}}) + \beta (\mathbf{u}_h, \mathbf{u}_h, \tilde{\mathbf{u}}) + (\nabla \mathbf{u}_h, \nabla \tilde{\mathbf{u}}) - (p_h, \nabla \cdot \tilde{\mathbf{u}}) = ((C_{1,h} - C_{2,h}) \mathbf{q}_h, \tilde{\mathbf{u}}), & \forall \tilde{\mathbf{u}} \in U_h, 0, \\ (\nabla \cdot \mathbf{u}_h, \tilde{p}) = 0, & \forall \tilde{p} \in W_h. \end{cases} \quad (3.4)$$

3.2 Semi-discrete Error Analysis

It is always necessary to decompose the finite element approximation error of the time-dependent and/or nonlinear PDE problems to two parts by introducing a linear and steady state H^1 -projection of the solution to the original PDE problem, and, such H^1 -projection shall satisfy the Galerkin orthogonality property. Hence, we introduce the H^1 -projection of (ϕ, \mathbf{q}, z) that is defined in (2.10), $(\Pi_h \phi, \Pi_h \mathbf{q}, \Pi_h z) \in W_h \times V_h \times Z_h$, such that the following system

$$\begin{cases} (\mathbf{q} - \Pi_h \mathbf{q}, \tilde{\mathbf{q}}) + (\nabla \cdot (\mathbf{q} - \Pi_h \mathbf{q}), \nabla \cdot \tilde{\mathbf{q}}) - (\phi - \Pi_h \phi, \nabla \cdot \tilde{\mathbf{q}}) = 0, & \forall \tilde{\mathbf{q}} \in V_h, \\ (\nabla \cdot (\mathbf{q} - \Pi_h \mathbf{q}), \tilde{\phi}) = 0, & \forall \tilde{\phi} \in W_h, \\ (\nabla (z - \Pi_h z), \nabla \tilde{z}) + (z - \Pi_h z, \tilde{z}) = 0, & \forall \tilde{z} \in Z_h. \end{cases} \quad (3.5)$$

Obviously, (3.5) satisfies all compatibility conditions (continuity, coercivity and *inf-sup* conditions) of $a_q(\cdot, \cdot)$, $b_q(\cdot, \cdot)$ and $a_z(\cdot, \cdot)$, and is thus well-posed according to Brezzi's theory. Then we have the following Lemma [36,38,39].

Lemma 3.1 *Let (ϕ, \mathbf{q}, z) be the solution to (2.10), and $(\Pi_h \phi, \Pi_h \mathbf{q}, \Pi_h z)$ be the solution to (3.5), then for any $t \in [0, T]$, the following error estimates hold*

$$\|\mathbf{q} - \Pi_h \mathbf{q}\|_V + \|\phi - \Pi_h \phi\|_0 \leq Mh^{k+1} (\|\mathbf{q}\|_{k+2} + \|\phi\|_{k+1}) \leq Mh^{k+1} \|\phi\|_{k+3}, \quad (3.6)$$

$$\|z - \Pi_h z\|_0 + h\|z - \Pi_h z\|_1 \leq Mh^{k+1} \|z\|_{k+1} \leq Mh^{k+1} \|\phi\|_{k+3}, \quad (3.7)$$

$$\|\partial_t (\mathbf{q} - \Pi_h \mathbf{q})\|_V + \|\partial_t (\phi - \Pi_h \phi)\|_0 \leq Mh^{k+1} \|\partial_t \phi\|_{k+3}, \quad (3.8)$$

$$\|\mathbf{q} - \Pi_h \mathbf{q}\|_\infty \leq Mh^{k+1} \|\mathbf{q}\|_{k+1,\infty} \leq Mh^{k+1} \|\phi\|_{k+2,\infty}, \quad (3.9)$$

$$\|\partial_t (\mathbf{q} - \Pi_h \mathbf{q})\|_\infty \leq Mh^{k+1} \|\partial_t \mathbf{q}\|_{k+1,\infty} \leq Mh^{k+1} \|\partial_t \phi\|_{k+2,\infty}. \quad (3.10)$$

Remark 3.1 The same L^∞ -error estimate as shown in (3.9) is presented in [39] for the mixed FEM using RT element, which relies on the study of a weighted L^2 -projection, R_h , in a divergence-free finite element space. In our case of using Taylor–Hood mixed finite element, to prove the L^∞ -error estimate (3.9), we only need to replace the kernel space and the weighted L^2 -projection which are used in [39] by the following kernel space $\mathring{V}_h = \{v_h \in V_h : (\nabla \cdot v_h, q_h) = 0, \forall q_h \in W_h\}$, and the following weighted L^2 -projection, $R_h : L^1(\Omega) \rightarrow \mathring{V}_h$ such that $\forall v \in L^1(\Omega)$, $R_h v \in \mathring{V}_h$, and

$$(v - R_h v, \tilde{v}) + (\nabla \cdot (v - R_h v), \nabla \cdot \tilde{v}) = 0, \quad \forall \tilde{v} \in \mathring{V}_h,$$

to account for the adoption of a stable Stokes-pair mixed finite element. Thereafter, the rest analyses are the same with [39, Theorem 3.1], then we can still obtain (3.9).

The following theorem is related with error estimates of $\phi - \phi_h, \mathbf{q} - \mathbf{q}_h$ and $z - z_h$ in their corresponding norms.

Theorem 3.1 *Let $(\phi_h, \mathbf{q}_h, z_h)$ be the solution to (3.2) and (ϕ, \mathbf{q}, z) be the solution to (2.10), and the regularity property (2.13) is held. Then for any $t \in [0, T]$, the following error estimates hold*

$$\|\mathbf{q} - \mathbf{q}_h\|_{L^\infty(V)} + \|\phi - \phi_h\|_{L^\infty(L^2)} \leq M \left(\sum_{i=1}^2 \|C_i - C_{i,h}\|_{L^\infty(L^2)} + h^{k+1} \right), \tag{3.11}$$

$$\|z - z_h\|_{L^\infty(L^2)} + h\|z - z_h\|_{L^\infty(H^1)} \leq M \left(\sum_{i=1}^2 \|C_i - C_{i,h}\|_{L^\infty(L^2)} + h^{k+1} \right), \tag{3.12}$$

$$\|\partial_t(\mathbf{q} - \mathbf{q}_h)\|_{L^2(V)} + \|\partial_t(\phi - \phi_h)\|_{L^2(L^2)} \leq M \left(\sum_{i=1}^2 \|\partial_t(C_i - C_{i,h})\|_{L^2(L^2)} + h^{k+1} \right). \tag{3.13}$$

Proof Subtract (3.2) from (2.10), and apply the H^1 -projection (3.5), yield

$$(\Pi_h \mathbf{q} - \mathbf{q}_h, \tilde{\mathbf{q}}) + (\nabla \cdot (\Pi_h \mathbf{q} - \mathbf{q}_h), \nabla \cdot \tilde{\mathbf{q}}) - (\Pi_h \phi - \phi_h, \nabla \cdot \tilde{\mathbf{q}}) = (z - z_h, \nabla \cdot \tilde{\mathbf{q}}), \quad \forall \tilde{\mathbf{q}} \in \mathbf{V}_h, \tag{3.14}$$

$$(\nabla \cdot (\Pi_h \mathbf{q} - \mathbf{q}_h), \tilde{\phi}) = (z - z_h, \tilde{\phi}), \quad \forall \tilde{\phi} \in W_h, \tag{3.15}$$

$$(\nabla(\Pi_h z - z_h), \nabla \tilde{z}) + (\Pi_h z - z_h, \tilde{z}) = ((C_1 - C_2) - (C_{1,h} - C_{2,h}), \tilde{z}), \quad \forall \tilde{z} \in Z_h. \tag{3.16}$$

Let $\tilde{z} = \Pi_h z - z_h \in Z_h$ in (3.16), utilize the Cauchy–Schwarz inequality, and Young’s inequality with ϵ : $pq \leq \epsilon p^2 + \frac{1}{4\epsilon} q^2$, results

$$\|\nabla(\Pi_h z - z_h)\|_0 + \|\Pi_h z - z_h\|_0 \leq M \sum_{i=1}^2 \|C_i - C_{i,h}\|_0. \tag{3.17}$$

Further combining with (3.7), we have (3.12).

Because the discrete *inf-sup* condition holds for $b_q(\tilde{\mathbf{q}}, \tilde{\phi})$ in Taylor–Hood finite element spaces [34,38], we attain

$$\begin{aligned} \|\Pi_h \phi - \phi_h\|_0 &\leq M \sup_{\tilde{\mathbf{q}} \in \mathbf{V}_h} \frac{(\Pi_h \phi - \phi_h, \nabla \cdot \tilde{\mathbf{q}})}{\|\tilde{\mathbf{q}}\|_V} \\ &\text{(by (3.14))} \leq M \sup_{\tilde{\mathbf{q}} \in \mathbf{V}_h} \frac{\|\Pi_h \mathbf{q} - \mathbf{q}_h\|_V \|\tilde{\mathbf{q}}\|_V + \|z - z_h\|_0 \|\tilde{\mathbf{q}}\|_V}{\|\tilde{\mathbf{q}}\|_V} \\ &\leq M (\|\Pi_h \mathbf{q} - \mathbf{q}_h\|_V + \|z - z_h\|_0). \end{aligned} \tag{3.18}$$

Let $\tilde{\mathbf{q}} = \Pi_h \mathbf{q} - \mathbf{q}_h, \tilde{\phi} = \Pi_h \phi - \phi_h$ in (3.14) and (3.15), then add them together, leads to

$$\begin{aligned} \|\Pi_h \mathbf{q} - \mathbf{q}_h\|_V^2 &= (z - z_h, \nabla \cdot (\Pi_h \mathbf{q} - \mathbf{q}_h)) + (z - z_h, \Pi_h \phi - \phi_h) \\ &\leq \|z - z_h\|_0 \|\nabla \cdot (\Pi_h \mathbf{q} - \mathbf{q}_h)\|_0 + \|z - z_h\|_0 \|\Pi_h \phi - \phi_h\|_0 \\ &\text{(by (3.18))} \leq M (\|z - z_h\|_0 \|\Pi_h \mathbf{q} - \mathbf{q}_h\|_V + \|z - z_h\|_0^2) \\ &\leq M \|z - z_h\|_0^2 + \epsilon \|\Pi_h \mathbf{q} - \mathbf{q}_h\|_V^2. \end{aligned} \tag{3.19}$$

Take a sufficiently small ϵ , and apply (3.18), yield

$$\|\Pi_h \mathbf{q} - \mathbf{q}_h\|_V + \|\Pi_h \phi - \phi_h\|_0 \leq M \|z - z_h\|_0. \tag{3.20}$$

Combining with (3.6) and (3.12), then we have (3.11).

Differentiating (3.14)–(3.16) with respect to time, we have

$$(\partial_t(\Pi_h \mathbf{q} - \mathbf{q}_h), \tilde{\mathbf{q}}) + (\nabla \cdot \partial_t(\Pi_h \mathbf{q} - \mathbf{q}_h), \nabla \cdot \tilde{\mathbf{q}}) - (\partial_t(\Pi_h \phi - \phi_h), \nabla \cdot \tilde{\mathbf{q}}) = (\partial_t(z - z_h), \nabla \cdot \tilde{\mathbf{q}}),$$

$$\begin{aligned} & \left(\nabla \cdot \partial_t \left((\Pi_h \mathbf{q} - \mathbf{q}_h), \tilde{\phi} \right), \tilde{\phi} \right) = \left(\partial_t (z - z_h), \tilde{\phi} \right), \\ & (\nabla \partial_t (\Pi_h z - z_h), \nabla \tilde{z}) + (\partial_t (\Pi_h z - z_h), \tilde{z}) = \left(\partial_t ((C_1 - C_2) - (C_{1,h} - C_{2,h}), \tilde{z}) \right). \end{aligned} \tag{3.21}$$

Taking $\tilde{\mathbf{q}} = \partial_t (\Pi_h \mathbf{q} - \mathbf{q}_h)$, $\tilde{\phi} = \partial_t (\Pi_h \phi - \phi_h)$, $\tilde{z} = \partial_t (\Pi_h z - z_h)$ in (3.21), and following the similar error estimate process at above, we can also attain (3.13). \square

We further define the H^1 -projection $(\Pi_h \mathbf{u}, \Pi_h p) \in \mathbf{U}_{h,0} \times W_h$ of (\mathbf{u}, p) that is the solution to (2.9) such that

$$\begin{cases} (\nabla \Pi_h \mathbf{u}, \nabla \tilde{\mathbf{u}}) - (\Pi_h p, \nabla \cdot \tilde{\mathbf{u}}) = (\nabla \mathbf{u}, \nabla \tilde{\mathbf{u}}) - (p, \nabla \cdot \tilde{\mathbf{u}}), & \forall \tilde{\mathbf{u}} \in \mathbf{U}_{h,0}, \\ (\nabla \cdot \Pi_h \mathbf{u}, \tilde{p}) = (\nabla \cdot \mathbf{u}, \tilde{p}), & \forall \tilde{p} \in W_h. \end{cases} \tag{3.22}$$

By [32, Theorems (12.6.7), (12.6.13)], and [29, Theorems 3.1-3.3], we have the following lemma.

Lemma 3.2 *Let (\mathbf{u}_h, p_h) be the finite element solution to (3.4). Suppose $(\Pi_h \mathbf{u}, \Pi_h p) \in \mathbf{U}_{h,0} \times W_h$ is defined in (3.22), then we have the following error estimates,*

$$\begin{aligned} & \|\mathbf{u} - \Pi_h \mathbf{u}\|_0 + h \|\mathbf{u} - \Pi_h \mathbf{u}\|_1 + h \|p - \Pi_h p\|_0 \leq M h^{k+2} (\|\mathbf{u}\|_{k+2} + \|p\|_{k+1}), \\ & \|\partial_t (\mathbf{u} - \Pi_h \mathbf{u})\|_0 + h \|\partial_t (\mathbf{u} - \Pi_h \mathbf{u})\|_1 \leq M h^{k+2} (\|\mathbf{u}\|_{k+2} + \|\partial_t \mathbf{u}\|_{k+2} + \|p\|_{k+1}), \\ & \|\mathbf{u} - \Pi_h \mathbf{u}\|_\infty + h |\ln h|^{\frac{1}{2}} \|\mathbf{u} - \Pi_h \mathbf{u}\|_{1,\infty} \leq M h^{k+2} |\ln h| (\|\mathbf{u}\|_{k+2,\infty} + \|p\|_{k+1,\infty}), \\ & \|\partial_t (\mathbf{u} - \Pi_h \mathbf{u})\|_\infty \leq M h^{k+2} |\ln h| (\|\mathbf{u}\|_{k+2,\infty} + \|\partial_t \mathbf{u}\|_{k+2,\infty} + \|p\|_{k+1,\infty}). \end{aligned}$$

Now we carry out error estimates for $\mathbf{u} - \mathbf{u}_h$ and $p - p_h$, as shown in the following theorem.

Theorem 3.2 *Let (\mathbf{u}_h, p_h) be the finite element solution to (3.4) and (\mathbf{u}, p) is defined in (2.9), and the regularity property (2.15) is held. Then the following error estimates hold*

$$\begin{aligned} & \|\mathbf{u} - \mathbf{u}_h\|_{L^\infty(L^2)} + \|\mathbf{u} - \mathbf{u}_h\|_{L^2(\mathbf{H}^1)} \\ & \leq M \left[\sum_{i=1}^2 \left(h^{-\frac{d}{2}} \|C_i - C_{i,h}\|_{L^2(L^2)}^2 + \|C_i - C_{i,h}\|_{L^2(L^2)} \right) + h^{k+1} \right]. \end{aligned} \tag{3.23}$$

$$\begin{aligned} & \|\partial_t (\mathbf{u} - \mathbf{u}_h)\|_{L^2(L^2)} + \|\mathbf{u} - \mathbf{u}_h\|_{L^\infty(\mathbf{H}^1)} \\ & \leq M \left[\sum_{i=1}^2 \left(h^{-\frac{d}{2}} \|C_i - C_{i,h}\|_{L^2(L^2)}^2 + \|C_i - C_{i,h}\|_{L^2(L^2)} \right) \right. \\ & \quad \left. + h^{k+1} + h^{-1} \sum_{i=1}^2 \left(h^{-d} \|C_i - C_{i,h}\|_{L^2(L^2)}^4 + \|C_i - C_{i,h}\|_{L^2(L^2)}^2 \right) \right]. \end{aligned} \tag{3.24}$$

$$\begin{aligned} & \|p - p_h\|_{L^2(L^2)} \\ & \leq M \left[\sum_{i=1}^2 \left(h^{-\frac{d}{2}} \|C_i - C_{i,h}\|_{L^2(L^2)}^2 + \|C_i - C_{i,h}\|_{L^2(L^2)} \right) + h^{k+1} \right. \\ & \quad \left. + h^{-1} \sum_{i=1}^2 \left(h^{-d} \|C_i - C_{i,h}\|_{L^2(L^2)}^4 + \|C_i - C_{i,h}\|_{L^2(L^2)}^2 \right) \right]. \end{aligned} \tag{3.25}$$

Proof Subtract (3.4) from (2.9), and use (3.22), yield

$$\begin{cases} (\partial_t (\mathbf{u} - \mathbf{u}_h), \tilde{\mathbf{u}}) + a_{\mathbf{u}} (\Pi_h \mathbf{u} - \mathbf{u}_h, \tilde{\mathbf{u}}) - b_{\mathbf{u}} (\tilde{\mathbf{u}}, \Pi_h p - p_h) \\ \quad + \beta (\mathbf{u}, \mathbf{u}, \tilde{\mathbf{u}}) - \beta (\mathbf{u}_h, \mathbf{u}_h, \tilde{\mathbf{u}}) = \sum_{i=1}^2 z_i (C_i \mathbf{q} - C_{i,h} \mathbf{q}_h, \tilde{\mathbf{u}}), \end{cases} \tag{3.26}$$

$$b_{\mathbf{u}} (\Pi_h \mathbf{u} - \mathbf{u}_h, \tilde{p}) = 0. \tag{3.27}$$

Let $\mathbf{u} - \mathbf{u}_h = (\mathbf{u} - \Pi_h \mathbf{u}) + (\Pi_h \mathbf{u} - \mathbf{u}_h) = \eta + \xi$, and choose $\tilde{\mathbf{u}} = \xi$, $\tilde{p} = \Pi_h p - p_h$ in (3.26) and (3.27). Then

$$(\partial_t (\eta + \xi), \xi) + a_{\mathbf{u}} (\xi, \xi) + \beta (\mathbf{u}, \mathbf{u}, \xi) - \beta (\mathbf{u}_h, \mathbf{u}_h, \xi) = \sum_{i=1}^2 z_i (C_i \mathbf{q} - C_{i,h} \mathbf{q}_h, \xi), \tag{3.28}$$

leading to

$$\begin{aligned} \frac{1}{2} \partial_t \|\xi\|_0^2 + \|\nabla \xi\|_0^2 &= -(\partial_t \eta, \xi) + \beta(\mathbf{u}_h, \mathbf{u}_h, \xi) - \beta(\Pi_h \mathbf{u}, \Pi_h \mathbf{u}, \xi) \\ &\quad + \beta(\Pi_h \mathbf{u}, \Pi_h \mathbf{u}, \xi) - \beta(\mathbf{u}, \mathbf{u}, \xi) + \sum_{i=1}^2 z_i (C_i \mathbf{q} - C_{i,h} \mathbf{q}_h, \xi). \end{aligned} \tag{3.29}$$

We first estimate terms involving $\beta(\cdot, \cdot, \cdot)$ as follows.

$$\begin{aligned} \beta(\mathbf{u}_h, \mathbf{u}_h, \xi) - \beta(\Pi_h \mathbf{u}, \Pi_h \mathbf{u}, \xi) &= -\beta(\mathbf{u}_h, \xi, \xi) - \beta(\xi, \Pi_h \mathbf{u}, \xi) = -\beta(\xi, \Pi_h \mathbf{u}, \xi) \\ &\quad \text{(by Lemma 2.1)} \leq M \|\nabla \Pi_h \mathbf{u}\|_0 \|\xi\|_0^{\frac{1}{2}} \|\nabla \xi\|_0^{\frac{3}{2}} \\ &\leq M \|\xi\|_0^2 + \epsilon \|\nabla \xi\|_0^2, \end{aligned} \tag{3.30}$$

where we employ the definition of $\beta(\cdot, \cdot, \cdot)$, the boundedness of $\|\Pi_h \mathbf{u}\|_1$ due to Lemma 3.2, and Young’s inequality with $\epsilon : pq \leq Mp^4 + \epsilon q^{4/3}$, and

$$\begin{aligned} \beta(\Pi_h \mathbf{u}, \Pi_h \mathbf{u}, \xi) - \beta(\mathbf{u}, \mathbf{u}, \xi) &= \beta(\mathbf{u} - \Pi_h \mathbf{u}, \mathbf{u} - \Pi_h \mathbf{u}, \xi) \\ &\quad - \beta(\mathbf{u} - \Pi_h \mathbf{u}, \mathbf{u}, \xi) - \beta(\mathbf{u}, \mathbf{u} - \Pi_h \mathbf{u}, \xi) \\ &\quad \text{(by Lemma 2.1)} \leq M \left(\|\nabla(\mathbf{u} - \Pi_h \mathbf{u})\|_0^2 + \|\mathbf{u} - \Pi_h \mathbf{u}\|_0 \right) \|\nabla \xi\|_0 \\ &\quad \text{(by Lemma 3.2)} \leq M \left(h^{4(k+1)} + h^{2(k+2)} \right) + \epsilon \|\nabla \xi\|_0^2. \end{aligned} \tag{3.31}$$

Next, we estimate the last term on the right hand side of (3.29).

$$\begin{aligned} &\sum_{i=1}^2 z_i (C_i \mathbf{q} - C_{i,h} \mathbf{q}_h, \xi) \\ &= \sum_{i=1}^2 z_i ((C_i - C_{i,h}) \mathbf{q}, \xi) + \sum_{i=1}^2 z_i (C_i (\mathbf{q} - \mathbf{q}_h), \xi) - \sum_{i=1}^2 z_i ((C_i - C_{i,h}) (\mathbf{q} - \mathbf{q}_h), \xi) \\ &\leq M \sum_{i=1}^2 (\|\mathbf{q}\|_{L^\infty} \|C_i - C_{i,h}\|_0 \|\xi\|_0 + \|C_i\|_{L^\infty} \|\mathbf{q} - \mathbf{q}_h\|_0 \|\xi\|_0 \\ &\quad + (\|\mathbf{q} - \Pi_h \mathbf{q}\|_{L^\infty} + \|\Pi_h \mathbf{q} - \mathbf{q}_h\|_{L^\infty}) \|C_i - C_{i,h}\|_0 \|\xi\|_0) \\ &\leq M \|\xi\|_0 \sum_{i=1}^2 (\|C_i - C_{i,h}\|_0 + \|\mathbf{q} - \mathbf{q}_h\|_0 \\ &\quad + (\|\mathbf{q} - \Pi_h \mathbf{q}\|_{L^\infty} + h^{-\frac{d}{2}} \|\Pi_h \mathbf{q} - \mathbf{q}_h\|_0) \|C_i - C_{i,h}\|_0) \\ &\leq M \|\xi\|_0 \left(\left(1 + h^{k+1-\frac{d}{2}}\right) \sum_{i=1}^2 \|C_i - C_{i,h}\|_0 + h^{k+1} + h^{-\frac{d}{2}} \sum_{i=1}^2 \|C_i - C_{i,h}\|_0^2 \right) \\ &\leq M \|\xi\|_0 \left(\sum_{i=1}^2 \|C_i - C_{i,h}\|_0 + h^{k+1} + h^{-\frac{d}{2}} \sum_{i=1}^2 \|C_i - C_{i,h}\|_0^2 \right), \end{aligned} \tag{3.32}$$

where we apply (3.9), (3.11) and the inverse inequality: $\|\Pi_h \mathbf{q} - \mathbf{q}_h\|_{L^\infty} \leq M h^{-\frac{d}{2}} \|\Pi_h \mathbf{q} - \mathbf{q}_h\|_0$.

Combining the above error estimates together and applying Young’s inequality, we have the following result for (3.29)

$$\frac{1}{2} \partial_t \|\xi\|_0^2 + \|\nabla \xi\|_0^2 \leq M \left[\left(h^{-\frac{d}{2}} \sum_{i=1}^2 \|C_i - C_{i,h}\|_0^2 \right)^2 \right]$$

$$+ \sum_{i=1}^2 \|C_i - C_{i,h}\|_0^2 + h^{2(k+1)} + \|\xi\|_0^2 \Big] + \epsilon \|\nabla \xi\|_0^2.$$

Take a sufficiently small ϵ , integrate both sides with respect to time from 0 to t , then apply Grönwall’s inequality with a proper choice on the initial condition $\mathbf{u}_h^0 = \Pi_h \mathbf{u}^0$, leads to

$$\|\xi\|_{L^\infty(L^2)} + \|\xi\|_{L^2(H^1)} \leq M \left(h^{-\frac{d}{2}} \sum_{i=1}^2 \|C_i - C_{i,h}\|_{L^2(L^2)}^2 + \sum_{i=1}^2 \|C_i - C_{i,h}\|_{L^2(L^2)} + h^{k+1} \right). \tag{3.33}$$

Then (3.23) is obtained by combining (3.33) with Lemma 3.2.

On the other hand, choose $\tilde{\mathbf{u}} = \partial_t \xi$ in (3.26), differentiate (3.27) in time and then choose $\tilde{p} = \Pi_h p - p_h$, yield

$$\begin{aligned} \|\partial_t \xi\|_0^2 + \frac{1}{2} \partial_t \|\nabla \xi\|_0^2 &= -(\partial_t \eta, \partial_t \xi) + \beta(\mathbf{u} - \mathbf{u}_h, \mathbf{u} - \mathbf{u}_h, \partial_t \xi) \\ &\quad - \beta(\mathbf{u}, \mathbf{u} - \mathbf{u}_h, \partial_t \xi) - \beta(\mathbf{u} - \mathbf{u}_h, \mathbf{u}, \partial_t \xi) \\ &\quad + \sum_{i=1}^2 z_i (C_i \mathbf{q} - C_{i,h} \mathbf{q}_h, \partial_t \xi). \end{aligned} \tag{3.34}$$

By Lemmas 2.1 and 3.2, we have

$$\begin{aligned} |\beta(\mathbf{u} - \mathbf{u}_h, \mathbf{u} - \mathbf{u}_h, \partial_t \xi)| &\leq M \|\nabla(\mathbf{u} - \mathbf{u}_h)\|_0^2 \|\nabla \partial_t \xi\|_0 \leq M \|\nabla(\mathbf{u} - \mathbf{u}_h)\|_0^2 h^{-1} \|\partial_t \xi\|_0 \\ &\leq M h^{-2} \|\nabla(\mathbf{u} - \mathbf{u}_h)\|_0^4 + \epsilon \|\partial_t \xi\|_0^2, \\ |-\beta(\mathbf{u}, \mathbf{u} - \mathbf{u}_h, \partial_t \xi) - \beta(\mathbf{u} - \mathbf{u}_h, \mathbf{u}, \partial_t \xi)| \\ &\leq M \|\mathbf{u}\|_\infty \|\nabla(\mathbf{u} - \mathbf{u}_h)\|_0 \|\partial_t \xi\|_0 + \|\nabla(\mathbf{u} - \mathbf{u}_h)\|_0 \|\mathbf{u}\|_2 \|\partial_t \xi\|_0 \\ &\leq M \|\nabla(\mathbf{u} - \mathbf{u}_h)\|_0^2 + \epsilon \|\partial_t \xi\|_0^2 \\ &\leq M \left(h^{2k+2} + \|\nabla \xi\|_0^2 \right) + \epsilon \|\partial_t \xi\|_0^2 \end{aligned}$$

Similar to (3.32), the last term on the right hand side of (3.34) can be estimated as

$$\begin{aligned} \sum_{i=1}^2 z_i (C_i \mathbf{q} - C_{i,h} \mathbf{q}_h, \partial_t \xi) &\leq M \|\partial_t \xi\|_0 \left(h^{-\frac{d}{2}} \sum_{i=1}^2 \|C_i - C_{i,h}\|_0^2 + \sum_{i=1}^2 \|C_i - C_{i,h}\|_0 + h^{k+1} \right) \\ &\leq M \left(h^{-\frac{d}{2}} \sum_{i=1}^2 \|C_i - C_{i,h}\|_0^2 + \sum_{i=1}^2 \|C_i - C_{i,h}\|_0 + h^{k+1} \right)^2 + \epsilon \|\partial_t \xi\|_0^2. \end{aligned} \tag{3.35}$$

Then, take a sufficiently small ϵ , (3.34) yields

$$\begin{aligned} \|\partial_t \xi\|_0 + \partial_t \|\nabla \xi\|_0 &\leq M \left(h^{-\frac{d}{2}} \sum_{i=1}^2 \|C_i - C_{i,h}\|_0^2 + \sum_{i=1}^2 \|C_i - C_{i,h}\|_0 + h^{k+1} + \|\nabla \xi\|_0 \right. \\ &\quad \left. + h^{-1} \|\mathbf{u} - \mathbf{u}_h\|_1^2 \right). \end{aligned}$$

Integrate both sides in time from 0 to t , and apply Grönwall’s inequality with $\mathbf{u}_h(0) = \Pi_h \mathbf{u}^0$, results

$$\begin{aligned} \|\partial_t \xi\|_{L^2(L^2)} + \|\nabla \xi\|_{L^\infty(L^2)} &\leq M \left(h^{-\frac{d}{2}} \sum_{i=1}^2 \|C_i - C_{i,h}\|_{L^2(L^2)}^2 + \sum_{i=1}^2 \|C_i - C_{i,h}\|_{L^2(L^2)} \right. \\ &\quad \left. + h^{k+1} + h^{-1} \|\mathbf{u} - \mathbf{u}_h\|_{L^2(H^1)}^2 \right). \end{aligned} \tag{3.36}$$

Applying (3.23), we obtain the desired (3.24) with Lemma 3.2.

To prove (3.25), we need to apply the discrete form of *inf-sup* condition $b_u(\cdot, \cdot)$, i.e., for any $\Pi_h p \in W_h$, we have [38]

$$\|\Pi_h p - p_h\|_0 \leq M \sup_{\forall \tilde{u} \in U_{h,0} \setminus \{0\}} \frac{b_u(\tilde{u}, \Pi_h p - p_h)}{\|\tilde{u}\|_1}. \tag{3.37}$$

Then from (3.26) we have

$$b_u(\tilde{u}, \Pi_h p - p_h) = (\partial_t(\mathbf{u} - \mathbf{u}_h), \tilde{u}) + a_u(\Pi_h \mathbf{u} - \mathbf{u}_h, \tilde{u}) + \beta(\mathbf{u}, \mathbf{u}, \tilde{u}) - \beta(\mathbf{u}_h, \mathbf{u}_h, \tilde{u}) - \sum_{i=1}^2 z_i (C_i \mathbf{q} - C_{i,h} \mathbf{q}_h, \tilde{u}).$$

By (3.37), the continuity of $a_u(\cdot, \cdot)$ and the same error analyses for (3.30)–(3.32), we can obtain

$$\|\Pi_h p - p_h\|_0 \leq M \left(\|\partial_t \xi\|_0 + \|\xi\|_1 + h^{k+1} + \sum_{i=1}^2 \|C_i - C_{i,h}\|_0 + h^{-\frac{d}{2}} \sum_{i=1}^2 \|C_i - C_{i,h}\|_0^2 \right).$$

Then integrate both sides in time from 0 to t , by (3.36), (3.23), Lemma 3.2 and the triangular inequality, we obtain (3.25). \square

Now we analyze error estimates of (3.3) between $(C_i, \mathbf{J}_i) \in L^2(\Omega) \times \mathbf{V}$ and $(C_{i,h}, \mathbf{J}_{i,h}) \in W_h \times \mathbf{V}_h$. We first introduce the H^1 -projection of (C_i, \mathbf{J}_i) , $(\Pi_h C_i, \Pi_h \mathbf{J}_i) \in W_h \times \mathbf{V}_h$, satisfying

$$\begin{cases} (\mathbf{J}_i - \Pi_h \mathbf{J}_i, \tilde{\mathbf{J}}_i) + (\nabla \cdot (\mathbf{J}_i - \Pi_h \mathbf{J}_i), \nabla \cdot \tilde{\mathbf{J}}_i) + (C_i - \Pi_h C_i, \nabla \cdot \tilde{\mathbf{J}}_i) = 0, & \forall \tilde{\mathbf{J}}_i \in \mathbf{V}_h, \\ -(\nabla \cdot (\mathbf{J}_i - \Pi_h \mathbf{J}_i), \tilde{C}_i) = 0, & \forall \tilde{C}_i \in W_h. \end{cases} \tag{3.38}$$

Clearly, (3.38) satisfies all compatibility conditions (continuity, coercivity and *inf-sup* conditions) of $a_{\mathbf{J}}(\cdot, \cdot)$ and $b_{\mathbf{J}}(\cdot, \cdot)$ in $W_h \times \mathbf{V}_h$, it is thus well-posed according to Brezzi’s theory, and holds the following Lemma [36,38].

Lemma 3.3 *Let (C_i, \mathbf{J}_i) be the solution to (2.12), and $(\Pi_h C_i, \Pi_h \mathbf{J}_i)$ be the solution to (3.38). Then for any $t \in [0, T]$, we have the following error estimates*

$$\|\mathbf{J}_i - \Pi_h \mathbf{J}_i\|_{\mathbf{V}} + \|C_i - \Pi_h C_i\|_0 \leq M h^{k+1} (\|\mathbf{J}_i\|_{k+2} + \|C_i\|_{k+1}), \tag{3.39}$$

$$\|\partial_t (\mathbf{J}_i - \Pi_h \mathbf{J}_i)\|_{\mathbf{V}} + \|\partial_t (C_i - \Pi_h C_i)\|_0 \leq M h^{k+1} (\|\partial_t \mathbf{J}_i\|_{k+2} + \|\partial_t C_i\|_{k+1}). \tag{3.40}$$

The following theorem demonstrates error estimates of (3.3) approximating to (2.12).

Theorem 3.3 *Let (C_i, \mathbf{J}_i) be the solution to (2.12) and $(C_{i,h}, \mathbf{J}_{i,h})$ be the finite element solution to (3.3), the regularity assumption (2.14) is held. Then we have the following error estimates*

$$\|\mathbf{J}_i - \mathbf{J}_{i,h}\|_{L^\infty(L^2)} + \|\mathbf{J}_i - \mathbf{J}_{i,h}\|_{L^2(\mathbf{V})} + \|C_i - C_{i,h}\|_{L^\infty(L^2)} \leq M h^{k+1}, \tag{3.41}$$

$$\|\partial_t (\mathbf{J}_i - \mathbf{J}_{i,h})\|_{L^2(L^2)} + \|\mathbf{J}_i - \mathbf{J}_{i,h}\|_{L^\infty(\mathbf{V})} + \|\partial_t (C_i - C_{i,h})\|_{L^2(L^2)} \leq M h^{k+1}. \tag{3.42}$$

Proof Subtract (3.3) from (2.12), and use (3.38), yield

$$\begin{aligned} & (\partial_t (\mathbf{J}_i - \mathbf{J}_{i,h}), \tilde{\mathbf{J}}_i) + (\Pi_h \mathbf{J}_i - \mathbf{J}_{i,h}, \tilde{\mathbf{J}}_i) \\ & + (\nabla \cdot (\Pi_h \mathbf{J}_i - \mathbf{J}_{i,h}), \nabla \cdot \tilde{\mathbf{J}}_i) + (\Pi_h C_i - C_{i,h}, \nabla \cdot \tilde{\mathbf{J}}_i) \\ & + z_i (\mathbf{q} C_i - \mathbf{q}_h C_{i,h}, \tilde{\mathbf{J}}_i) + (\mathbf{u} C_i - \mathbf{u}_h C_{i,h}, \tilde{\mathbf{J}}_i) + z_i (\partial_t (\mathbf{q} C_i - \mathbf{q}_h C_{i,h}), \tilde{\mathbf{J}}_i) \\ & + (\partial_t (\mathbf{u} C_i - \mathbf{u}_h C_{i,h}), \tilde{\mathbf{J}}_i) = 0, \quad \forall \tilde{\mathbf{J}}_i \in \mathbf{V}_h, \end{aligned} \tag{3.43}$$

$$(\partial_t (C_i - C_{i,h}), \tilde{C}_i) - (\nabla \cdot (\Pi_h \mathbf{J}_i - \mathbf{J}_{i,h}), \tilde{C}_i) = 0, \quad \forall \tilde{C}_i \in W_h. \tag{3.44}$$

Let $\mathbf{J}_i - \mathbf{J}_{i,h} = (\mathbf{J}_i - \Pi_h \mathbf{J}_i) + (\Pi_h \mathbf{J}_i - \mathbf{J}_{i,h}) = \mathbf{e}_i + \theta_i$, $C_i - C_{i,h} = (C_i - \Pi_h C_i) + (\Pi_h C_i - C_{i,h}) = \sigma_i + \delta_i$, choose $\tilde{\mathbf{J}}_i = \theta_i$, $\tilde{C}_i = \delta_i$ in (3.43) and (3.44), and add them together, results

$$\begin{aligned} & (\partial_t (e_i + \theta_i), \theta_i) + (\theta_i, \theta_i) \\ & + (\nabla \cdot \theta_i, \nabla \cdot \theta_i) + (\partial_t (\sigma_i + \delta_i), \delta_i) \\ & + z_i (\mathbf{q} C_i - \mathbf{q}_h C_{i,h}, \theta_i) + (\mathbf{u} C_i - \mathbf{u}_h C_{i,h}, \theta_i) + z_i (\partial_t (\mathbf{q} C_i - \mathbf{q}_h C_{i,h}), \theta_i) \\ & + (\partial_t (\mathbf{u} C_i - \mathbf{u}_h C_{i,h}), \theta_i) = 0. \end{aligned}$$

Then,

$$\begin{aligned} & \frac{1}{2} \partial_t \|\theta_i\|_0^2 + \|\theta_i\|_V^2 + \frac{1}{2} \partial_t \|\delta_i\|_0^2 \\ & = -(\partial_t e_i, \theta_i) - (\partial_t \sigma_i, \delta_i) - z_i (\mathbf{q} C_i - \mathbf{q}_h C_{i,h}, \theta_i) - (\mathbf{u} C_i - \mathbf{u}_h C_{i,h}, \theta_i) \\ & \quad - z_i (\partial_t (\mathbf{q} C_i - \mathbf{q}_h C_{i,h}), \theta_i) - (\partial_t (\mathbf{u} C_i - \mathbf{u}_h C_{i,h}), \theta_i) = \sum_{j=1}^6 G_j. \end{aligned} \tag{3.45}$$

By Cauchy–Schwarz inequality, Young’s inequality with ϵ and Lemma (3.3), we have

$$G_1 \leq M \|\partial_t e_i\|_0^2 + \epsilon \|\theta_i\|_0^2 \leq M h^{2(k+1)} + \epsilon \|\theta_i\|_0^2, \tag{3.46}$$

$$G_2 \leq M \|\partial_t \sigma_i\|_0^2 + \epsilon \|\delta_i\|_0^2 \leq M h^{2(k+1)} + \epsilon \|\delta_i\|_0^2. \tag{3.47}$$

Utilize the same analysis skills for estimating (3.32), and apply Lemmas 3.1 and 3.2, Theorems 3.1 and 3.2 as well as corresponding inverse inequalities, leads to

$$\begin{aligned} G_3 & = -z_i ((C_i - C_{i,h}) \mathbf{q}, \theta_i) - z_i (C_i (\mathbf{q} - \mathbf{q}_h), \theta_i) + z_i ((C_i - C_{i,h}) (\mathbf{q} - \mathbf{q}_h), \theta_i) \\ & \leq M \|\theta_i\|_0 (\|\mathbf{q}\|_{L^\infty} \|C_i - C_{i,h}\|_0 + \|C_i\|_{L^\infty} \|\mathbf{q} - \mathbf{q}_h\|_0 + \|\mathbf{q} - \mathbf{q}_h\|_{L^\infty} \|C_i - C_{i,h}\|_0) \\ & \leq M \|\theta_i\|_0 (\|C_i - C_{i,h}\|_0 + \|\mathbf{q} - \mathbf{q}_h\|_0 + h^{-\frac{d}{2}} \|\Pi_h \mathbf{q} - \mathbf{q}_h\|_0 \|C_i - C_{i,h}\|_0) \\ & \leq M \left[\sum_{i=1}^2 \|\delta_i\|_0^2 + h^{2(k+1)} + \left(h^{-\frac{d}{2}} \|\delta_i\|_0 \sum_{j=1}^2 \|\delta_j\|_0 \right)^2 + \|\theta_i\|_0^2 \right], \end{aligned} \tag{3.48}$$

$$\begin{aligned} G_4 & = ((C_i - C_{i,h}) \mathbf{u}, \theta_i) + ((C_i (\mathbf{u} - \mathbf{u}_h), \theta_i) - ((C_i - C_{i,h}) (\mathbf{u} - \mathbf{u}_h), \theta_i)) \\ & \leq M \|\theta_i\|_0 (\|\mathbf{u}\|_{L^\infty} \|C_i - C_{i,h}\|_0 + \|C_i\|_{L^\infty} \|\mathbf{u} - \mathbf{u}_h\|_0 + \|\mathbf{u} - \mathbf{u}_h\|_{L^\infty} \|C_i - C_{i,h}\|_0) \\ & \leq M \|\theta_i\|_0 (\|C_i - C_{i,h}\|_0 + \|\mathbf{u} - \mathbf{u}_h\|_0 + h^{-\frac{d}{2}} \|\Pi_h \mathbf{u} - \mathbf{u}_h\|_0 \|C_i - C_{i,h}\|_0) \\ & \leq M \left[\sum_{i=1}^2 \|\delta_i\|_0^2 + \left(h^{-\frac{d}{2}} \|\delta_i\|_0 \sum_{j=1}^2 \|\delta_j\|_0 \right)^2 + \left(h^{-d} \|\delta_i\|_0 \sum_{j=1}^2 \|\delta_j\|_0^2 \right)^2 + h^{2(k+1)} + \|\theta_i\|_0^2 \right], \end{aligned} \tag{3.49}$$

$$\begin{aligned} G_5 & = -z_i (\partial_t ((C_i - C_{i,h}) \mathbf{q}), \theta_i) - z_i (\partial_t (C_i (\mathbf{q} - \mathbf{q}_h)), \theta_i) + z_i (\partial_t ((C_i - C_{i,h}) (\mathbf{q} - \mathbf{q}_h)), \theta_i) \\ & \leq M \|\theta_i\|_0 (\|\partial_t \mathbf{q}\|_{L^\infty} \|C_i - C_{i,h}\|_0 + \|\mathbf{q}\|_{L^\infty} \|\partial_t (C_i - C_{i,h})\|_0 \\ & \quad + \|\partial_t C_i\|_{L^\infty} \|\mathbf{q} - \mathbf{q}_h\|_0 + \|C_i\|_{L^\infty} \|\partial_t (\mathbf{q} - \mathbf{q}_h)\|_0 \\ & \quad + \|\mathbf{q} - \mathbf{q}_h\|_{L^\infty} \|\partial_t (C_i - C_{i,h})\|_0 + \|\partial_t (\mathbf{q} - \mathbf{q}_h)\|_{L^\infty} \|C_i - C_{i,h}\|_0) \\ & \leq M \|\theta_i\|_0 (\|C_i - C_{i,h}\|_0 + \|\partial_t (C_i - C_{i,h})\|_0 + \|\mathbf{q} - \mathbf{q}_h\|_0 + \|\partial_t (\mathbf{q} - \mathbf{q}_h)\|_0 \\ & \quad + h^{-\frac{d}{2}} \|\Pi_h \mathbf{q} - \mathbf{q}_h\|_0 \|\partial_t (C_i - C_{i,h})\|_0 + h^{-\frac{d}{2}} \|\partial_t (\Pi_h \mathbf{q} - \mathbf{q}_h)\|_0 \|C_i - C_{i,h}\|_0) \\ & \leq M \left[\sum_{i=1}^2 \|\delta_i\|_0^2 + h^{2(k+1)} + \|\theta_i\|_0^2 + \left(h^{-\frac{d}{2}} \|\theta_i\|_0 \sum_{j=1}^2 \|\delta_j\|_0 \right)^2 + \left(h^{-\frac{d}{2}} \|\delta_i\|_0 \|\theta_i\|_0 \right)^2 \right] \end{aligned}$$

$$+\epsilon \sum_{i=1}^2 \|\partial_t \delta_i\|_0^2. \tag{3.50}$$

By conducting the same analysis as for (3.49) and (3.50), we have

$$\begin{aligned} G_6 &= -(\partial_t((C_i - C_{i,h})\mathbf{u}), \theta_i) - (\partial_t(C_i(\mathbf{u} - \mathbf{u}_h)), \theta_i) + z_i(\partial_t((C_i - C_{i,h})(\mathbf{u} - \mathbf{u}_h)), \theta_i) \\ &\leq M\|\theta_i\|_0(\|\partial_t \mathbf{u}\|_{L^\infty}\|C_i - C_{i,h}\|_0 + \|\mathbf{u}\|_{L^\infty}\|\partial_t(C_i - C_{i,h})\|_0 \\ &\quad + \|\partial_t C_i\|_{L^\infty}\|\mathbf{u} - \mathbf{u}_h\|_0 + \|C_i\|_{L^\infty}\|\partial_t(\mathbf{u} - \mathbf{u}_h)\|_0 \\ &\quad + \|\mathbf{u} - \mathbf{u}_h\|_{L^\infty}\|\partial_t(C_i - C_{i,h})\|_0 + \|\partial_t(\mathbf{u} - \mathbf{u}_h)\|_{L^\infty}\|C_i - C_{i,h}\|_0) \\ &\leq M\|\theta_i\|_0(\|C_i - C_{i,h}\|_0 + \|\partial_t(C_i - C_{i,h})\|_0 + \|\mathbf{u} - \mathbf{u}_h\|_0 + \|\partial_t(\mathbf{u} - \mathbf{u}_h)\|_0 \\ &\quad + h^{-\frac{d}{2}}\|\Pi_h \mathbf{u} - \mathbf{u}_h\|_0\|\partial_t(C_i - C_{i,h})\|_0 + h^{-\frac{d}{2}}\|\partial_t(\Pi_h \mathbf{u} - \mathbf{u}_h)\|_0\|C_i - C_{i,h}\|_0) \\ &\leq M \left[\sum_{i=1}^2 \|\delta_i\|_0^2 + \|\theta\|_0^2 + h^{2(k+1)} + \left(h^{-\frac{d}{2}} \sum_{j=1}^2 \|\delta_j\|_0^2\right)^2 + \left(h^{-d-1} \sum_{j=1}^2 \|\delta_j\|_0^4\right)^2 \right. \\ &\quad + \left(h^{-1} \sum_{j=1}^2 \|\delta_j\|_0^2\right)^2 + \left(h^{-d}\|\theta_i\|_0 \sum_{j=1}^2 \|\delta_j\|_0^2\right)^2 + \left(h^{-\frac{d}{2}}\|\theta_i\|_0 \sum_{j=1}^2 \|\delta_j\|_0\right)^2 \\ &\quad \left. + \left(h^{-\frac{3}{2}d-1}\|\theta_i\|_0 \sum_{j=1}^2 \|\delta_j\|_0^4\right)^2 + \left(h^{-\frac{d}{2}-1}\|\theta_i\|_0 \sum_{j=1}^2 \|\delta_j\|_0^2\right)^2 \right] + \epsilon \|\partial_t \delta_i\|_0^2. \tag{3.51} \end{aligned}$$

Now we conduct a mathematical induction process and propose the following induction hypothesis:

$$h^{-\frac{d}{2}}\|\delta_i(t)\|_0 \leq M, \forall t \in [0, T], i = 1, 2, d = 2, 3. \tag{3.52}$$

When $t = 0$, by a properly chose initial value $C_{i,h}(0) = \Pi_h C_i^0$, we have $\delta_i(0) = 0$, thus (3.52) is satisfied. Assume that (3.52) holds for G_3, G_4, G_5 and G_6 for $t \in [0, T^*], T^* < T$, then

$$G_3 + G_4 + G_5 + G_6 \leq M \left(\sum_{i=1}^2 \|\delta_i\|_0^2 + h^{2(k+1)} + \|\theta_i\|_0^2 \right) + \epsilon \sum_{i=1}^2 \|\partial_t \delta_i\|_0^2. \tag{3.53}$$

On the other hand, let $\tilde{C}_i = \partial_t \delta_i$ in (3.44), we have

$$(\partial_t(\sigma_i + \delta_i), \partial_t \delta_i) - (\nabla \cdot \theta_i, \partial_t \delta_i) = 0, \tag{3.54}$$

thus

$$\|\partial_t \delta_i\|_0 \leq \|\partial_t \sigma_i\|_0 + \|\nabla \cdot \theta_i\|_0. \tag{3.55}$$

Substitute (3.55) into (3.53), then (3.45) can be estimated as

$$\frac{1}{2}\partial_t \|\theta_i\|_0^2 + \|\theta_i\|_V^2 + \frac{1}{2}\partial_t \|\delta_i\|_0^2 \leq M \left(\sum_{i=1}^2 \|\delta_i\|_0^2 + h^{2(k+1)} + \|\theta_i\|_0^2 \right) + \epsilon \sum_{i=1}^2 \|\theta_i\|_V^2. \tag{3.56}$$

Sum over i from 1 to 2, take a sufficiently small ϵ , integrate both sides of (3.56) in time from 0 to t , then apply Grönwall's inequality with $C_{i,h}(0) = \Pi_h C_i^0$ and $\mathbf{J}_{i,h}(0) = \Pi_h \mathbf{J}_i^0$ (see Remark 3.2), yield

$$\sum_{i=1}^2 \left(\|\theta_i\|_{L^\infty(L^2)} + \|\theta_i\|_{L^2(V)} + \|\delta_i\|_{L^\infty(L^2)} \right) \leq M h^{k+1}, \tag{3.57}$$

which is true for any $t \in [0, T^*]$. (3.57) also shows that for $k \geq 1$ and $d = 2, 3$, we always have

$$h^{-\frac{d}{2}} \|\delta_i(t)\|_0 \leq Mh^{k+1-\frac{d}{2}} \leq M.$$

On the other hand, since $h^{-\frac{d}{2}} \|\delta_i(t)\|_0$ is a continuous function with respect to $t \in [0, T]$, thus due to the uniform continuity in time, there exists ϵ such that for any $t \in [0, T^* + \epsilon]$, we have $h^{-\frac{d}{2}} \|\delta_i(t)\|_0 \leq M$. Because $[0, T]$ is a finite interval, so the induction hypothesis (3.52) holds true for all $t \in [0, T]$. Therefore, for any $t \in [0, T]$ we have (3.57).

Combine (3.57) with (3.55), apply Lemma 3.3 and the triangular inequality, (3.41) is then obtained. On the other hand, choose $\tilde{J}_i = \partial_t \theta_i$, $\tilde{C}_i = \partial_t \delta_i$ in (3.43) and (3.44), yields

$$\begin{aligned} & \|\partial_t \theta_i\|_0^2 + \frac{1}{2} \partial_t \|\theta_i\|_0^2 + \frac{1}{2} \partial_t \|\nabla \cdot \theta_i\|_0^2 = -(\partial_t e_i, \partial_t \theta_i) + (\partial_t (\sigma_i + \delta_i), \partial_t \delta_i) - \partial_t (\delta_i, \nabla \cdot \theta_i) \\ & - z_i (\mathbf{q} C_i - \mathbf{q}_h C_{i,h}, \partial_t \theta_i) - (\mathbf{u} C_i - \mathbf{u}_h C_{i,h}, \partial_t \theta_i) - z_i (\partial_t (\mathbf{q} C_i - \mathbf{q}_h C_{i,h}), \partial_t \theta_i) \\ & - (\partial_t (\mathbf{u} C_i - \mathbf{u}_h C_{i,h}), \partial_t \theta_i) = \sum_{j=1}^7 R_j. \end{aligned} \tag{3.58}$$

By Cauchy–Schwarz inequality, Young’s inequality with ϵ , Lemma 3.3 and (3.55), we have

$$R_1 \leq M \|\partial_t e_i\|_0^2 + \epsilon \|\partial_t \theta_i\|_0^2 \leq Mh^{2(k+1)} + \epsilon \|\partial_t \theta_i\|_0^2, \tag{3.59}$$

$$R_2 \leq M \left(\|\partial_t \sigma_i\|_0^2 + \|\partial_t \delta_i\|_0^2 \right) \leq M \left(h^{2(k+1)} + \|\nabla \cdot \theta_i\|_0^2 \right). \tag{3.60}$$

Utilize the same analysis skills as conducted in (3.48), (3.49), (3.50) and (3.51) for Terms R_4 – R_7 , results

$$R_4 + R_5 + R_6 + R_7 \leq M \left(\sum_{i=1}^2 \left(\|\delta_i\|_0^2 + \|\nabla \cdot \theta_i\|_0^2 \right) + h^{2(k+1)} \right) + \epsilon \|\partial_t \theta_i\|_0^2. \tag{3.61}$$

Take a sufficiently small ϵ , and apply (3.57), then (3.58) can be estimated as

$$\|\partial_t \theta_i\|_0^2 + \frac{1}{2} \partial_t \|\theta_i\|_V^2 \leq M(h^{2(k+1)} + \|\nabla \cdot \theta_i\|_0^2) - \partial_t (\delta_i, \nabla \cdot \theta_i). \tag{3.62}$$

Integrate both sides in time from 0 to t , yields

$$\begin{aligned} \int_0^t \|\partial_t \theta_i\|_0^2 d\tau + \|\theta_i\|_V^2 & \leq M \left(h^{2(k+1)} + \int_0^t \|\theta_i\|_V^2 d\tau \right) - (\delta_i, \nabla \cdot \theta_i) \\ & \leq M \left(h^{2(k+1)} + \int_0^t \|\theta_i\|_V^2 d\tau \right) + \|\delta_i\|_0^2 + \epsilon \|\theta_i\|_V^2. \end{aligned} \tag{3.63}$$

Then, further take a sufficiently small ϵ , apply Grönwall’s inequality and (3.57), leads to

$$\|\partial_t \theta_i\|_{L^2(L^2)} + \|\theta_i\|_{L^\infty(V)} \leq Mh^{k+1}. \tag{3.64}$$

Combine (3.64) with (3.55), apply Lemma 3.3 and the triangular inequality, (3.42) is then obtained. \square

Combining Theorems 3.1, 3.2, 3.3, we finally obtain a complete convergence theorem for the semi-discrete scheme (3.2)–(3.4) as follows.

Theorem 3.4 *Let $(\phi, \mathbf{q}, z, u, p, C_i, \mathbf{J}_i)$ be the solution to (2.7a)–(2.9) satisfying the regularity properties (2.13)–(2.15), and $(\phi_h, \mathbf{q}_h, z_h, u_h, p_h, C_{i,h}, \mathbf{J}_{i,h})$ be the solution to (3.2)–(3.4). Then the following error estimates hold*

$$\begin{aligned} & \|\mathbf{q} - \mathbf{q}_h\|_{L^\infty(V)} + \|\partial_t (\mathbf{q} - \mathbf{q}_h)\|_{L^2(V)} + \|\phi - \phi_h\|_{L^\infty(L^2)} + \|\partial_t (\phi - \phi_h)\|_{L^2(L^2)} \\ & + \|z - z_h\|_{L^\infty(L^2)} + h \|z - z_h\|_{L^\infty(H^1)} \leq Mh^{k+1}, \\ & \|\mathbf{u} - \mathbf{u}_h\|_{L^\infty(L^2)} + \|\mathbf{u} - \mathbf{u}_h\|_{L^\infty(H^1)} + \|\partial_t (\mathbf{u} - \mathbf{u}_h)\|_{L^2(L^2)} \end{aligned} \tag{3.65}$$

$$+\|p - p_h\|_{L^2(L^2)} \leq Mh^{k+1}, \tag{3.66}$$

$$\begin{aligned} &\|C_i - C_{i,h}\|_{L^\infty(L^2)} + \|\partial_t(C_i - C_{i,h})\|_{L^2(L^2)} \\ &+\|J_i - J_{i,h}\|_{L^\infty(V)} + \|J_i - J_{i,h}\|_{L^\infty(L^2)} \leq Mh^{k+1}. \end{aligned} \tag{3.67}$$

Remark 3.2 Given initial values C_i^0 and u^0 , we can obtain $\phi^0 = \phi(0)$ that is determined by the fourth-order elliptic equation in (2.1) at $t = 0$ with the boundary condition shown in (2.2). Thereafter, by the definition (2.4), we have $J_i^0 = J_i(0) = \nabla C_i^0 + z_i \nabla \phi^0 C_i^0 - u^0 C_i^0$. Thus, all discrete initial values can be defined as: $C_{i,h}(0) = \Pi_h C_i^0$, $J_{i,h}(0) = \Pi_h J_i^0$ and $u_h(0) = \Pi_h u^0$ by their own H^1 -projection.

4 Fully Discrete Mixed Finite Element Approximation

In order to develop a full discretization for (2.9), (2.10) and (2.12), we first define a uniform partition in the time interval $[0, T]$: $0 = t_0 < t_1 < \dots < t_N = T$ with the time-step size $\Delta t = T/N$, then set $t_n = n \Delta t$ ($0 \leq n \leq N$). Let $\varphi^n = \varphi(t^n)$, and $d_t \varphi^{n+1} = \frac{\varphi^{n+1} - \varphi^n}{\Delta t}$. In what follows, we employ the backward Euler scheme together with Taylor–Hood mixed finite element approximation to define the fully discrete scheme of (2.9), (2.10) and (2.12).

4.1 Fully Discrete Mixed Finite Element Discretization

For $n = 0, 1, \dots, N - 1$, suppose $(\phi_h^n, q_h^n, z_h^n, C_{i,h}^n, J_{i,h}^n, u_h^n, p_h^n)$ are given, find $(\phi_h^{n+1}, q_h^{n+1}, z_h^{n+1}) \in W_h, f_1 \times V_h \times Z_h, (C_{i,h}^{n+1}, J_{i,h}^{n+1}) \in W_h, g_i \times V_h, (u_h^{n+1}, p_h^{n+1}) \in U_h, 0 \times W_h, \forall (\tilde{q}, \tilde{\phi}, \tilde{z}, \tilde{J}_i, \tilde{C}_i, \tilde{u}, \tilde{p}) \in V_h \times W_h \times Z_h \times V_h \times W_h \times U_h, 0 \times W_h$, such that

$$\begin{cases} (q_h^{n+1}, \tilde{q}) + (\nabla \cdot q_h^{n+1}, \nabla \cdot \tilde{q}) - (\phi_h^{n+1}, \nabla \cdot \tilde{q}) = (z_h^{n+1}, \nabla \cdot \tilde{q}) - \langle f_1^{n+1}, \tilde{q} \cdot \mathbf{n} \rangle_{\partial\Omega}, \\ (\nabla \cdot q_h^{n+1}, \tilde{\phi}) = (z_h^{n+1}, \tilde{\phi}), \\ (\nabla z_h^{n+1}, \nabla \tilde{z}) + (z_h^{n+1}, \tilde{z}) = (C_{1,h}^{n+1} - C_{2,h}^{n+1}, \tilde{z}) - \langle f_2^{n+1}, \tilde{z} \rangle_{\partial\Omega}, \end{cases} \tag{4.1}$$

$$\begin{cases} (d_t J_{i,h}^{n+1}, \tilde{J}_i) + (J_{i,h}^{n+1}, \tilde{J}_i) + (\nabla \cdot J_{i,h}^{n+1}, \nabla \cdot \tilde{J}_i) + (C_{i,h}^{n+1}, \nabla \cdot \tilde{J}_i) + z_i (q_h^{n+1} C_{i,h}^{n+1}, \tilde{J}_i) \\ + (u_h^{n+1} C_{i,h}^{n+1}, \tilde{J}_i) + z_i (d_t (C_{i,h}^{n+1} q_h^{n+1}), \tilde{J}_i) + (d_t (C_{i,h}^{n+1} u_h^{n+1}), \tilde{J}_i) \\ = \langle g_i^{n+1}, \tilde{J}_i \cdot \mathbf{n} \rangle_{\partial\Omega} + \langle \partial_t g_i^{n+1}, \tilde{J}_i \cdot \mathbf{n} \rangle_{\partial\Omega}, \\ (d_t C_{i,h}^{n+1}, \tilde{C}_i) - (\nabla \cdot J_{i,h}^{n+1}, \tilde{C}_i) = 0, \end{cases} \tag{4.2}$$

$$\begin{cases} (d_t u_h^{n+1}, \tilde{u}) + \beta (u_h^{n+1}, u_h^{n+1}, \tilde{u}) + (\nabla u_h^{n+1}, \nabla \tilde{u}) - (p_h^{n+1}, \nabla \cdot \tilde{u}) \\ = ((C_{1,h}^{n+1} - C_{2,h}^{n+1}) q_h^{n+1}, \tilde{u}), \\ (\nabla \cdot u_h^{n+1}, \tilde{p}) = 0. \end{cases} \tag{4.3}$$

We use Picard’s method to linearize nonlinear terms in (4.1)–(4.3), and implement the following Algorithm 4.1 to carry out the mixed finite element computation for the presented modified PNP/NS coupling system (2.1).

- Algorithm 4.1**
1. Initialization of time marching: set $n = 0$ and adopt the discrete initial values $(C_{i,h}^0, J_{i,h}^0, u_h^0)$ as shown in Remark 3.2.
 2. Initialization of nonlinear iteration: let $(\phi_h^{n+1,0}, q_h^{n+1,0}, z_h^{n+1,0}, C_{i,h}^{n+1,0}, J_{i,h}^{n+1,0}, u_h^{n+1,0}, p_h^{n+1,0}) = (\phi_h^n, q_h^n, z_h^n, C_{i,h}^n, J_{i,h}^n, u_h^n, p_h^n)$ as $n \geq 0$. Set $m = 0$.
 3. Mixed finite element computation at each nonlinear iteration: for $m \geq 0$, find

$(\phi_h^{n+1,m+1}, \mathbf{q}_h^{n+1,m+1}, z_h^{n+1,m+1}, C_{i,h}^{n+1,m+1}, \mathbf{J}_{i,h}^{n+1,m+1}, \mathbf{u}_h^{n+1,m+1}, p_h^{n+1,m+1}) \in W_h \times V_h \times Z_h \times W_h \times V_h \times \mathbf{U}_h \times W_h, \forall (\tilde{\mathbf{q}}, \tilde{\phi}, \tilde{z}, \tilde{\mathbf{J}}_i, \tilde{C}_i, \tilde{\mathbf{u}}, \tilde{p}) \in V_h \times W_h \times Z_h \times V_h \times W_h \times \mathbf{U}_h \times W_h$ such that

$$\begin{cases} (\mathbf{q}_h^{n+1,m+1}, \tilde{\mathbf{q}}) + (\nabla \cdot \mathbf{q}_h^{n+1,m+1}, \nabla \cdot \tilde{\mathbf{q}}) - (\phi_h^{n+1,m+1}, \nabla \cdot \tilde{\mathbf{q}}) - (z_h^{n+1,m+1}, \nabla \cdot \tilde{\mathbf{q}}) \\ \quad = - \langle f_1^{n+1}, \tilde{\mathbf{q}} \cdot \mathbf{n} \rangle_{\partial\Omega}, \\ (\nabla \cdot \mathbf{q}_h^{n+1,m+1}, \tilde{\phi}) - (z_h^{n+1,m+1}, \tilde{\phi}) = 0, \\ (\nabla z_h^{n+1,m+1}, \nabla \tilde{z}) + (z_h^{n+1,m+1}, \tilde{z}) = (C_{1,h}^{n+1,m} - C_{2,h}^{n+1,m}, \tilde{z}) - \langle f_2^{n+1}, \tilde{z} \rangle_{\partial\Omega}, \\ \left(\frac{J_{i,h}^{n+1,m+1} - J_{i,h}^n}{\Delta t}, \tilde{\mathbf{J}}_i \right) + (\mathbf{J}_{i,h}^{n+1,m+1}, \tilde{\mathbf{J}}_i) + (\nabla \cdot \mathbf{J}_{i,h}^{n+1,m+1}, \nabla \cdot \tilde{\mathbf{J}}_i) + (C_{i,h}^{n+1,m+1}, \nabla \cdot \tilde{\mathbf{J}}_i) \\ \quad + (z_i \mathbf{q}_h^{n+1,m} C_{i,h}^{n+1,m+1}, \tilde{\mathbf{J}}_i) + (\mathbf{u}_h^{n+1,m} C_{i,h}^{n+1,m+1}, \tilde{\mathbf{J}}_i) + \left(z_i \frac{q_h^{n+1,m} - q_h^n}{\Delta t} C_{i,h}^{n+1,m+1}, \tilde{\mathbf{J}}_i \right) \\ \quad + \left(z_i \mathbf{q}_h^{n+1,m} \frac{C_{i,h}^{n+1,m+1} - C_{i,h}^n}{\Delta t}, \tilde{\mathbf{J}}_i \right) + \left(\frac{u_h^{n+1,m} - u_h^n}{\Delta t} C_{i,h}^{n+1,m+1}, \tilde{\mathbf{J}}_i \right) + \left(\mathbf{u}_h^{n+1,m} \frac{C_{i,h}^{n+1,m+1} - C_{i,h}^n}{\Delta t}, \tilde{\mathbf{J}}_i \right) \\ \quad = \langle g_i^{n+1}, \tilde{\mathbf{J}}_i \cdot \mathbf{n} \rangle_{\partial\Omega} + \langle \partial_t g_i^{n+1}, \tilde{\mathbf{J}}_i \cdot \mathbf{n} \rangle_{\partial\Omega}, \\ \left(\frac{C_{i,h}^{n+1,m+1} - C_{i,h}^n}{\Delta t}, \tilde{C}_i \right) - (\nabla \cdot \mathbf{J}_{i,h}^{n+1,m+1}, \tilde{C}_i) = 0, \\ \left(\frac{u_h^{n+1,m+1} - u_h^n}{\Delta t}, \tilde{\mathbf{u}} \right) + \beta (\mathbf{u}_h^{n+1,m}, \mathbf{u}_h^{n+1,m+1}, \tilde{\mathbf{u}}) + (\nabla \mathbf{u}_h^{n+1,m+1}, \nabla \tilde{\mathbf{u}}) - (p_h^{n+1,m+1}, \nabla \cdot \tilde{\mathbf{u}}) \\ \quad = \left((C_{1,h}^{n+1,m} - C_{2,h}^{n+1,m}) \mathbf{q}_h^{n+1,m}, \tilde{\mathbf{u}} \right), \\ (\nabla \cdot \mathbf{u}_h^{n+1,m+1}, \tilde{p}) = 0. \end{cases}$$

4. Check stopping criteria for the nonlinear iteration: for a given tolerance ϵ , stop the iteration if

$$\begin{aligned} & \| \mathbf{q}_h^{n+1,m+1} - \phi_h^{n+1,m} \|_0 + \| \mathbf{q}_h^{n+1,m+1} - \mathbf{q}_h^{n+1,m} \|_0 + \| z_h^{n+1,m+1} - z_h^{n+1,m} \|_0 \\ & + \sum_{i=1}^2 \| C_{i,h}^{n+1,m+1} - C_{i,h}^{n+1,m} \|_0 + \| \mathbf{u}_h^{n+1,m+1} - \mathbf{u}_h^{n+1,m} \|_0 + \| p_h^{n+1,m+1} - p_h^{n+1,m} \|_0 \leq \epsilon, \end{aligned}$$

and set

$$\begin{aligned} & (\phi_h^{n+1}, \mathbf{q}_h^{n+1}, z_h^{n+1}, C_{i,h}^{n+1}, \mathbf{J}_{i,h}^{n+1}, \mathbf{u}_h^{n+1}, p_h^{n+1}) \\ & = (\phi_h^{n+1,m+1}, \mathbf{q}_h^{n+1,m+1}, z_h^{n+1,m+1}, C_{i,h}^{n+1,m+1}, \mathbf{J}_{i,h}^{n+1,m+1}, \mathbf{u}_h^{n+1,m+1}, p_h^{n+1,m+1}). \end{aligned}$$

Otherwise, set $m \leftarrow m + 1$ and go to Step 3 to continue.

5. Time marching: stop marching if $n + 1 = N$, otherwise set $n \leftarrow n + 1$ and go to Step 2 to continue.

4.2 Fully Discrete Error Analysis

First, let each term in weak formulations (2.9), (2.10) and (2.12) take the value at t_{n+1} , yields

$$\begin{cases} (\mathbf{q}^{n+1}, \tilde{\mathbf{q}}) + (\nabla \cdot \mathbf{q}^{n+1}, \nabla \cdot \tilde{\mathbf{q}}) - (\phi^{n+1}, \nabla \cdot \tilde{\mathbf{q}}) = (z^{n+1}, \nabla \cdot \tilde{\mathbf{q}}) - \langle f_1^{n+1}, \tilde{\mathbf{q}} \cdot \mathbf{n} \rangle_{\partial\Omega}, \\ (\nabla \cdot \mathbf{q}^{n+1}, \tilde{\phi}) = (z^{n+1}, \tilde{\phi}), \\ (\nabla z^{n+1}, \nabla \tilde{z}) + (z^{n+1}, \tilde{z}) = (C_1^{n+1} - C_2^{n+1}, \tilde{z}) - \langle f_2^{n+1}, \tilde{z} \rangle_{\partial\Omega}. \end{cases} \tag{4.4}$$

$$\begin{cases} (\partial_t \mathbf{u}^{n+1}, \tilde{\mathbf{u}}) + \beta (\mathbf{u}^{n+1}, \mathbf{u}^{n+1}, \tilde{\mathbf{u}}) + (\nabla \mathbf{u}^{n+1}, \nabla \tilde{\mathbf{u}}) - (p^{n+1}, \nabla \cdot \tilde{\mathbf{u}}) = \left((C_1^{n+1} - C_2^{n+1}) \mathbf{q}^{n+1}, \tilde{\mathbf{u}} \right), \\ (\nabla \cdot \mathbf{u}^{n+1}, \tilde{p}) = 0. \end{cases} \tag{4.5}$$

$$\begin{cases} (\partial_t \mathbf{J}_i^{n+1}, \tilde{\mathbf{J}}_i) + (\mathbf{J}_i^{n+1}, \tilde{\mathbf{J}}_i) + (\nabla \cdot \mathbf{J}_i^{n+1}, \nabla \cdot \tilde{\mathbf{J}}_i) + (C_i^{n+1}, \nabla \cdot \tilde{\mathbf{J}}_i) + (z_i \mathbf{q}^{n+1} C_i^{n+1}, \tilde{\mathbf{J}}_i) \\ \quad + (\mathbf{u}^{n+1} C_i^{n+1}, \tilde{\mathbf{J}}_i) + (z_i \partial_t (\mathbf{q}^{n+1} C_i^{n+1}), \tilde{\mathbf{J}}_i) + (\partial_t (\mathbf{u}^{n+1} C_i^{n+1}), \tilde{\mathbf{J}}_i) \\ \quad = \langle g_i^{n+1}, \tilde{\mathbf{J}}_i \cdot \mathbf{n} \rangle_{\partial\Omega} + \langle \partial_t g_i^{n+1}, \tilde{\mathbf{J}}_i \cdot \mathbf{n} \rangle_{\partial\Omega}, \\ (\partial_t C_i^{n+1}, \tilde{C}_i) - (\nabla \cdot \mathbf{J}_i^{n+1}, \tilde{C}_i) = 0. \end{cases} \tag{4.6}$$

Subtracting (4.1) from (4.4), and utilizing the H^1 -projection (3.5) at t_{n+1} , we can have the following lemma by doing an analogous proof as for Theorem 3.1 because of its steady state feature.

Lemma 4.1 *Let $(\phi_h^{n+1}, \mathbf{q}_h^{n+1}, z_h^{n+1})$ be the solution to (4.1), and $(\phi^{n+1}, \mathbf{q}^{n+1}, z^{n+1})$ be the solution to (4.4). Then the following error estimates hold*

$$\|\mathbf{q}^{n+1} - \mathbf{q}_h^{n+1}\|_V + \|\phi^{n+1} - \phi_h^{n+1}\|_0 \leq M \left(\sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0 + h^{k+1} \right), \tag{4.7}$$

$$\|z^{n+1} - z_h^{n+1}\|_0 + h\|z^{n+1} - z_h^{n+1}\|_1 \leq M \left(\sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0 + h^{k+1} \right). \tag{4.8}$$

Next, we analysis the fully discrete error estimates for $\mathbf{u}^{n+1} - \mathbf{u}_h^{n+1}$, $\mathbf{J}_i^{n+1} - \mathbf{J}_{i,h}^{n+1}$ and $C_i^{n+1} - C_{i,h}^{n+1}$, respectively. Subtract (4.2) from (4.5), and use (3.22) at t_{n+1} , reads

$$\begin{aligned} & (\partial_t \mathbf{u}^{n+1} - d_t \mathbf{u}_h^{n+1}, \tilde{\mathbf{u}}) + a_u (\Pi_h \mathbf{u}^{n+1} - \mathbf{u}_h^{n+1}, \tilde{\mathbf{u}}) - b_u (\tilde{\mathbf{u}}, \Pi_h p^{n+1} - p_h^{n+1}) \\ & + \beta (\mathbf{u}^{n+1}, \mathbf{u}^{n+1}, \tilde{\mathbf{u}}) - \beta (\mathbf{u}_h^{n+1}, \mathbf{u}_h^{n+1}, \tilde{\mathbf{u}}) = \sum_{i=1}^2 z_i (C_i^{n+1} \mathbf{q}^{n+1} - C_{i,h}^{n+1} \mathbf{q}_h^{n+1}, \tilde{\mathbf{u}}), \end{aligned} \tag{4.9}$$

$$b_u (\Pi_h \mathbf{u}^{n+1} - \mathbf{u}_h^{n+1}, \tilde{p}) = 0. \tag{4.10}$$

Let $\mathbf{u}^{n+1} - \mathbf{u}_h^{n+1} = (\mathbf{u}^{n+1} - \Pi_h \mathbf{u}^{n+1}) + (\Pi_h \mathbf{u}^{n+1} - \mathbf{u}_h^{n+1}) = \eta^{n+1} + \xi^{n+1}$, choose $\tilde{\mathbf{u}} = \xi^{n+1}$, $\tilde{p} = \Pi_h p^{n+1} - p_h^{n+1}$, and then add (4.9) and (4.10), yield

$$\begin{aligned} & (d_t \xi^{n+1}, \xi^{n+1}) + a_u (\xi^{n+1}, \xi^{n+1}) \\ & = -(\partial_t \mathbf{u}^{n+1} - d_t \mathbf{u}^{n+1}, \xi^{n+1}) + (\partial_t \eta^{n+1} - d_t \eta^{n+1}, \xi^{n+1}) - (\partial_t \eta^{n+1}, \xi^{n+1}) \\ & + \beta (\mathbf{u}_h^{n+1}, \mathbf{u}_h^{n+1}, \xi^{n+1}) - \beta (\mathbf{u}^{n+1}, \mathbf{u}^{n+1}, \xi^{n+1}) + \sum_{i=1}^2 z_i (C_i^{n+1} \mathbf{q}^{n+1} - C_{i,h}^{n+1} \mathbf{q}_h^{n+1}, \xi^{n+1}). \end{aligned} \tag{4.11}$$

By Taylor’s expansion, we have

$$\partial_t \varphi^{n+1} - d_t \varphi^{n+1} = \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} (\tilde{t} - t_n) \frac{\partial^2 \varphi}{\partial t^2} d\tilde{t}, \quad \forall \varphi \in H^2(0, T; L^2(\Omega)), \tag{4.12}$$

then

$$\|\partial_t \varphi^{n+1} - d_t \varphi^{n+1}\|_0 \leq M(\Delta t) \left\| \frac{\partial^2 \varphi}{\partial t^2} \right\|_0. \tag{4.13}$$

Thus, we have

$$(\partial_t \mathbf{u}^{n+1} - d_t \mathbf{u}^{n+1}, \xi^{n+1}) \leq M(\Delta t) \|\mathbf{u}\|_{H^2(L^2)} \|\xi^{n+1}\|_0 \leq M \left((\Delta t)^2 + \|\xi^{n+1}\|_0^2 \right), \tag{4.14}$$

$$(\partial_t \eta^{n+1} - d_t \eta^{n+1}, \xi^{n+1}) \leq M(\Delta t) \|\eta\|_{H^2(L^2)} \|\xi^{n+1}\|_0 \leq M \left((\Delta t)^2 + \|\xi^{n+1}\|_0^2 \right), \tag{4.15}$$

$$(\partial_t \eta^{n+1}, \xi^{n+1}) \leq M \|\partial_t \eta^{n+1}\|_0 \|\xi^{n+1}\|_0 \leq M \left(h^{2(k+2)} + \|\xi^{n+1}\|_0^2 \right). \tag{4.16}$$

Analyses of the rest terms in (4.11) are similar with (3.30), (3.31) and (3.32) in the proof of Theorem 3.2 and are thus omitted here, then we obtain

$$\|\xi^{n+1}\|_0^2 + \Delta t \|\nabla \xi^{n+1}\|_0^2 \leq (\xi^n, \xi^{n+1}) + M \Delta t \left(h^{-d} \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^4 + \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^2 \right)$$

$$+ \|\xi^{n+1}\|_0^2 + (\Delta t)^2 + h^{2(k+1)}) + \epsilon \Delta t \|\nabla \xi^{n+1}\|_0^2.$$

Apply Cauchy–Schwarz inequality and Young’s inequality with $\epsilon = \frac{1}{2}$ to the first term on the right hand side, and take a sufficiently small ϵ , yield

$$\begin{aligned} \frac{1}{2} \|\xi^{n+1}\|_0^2 + \Delta t \|\nabla \xi^{n+1}\|_0^2 &\leq M \Delta t \left(h^{-d} \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^4 + \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^2 \right. \\ &\quad \left. + \|\xi^{n+1}\|_0^2 + (\Delta t)^2 + h^{2(k+1)} \right) + \frac{1}{2} \|\xi^n\|_0^2. \end{aligned}$$

Sum over the time step n from 0 to $L - 1$ ($1 \leq L \leq N$), and apply the telescoping technique, results

$$\begin{aligned} \frac{1}{2} \|\xi^L\|_0^2 + \Delta t \sum_{n=0}^{L-1} \|\nabla \xi^{n+1}\|_0^2 &\leq \frac{1}{2} \|\xi^0\|_0^2 + M \Delta t \sum_{n=0}^{L-1} \left(h^{-d} \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^4 \right. \\ &\quad \left. + \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^2 + \|\xi^{n+1}\|_0^2 + (\Delta t)^2 + h^{2(k+1)} \right). \end{aligned}$$

Then, by the discrete Grönwall’s inequality, and properly choosing the initial value $u_h^0 = \Pi_h u^0$, we have

$$\begin{aligned} &\|\xi^L\|_0^2 + \Delta t \sum_{n=0}^{L-1} \|\nabla \xi^{n+1}\|_0^2 \\ &\leq M \left[\Delta t \sum_{n=0}^{L-1} \left(h^{-d} \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^4 + \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^2 \right) + (\Delta t)^2 + h^{2(k+1)} \right]. \end{aligned} \tag{4.17}$$

If choose $\tilde{u} = d_t \xi^{n+1}$, $\tilde{p} = d_t (\Pi_h p^{n+1} - p_h^{n+1})$ in (4.9) and (4.10), then

$$\begin{aligned} &(d_t \xi^{n+1}, d_t \xi^{n+1}) + a_u (\xi^{n+1}, d_t \xi^{n+1}) \\ &= -(\partial_t u^{n+1} - d_t u^{n+1}, d_t \xi^{n+1}) + (\partial_t \eta^{n+1} - d_t \eta^{n+1}, d_t \xi^{n+1}) - (\partial_t \eta^{n+1}, d_t \xi^{n+1}) \\ &\quad + \beta (u_h^{n+1}, u_h^{n+1}, d_t \xi^{n+1}) - \beta (u^{n+1}, u^{n+1}, d_t \xi^{n+1}) \\ &\quad + \sum_{i=1}^2 z_i (C_i^{n+1} q^{n+1} - C_{i,h}^{n+1} q_h^{n+1}, d_t \xi^{n+1}). \end{aligned}$$

By similar analysis skills as for (4.11) and (3.34), we can have

$$\begin{aligned} &\Delta t \sum_{n=0}^{L-1} \|d_t \xi^{n+1}\|_0^2 + \|\nabla \xi^L\|_0^2 \\ &\leq M \left[\Delta t \sum_{n=0}^{L-1} \left(h^{-2} \|\nabla (u^{n+1} - u_h^{n+1})\|_0^4 + \|\nabla (u^{n+1} - u_h^{n+1})\|_0^2 \right. \right. \\ &\quad \left. \left. + h^{-d} \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^4 + \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^2 \right) + (\Delta t)^2 + h^{2(k+1)} \right]. \end{aligned} \tag{4.18}$$

Then by (4.17) we obtain

$$\begin{aligned} &\Delta t \sum_{n=0}^{L-1} \|d_t \xi^{n+1}\|_0^2 + \|\nabla \xi^L\|_0^2 \\ &\leq M \left[\Delta t \sum_{n=0}^{L-1} \left(h^{-2} \left(h^{-2d} \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^8 + \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^4 \right) \right. \right. \end{aligned}$$

$$+h^{-d} \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^4 + \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^2 \Big) + (\Delta t)^2 + h^{2(k+1)} \Big]. \tag{4.19}$$

As for the fully discrete error estimates of Nernst-Planck equations, we subtract (4.3) from (4.6), and utilize (3.38) at t_{n+1} to have

$$\begin{aligned} & \left(\partial_t J_i^{n+1} - d_t J_{i,h}^{n+1}, \tilde{J}_i \right) + \left(\Pi_h J_i^{n+1} - J_{i,h}^{n+1}, \tilde{J}_i \right) + \left(\nabla \cdot \left(\Pi_h J_i^{n+1} - J_{i,h}^{n+1} \right), \nabla \cdot \tilde{J}_i \right) \\ & + \left(\Pi_h C_i^{n+1} - C_{i,h}^{n+1}, \nabla \cdot \tilde{J}_i \right) + z_i \left(q^{n+1} C_i^{n+1} - q_h^{n+1} C_{i,h}^{n+1}, \tilde{J}_i \right) \\ & + \left(u^{n+1} C_i^{n+1} - u_h^{n+1} C_{i,h}^{n+1}, \tilde{J}_i \right) + z_i \left(\partial_t \left(q^{n+1} C_i^{n+1} \right) - d_t \left(q_h^{n+1} C_{i,h}^{n+1} \right), \tilde{J}_i \right) \\ & + \left(\partial_t \left(u^{n+1} C_i^{n+1} \right) - d_t \left(u_h^{n+1} C_{i,h}^{n+1} \right), \tilde{J}_i \right) = 0, \quad \forall \tilde{J}_i \in V_h, \end{aligned} \tag{4.20}$$

$$\left(\partial_t C_i^{n+1} - d_t C_{i,h}^{n+1}, \tilde{C}_i \right) - \left(\nabla \cdot \left(\Pi_h J_i^{n+1} - J_{i,h}^{n+1} \right), \tilde{C}_i \right) = 0, \quad \forall \tilde{C}_i \in W_h. \tag{4.21}$$

Let $J_i^{n+1} - J_{i,h}^{n+1} = (J_i^{n+1} - \Pi_h J_i^{n+1}) + (\Pi_h J_i^{n+1} - J_{i,h}^{n+1}) = e_i^{n+1} + \theta_i^{n+1}$, $C_i^{n+1} - C_{i,h}^{n+1} = (C_i^{n+1} - \Pi_h C_i^{n+1}) + (\Pi_h C_i^{n+1} - C_{i,h}^{n+1}) = \sigma_i^{n+1} + \delta_i^{n+1}$, choose $\tilde{J}_i = \theta_i^{n+1}$, $\tilde{C}_i = \delta_i^{n+1}$ in (4.20) and (4.21), and add them together, yield

$$\begin{aligned} & \left(d_t \theta_i^{n+1}, \theta_i^{n+1} \right) + \left(\theta_i^{n+1}, \theta_i^{n+1} \right) + \left(\nabla \cdot \theta_i^{n+1}, \nabla \cdot \theta_i^{n+1} \right) + \left(d_t \delta_i^{n+1}, \delta_i^{n+1} \right) \\ & = - \left(\partial_t J_i^{n+1} - d_t J_i^{n+1}, \theta_i^{n+1} \right) + \left(\partial_t e_i^{n+1} - d_t e_i^{n+1}, \theta_i^{n+1} \right) - \left(\partial_t e_i^{n+1}, \theta_i^{n+1} \right) \\ & - \left(\partial_t C_i^{n+1} - d_t C_i^{n+1}, \delta_i^{n+1} \right) + \left(\partial_t \sigma_i^{n+1} - d_t \sigma_i^{n+1}, \delta_i^{n+1} \right) - \left(\partial_t \sigma_i^{n+1}, \delta_i^{n+1} \right) \\ & - z_i \left(q^{n+1} C_i^{n+1} - q_h^{n+1} C_{i,h}^{n+1}, \theta_i^{n+1} \right) - \left(u^{n+1} C_i^{n+1} - u_h^{n+1} C_{i,h}^{n+1}, \theta_i^{n+1} \right) \\ & - z_i \left(\partial_t \left(q^{n+1} C_i^{n+1} \right) - d_t \left(q_h^{n+1} C_{i,h}^{n+1} \right), \theta_i^{n+1} \right) - \left(\partial_t \left(u^{n+1} C_i^{n+1} \right) - d_t \left(u_h^{n+1} C_{i,h}^{n+1} \right), \theta_i^{n+1} \right) \\ & = \sum_{k=1}^{10} T_k. \end{aligned} \tag{4.22}$$

The analysis of Terms T_1 – T_6 are similar to (4.14), (4.15) and (4.16), leading to

$$\begin{aligned} T_1 + T_2 + T_3 & \leq M \left((\Delta t)^2 + h^{2(k+1)} + \|\theta_i^{n+1}\|_0^2 \right), \\ T_4 + T_5 + T_6 & \leq M \left((\Delta t)^2 + h^{2(k+1)} + \|\delta_i^{n+1}\|_0^2 \right). \end{aligned}$$

As for T_7 and T_8 , we will do an analogous error estimate with (3.48) and (3.49), i.e., we need to conduct a mathematical induction by assuming the following induction hypothesis for any $n = 0, 1, \dots, N$:

$$h^{-\frac{d}{2}} \|\delta_i^n\|_0 \leq M, \quad i = 1, 2, \tag{4.23}$$

which is obviously true when $n = 0$ since $\delta_i^0 = 0$ by choosing $C_{i,h}(0) = \Pi_h C_i^0$. Now we assume (4.23) holds for any $n = 0, 1, \dots, L - 1$, where $1 \leq L \leq N$. Then,

$$T_7 + T_8 \leq M \left(\sum_{i=1}^2 \|\delta_i^{n+1}\|_0^2 + \|\theta_i^{n+1}\|_0^2 + h^{2(k+1)} \right).$$

Next we estimate T_9 and T_{10} . Let $\tilde{C}_i = d_t \delta_i^{n+1}$ in (4.21), yields

$$\left(\partial_t C_i^{n+1} - d_t C_{i,h}^{n+1}, d_t \delta_i^{n+1} \right) - \left(\nabla \cdot \theta_i^{n+1}, d_t \delta_i^{n+1} \right) = 0, \tag{4.24}$$

that is

$$\left(\partial_t C_i^{n+1} - d_t C_i^{n+1}, d_t \delta_i^{n+1} \right) + \left(d_t \sigma_i^{n+1} - \partial_t \sigma_i^{n+1}, d_t \delta_i^{n+1} \right) + \left(\partial_t \sigma_i^{n+1}, d_t \delta_i^{n+1} \right)$$

$$+ \left(d_t \delta_i^{n+1}, d_t \delta_i^{n+1} \right) - \left(\nabla \cdot \theta_i^{n+1}, d_t \delta_i^{n+1} \right) = 0. \tag{4.25}$$

By Cauchy–Schwarz inequality and applying similar estimates as in (4.14), (4.15) and (4.16), we obtain

$$\|d_t \delta_i^{n+1}\|_0 \leq M \left(\Delta t + h^{k+1} \right) + \|\nabla \cdot \theta_i^{n+1}\|_0. \tag{4.26}$$

Then,

$$\begin{aligned} \|\partial_t C_i^{n+1} - d_t C_{i,h}^{n+1}\|_0 &\leq \|\partial_t C_i^{n+1} - d_t C_i^{n+1}\|_0 + \|d_t \sigma_i^{n+1} \\ &\quad - \partial_t \sigma_i^{n+1}\|_0 + \|\partial_t \sigma_i^{n+1}\|_0 + \|d_t \delta_i^{n+1}\|_0 \\ &\leq M \left(\Delta t + h^{k+1} \right) + \|\nabla \cdot \theta_i^{n+1}\|_0. \end{aligned} \tag{4.27}$$

On the other hand, differentiate (2.10) in time, and then fully discretize it in both space and time as done for (4.2). The error equation between them can then be obtained by means of the differentiation of (3.5) in time, where, we choose $\tilde{q} = d_t (\Pi_h q^{n+1} - q_h^{n+1})$ and $\tilde{\phi} = d_t (\Pi_h \phi^{n+1} - \phi_h^{n+1})$. By Taylor Expansion (4.12) and the same analysis techniques for proving Theorem 3.1, we can obtain

$$\|d_t (\Pi_h q^{n+1} - q_h^{n+1})\|_0 \leq M \left(\Delta t + h^{k+1} \right) + \sum_{i=1}^2 \|\partial_t C_i^{n+1} - d_t C_{i,h}^{n+1}\|_0. \tag{4.28}$$

Thus by the triangular inequality, (4.13), Lemma 3.1, (4.28) and (4.27), we have

$$\begin{aligned} \|\partial_t q^{n+1} - d_t q_h^{n+1}\|_0 &\leq \|\partial_t q^{n+1} - d_t q^{n+1}\|_0 \\ &\quad + \|d_t (q^{n+1} - \Pi_h q^{n+1})\|_0 + \|d_t (\Pi_h q^{n+1} - q_h^{n+1})\|_0 \\ &\leq M \left((\Delta t) + h^{k+1} \right) + \|\nabla \cdot \theta_i^{n+1}\|_0. \end{aligned} \tag{4.29}$$

Therefore, apply an analogous analysis as for (3.50) and (3.51), and utilize Lemma 4.1, (4.29), (4.27) and the mathematical induction (4.23), yield

$$\begin{aligned} T_9 &= -z_i \left(q^{n+1} \partial_t C_i^{n+1} - q_h^{n+1} d_t C_{i,h}^{n+1}, \theta_i^{n+1} \right) - z_i \left(C_i^{n+1} \partial_t q^{n+1} - C_{i,h}^{n+1} d_t q_h^{n+1}, \theta_i^{n+1} \right) \\ &= -z_i \left((q^{n+1} - q_h^{n+1}) \partial_t C_i^{n+1}, \theta_i^{n+1} \right) - z_i \left(q_h^{n+1} (\partial_t C_i^{n+1} - d_t C_{i,h}^{n+1}), \theta_i^{n+1} \right) \\ &\quad - z_i \left((C_i^{n+1} - C_{i,h}^{n+1}) \partial_t q^{n+1}, \theta_i^{n+1} \right) - z_i \left(C_{i,h}^{n+1} (\partial_t q^{n+1} - d_t q_h^{n+1}), \theta_i^{n+1} \right) \\ &\leq M \left(\sum_{i=1}^2 \|\delta_i^{n+1}\|_0^2 + \|\theta_i^{n+1}\|_0^2 + (\Delta t)^2 + h^{2(k+1)} \right) + \epsilon \|\nabla \cdot \theta_i^{n+1}\|_0^2, \\ T_{10} &= - \left(u^{n+1} \partial_t C_i^{n+1} - u_h^{n+1} d_t C_{i,h}^{n+1}, \theta_i^{n+1} \right) - \left(C_i^{n+1} \partial_t u^{n+1} - C_{i,h}^{n+1} d_t u_h^{n+1}, \theta_i^{n+1} \right) \\ &= - \left((u^{n+1} - u_h^{n+1}) \partial_t C_i^{n+1}, \theta_i^{n+1} \right) - \left(u_h^{n+1} (\partial_t C_i^{n+1} - d_t C_{i,h}^{n+1}), \theta_i^{n+1} \right) \\ &\quad - \left((C_i^{n+1} - C_{i,h}^{n+1}) \partial_t u^{n+1}, \theta_i^{n+1} \right) - \left(C_{i,h}^{n+1} (\partial_t u^{n+1} - d_t u_h^{n+1}), \theta_i^{n+1} \right) \\ &\leq M \left(\sum_{i=1}^2 \|\delta_i^{n+1}\|_0^2 + \|\theta_i^{n+1}\|_0^2 + (\Delta t)^2 + h^{2(k+1)} + \|\xi^{n+1}\|_0^2 + \|d_t \xi^{n+1}\|_0^2 \right) + \epsilon \|\nabla \cdot \theta_i^{n+1}\|_0^2. \end{aligned}$$

Then, (4.22) finally yields

$$\begin{aligned} &\left(\frac{\theta_i^{n+1} - \theta_i^n}{\Delta t}, \theta_i^{n+1} \right) + \|\theta_i^{n+1}\|_0^2 + \|\nabla \cdot \theta_i^{n+1}\|_0^2 + \left(\frac{\delta_i^{n+1} - \delta_i^n}{\Delta t}, \delta_i^{n+1} \right) \\ &\leq M \left(\sum_{i=1}^2 \|\delta_i^{n+1}\|_0^2 + \|\theta_i^{n+1}\|_0^2 + (\Delta t)^2 + h^{2(k+1)} + \|\xi^{n+1}\|_0^2 + \|d_t \xi^{n+1}\|_0^2 \right) + \epsilon \|\nabla \cdot \theta_i^{n+1}\|_0^2. \end{aligned}$$

Take a sufficiently small ϵ , apply Cauchy–Schwarz inequality and Young’s inequality with $\epsilon = \frac{1}{2}$, yield

$$\begin{aligned} & \frac{1}{2} \left(\|\theta_i^{n+1}\|_0^2 + \|\delta_i^{n+1}\|_0^2 \right) + \Delta t \|\theta_i^{n+1}\|_0^2 + \Delta t \|\nabla \cdot \theta_i^{n+1}\|_0^2 \\ & \leq M \Delta t \left(\sum_{i=1}^2 \|\delta_i^{n+1}\|_0^2 + \|\theta_i^{n+1}\|_0^2 + (\Delta t)^2 + h^{2(k+1)} + \|\xi^{n+1}\|_0^2 + \|d_t \xi^{n+1}\|_0^2 \right) \\ & \quad + \frac{1}{2} \left(\|\theta_i^n\|_0^2 + \|\delta_i^n\|_0^2 \right). \end{aligned}$$

Sum over the time step n from 0 to $L - 1$ ($1 \leq L \leq N$) on both sides, apply the telescoping technique, and properly choose initial values $C_{i,h}^0 = \Pi_h C_i^0$ and $J_h^0 = \Pi_h J^0$, yield

$$\begin{aligned} & \|\theta_i^L\|_0^2 + \|\delta_i^L\|_0^2 + \Delta t \sum_{n=0}^{L-1} \|\theta_i^{n+1}\|_V^2 \\ & \leq M \Delta t \sum_{n=0}^{L-1} \left(\sum_{i=1}^2 \|\delta_i^{n+1}\|_0^2 + \|\theta_i^{n+1}\|_0^2 + \|\xi^{n+1}\|_0^2 + \|d_t \xi^{n+1}\|_0^2 + (\Delta t)^2 + h^{2(k+1)} \right). \end{aligned} \tag{4.30}$$

Due to the mathematical induction (4.23) and Poincaré inequality, (4.17) leads to

$$\Delta t \sum_{n=0}^{L-1} \|\xi^{n+1}\|_0^2 \leq M \Delta t \sum_{n=0}^{L-1} \|\nabla \xi^{n+1}\|_0^2 \leq M \left[\Delta t \sum_{n=0}^{L-1} \sum_{i=0}^2 \|\delta_i^{n+1}\|_0^2 + (\Delta t)^2 + h^{2(k+1)} \right], \tag{4.31}$$

and so does (4.19), resulting in

$$\Delta t \sum_{n=0}^{L-1} \|d_t \xi^{n+1}\|_0^2 \leq M \left[\Delta t \sum_{n=0}^{L-1} \sum_{i=0}^2 \|\delta_i^{n+1}\|_0^2 + (\Delta t)^2 + h^{2(k+1)} \right]. \tag{4.32}$$

Take the sum over i from 1 to 2 in (4.30), then apply the discrete Grönwall’s inequality, results

$$\sum_{i=1}^2 \left[\|\theta_i^L\|_0^2 + \|\delta_i^L\|_0^2 + \Delta t \sum_{n=0}^{L-1} \|\theta_i^{n+1}\|_V^2 \right] \leq M \left((\Delta t)^2 + h^{2(k+1)} \right). \tag{4.33}$$

Because $k + 1 - \frac{d}{2} > 0$ for $k \geq 1$ and $d = 2, 3$, (4.33) implies that when Δt is sufficiently small, we have

$$h^{-\frac{d}{2}} \|\delta_i^L\|_0 \leq M,$$

which proves the mathematical induction hypothesis (4.23) uniformly holds for all $1 \leq n \leq N$.

Combining (4.33) with Lemma 3.3 at $t = t_L$ ($1 \leq L \leq N$), by the triangular inequality we obtain

$$\|J_i^L - J_{i,h}^L\|_0 + \|C_i^L - C_{i,h}^L\|_0 \leq M \left(\Delta t + h^{k+1} \right). \tag{4.34}$$

Then Lemma 4.1 results

$$\|q^L - q_h^L\|_V + \|\phi^L - \phi_h^L\|_0 \leq M \left(\Delta t + h^{k+1} \right), \tag{4.35}$$

$$\|z^L - z_h^L\|_0 + h \|z^L - z_h^L\|_1 \leq M (\Delta t + h^{k+1}). \tag{4.36}$$

Further combining (4.17) and (4.19) with Lemma 3.2 at $t = t_L$ ($1 \leq L \leq N$), we have

$$\|u^L - u_h^L\|_0 + \|u^L - u_h^L\|_1 \leq M (\Delta t + h^{k+1}). \tag{4.37}$$

On the other hand, taking $\tilde{J}_i = d_t \theta_i^{n+1}$, $\tilde{C}_i = d_t \delta_i^{n+1}$ in (4.20) and (4.21), we have

$$\left(d_t \theta_i^{n+1}, d_t \theta_i^{n+1} \right) + \left(\theta_i^{n+1}, d_t \theta_i^{n+1} \right) + \left(\nabla \cdot \theta_i^{n+1}, d_t \nabla \cdot \theta_i^{n+1} \right)$$

$$\begin{aligned}
 &= -\left(\partial_t J_i^{n+1} - d_t J_i^{n+1}, d_t \theta_i^{n+1}\right) + \left(\partial_t e_i^{n+1} - d_t e_i^{n+1}, d_t \theta_i^{n+1}\right) \\
 &\quad - \left(\partial_t e_i^{n+1}, d_t \theta_i^{n+1}\right) - \left(\delta_i^{n+1}, d_t \nabla \cdot \theta_i^{n+1}\right) \\
 &\quad - z_i \left(\mathbf{q}^{n+1} C_i^{n+1} - \mathbf{q}_h^{n+1} C_{i,h}^{n+1}, d_t \theta_i^{n+1}\right) - \left(\mathbf{u}^{n+1} C_i^{n+1} - \mathbf{u}_h^{n+1} C_{i,h}^{n+1}, d_t \theta_i^{n+1}\right) \\
 &\quad - z_i \left(\partial_t \left(\mathbf{q}^{n+1} C_i^{n+1}\right) - d_t \left(\mathbf{q}_h^{n+1} C_{i,h}^{n+1}\right), d_t \theta_i^{n+1}\right) - \left(\partial_t \left(\mathbf{u}^{n+1} C_i^{n+1}\right) - d_t \left(\mathbf{u}_h^{n+1} C_{i,h}^{n+1}\right), d_t \theta_i^{n+1}\right).
 \end{aligned}$$

By using similar analysis techniques as for (4.22), we can obtain the following estimate for any $1 \leq L \leq N$:

$$\begin{aligned}
 &\Delta t \sum_{i=0}^{L-1} \|d_t \theta_i^{n+1}\|_0^2 + \|\theta_i^L\|_V^2 \\
 &\leq \Delta t \sum_{n=0}^{L-1} \left[M \left(\sum_{i=1}^2 \|\delta_i^{n+1}\|_0^2 + \|\theta_i^{n+1}\|_V^2 + (\Delta t)^2 + h^{2(k+1)} \right) + \epsilon \|d_t \theta_i^{n+1}\|_0^2 \right].
 \end{aligned}$$

Take a sufficiently small ϵ , apply the discrete Grönwall’s inequality and (4.34), yield

$$\|\theta_i^L\|_V \leq M(h^{k+1} + \Delta t).$$

Further, we have

$$\|\mathbf{J}_i^L - \mathbf{J}_{i,h}^L\|_V \leq M(h^{k+1} + \Delta t). \tag{4.38}$$

To estimate $p^{n+1} - p_h^{n+1}$, we need the discrete form of *inf-sup* condition for $b_u(\cdot, \cdot)$ in (3.37). First, apply (4.9), the continuity of $a_u(\cdot, \cdot)$ and the same error analyses for (4.14) and (3.30)–(3.32), yield

$$\begin{aligned}
 b_u(\tilde{\mathbf{u}}, \Pi_h p^{n+1} - p_h^{n+1}) &= \left(\partial_t \mathbf{u}^{n+1} - d_t \mathbf{u}_h^{n+1}, \tilde{\mathbf{u}}\right) + a_u\left(\Pi_h \mathbf{u}^{n+1} - \mathbf{u}_h^{n+1}, \tilde{\mathbf{u}}\right) \\
 &\quad + \beta\left(\mathbf{u}^{n+1}, \mathbf{u}^{n+1}, \tilde{\mathbf{u}}\right) \\
 &\quad - \beta\left(\mathbf{u}_h^{n+1}, \mathbf{u}_h^{n+1}, \tilde{\mathbf{u}}\right) - \sum_{i=1}^2 z_i \left(C_i^{n+1} \mathbf{q}^{n+1} - C_{i,h}^{n+1} \mathbf{q}_h^{n+1}, \tilde{\mathbf{u}}\right). \\
 &\leq M \left[(\Delta t + h^{k+1} + \|d_t \xi^{n+1}\|_0) \|\tilde{\mathbf{u}}\|_0 + \|\nabla \xi^{n+1}\|_0 \|\tilde{\mathbf{u}}\|_1 \right. \\
 &\quad + \left(\|\nabla \left(\mathbf{u}^{n+1} - \mathbf{u}_h^{n+1}\right)\|_0^2 + \|\nabla \mathbf{u}^{n+1}\|_0 \|\nabla \left(\mathbf{u}^{n+1} - \mathbf{u}_h^{n+1}\right)\|_0 \right) \|\tilde{\mathbf{u}}\|_1 \\
 &\quad + \left(h^{-\frac{d}{2}} \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0^2 \right. \\
 &\quad \left. + \sum_{i=1}^2 \|C_i^{n+1} - C_{i,h}^{n+1}\|_0 + h^{k+1} \right) \|\tilde{\mathbf{u}}\|_0 \left. \right].
 \end{aligned}$$

After combining the above inequality with (4.34) and (4.37), we can obtain the following error estimate through (3.37) as:

$$\|\Pi_h p^{n+1} - p_h^{n+1}\|_0 \leq M \left(\Delta t + h^{k+1} + \|d_t \xi^{n+1}\|_0 \right).$$

Then apply (4.32) and (4.33), and combine with Lemma 3.2, yield

$$\left(\Delta t \sum_{n=0}^{L-1} \|p^{n+1} - p_h^{n+1}\|_0^2 \right)^{\frac{1}{2}} \leq M \left(\Delta t + h^{k+1} \right).$$

Therefore, the following convergence theorem is eventually derived for the fully discrete scheme (4.1)–(4.3).

Theorem 4.1 Let $(\phi^{n+1}, \mathbf{q}^{n+1}, z^{n+1}, \mathbf{u}^{n+1}, p^{n+1}, C_i^{n+1}, \mathbf{J}_i^{n+1})$ be the solution to (2.7a)–(2.9) satisfying the regularity properties (2.13)–(2.15), and $(\phi_h^{n+1}, \mathbf{q}_h^{n+1}, z_h^{n+1}, \mathbf{u}_h^{n+1}, p_h^{n+1}, C_{i,h}^{n+1}, \mathbf{J}_{i,h}^{n+1})$ be the solution to (4.1)–(4.3). Then for $1 \leq L \leq N$, we have the following error estimates,

$$\begin{aligned} & \|\mathbf{q}^L - \mathbf{q}_h^L\|_V + \|\phi^L - \phi_h^L\|_0 + \|z^L - z_h^L\|_0 + h\|z^L - z_h^L\|_1 \leq M \left(h^{k+1} + \Delta t \right), \\ & \|\mathbf{u}^L - \mathbf{u}_h^L\|_0 + \|\mathbf{u}^L - \mathbf{u}_h^L\|_1 + \left(\Delta t \sum_{n=1}^L \|p^n - p_h^n\|_0^2 \right)^{\frac{1}{2}} \leq M(h^{k+1} + \Delta t), \\ & \|C_i^L - C_{i,h}^L\|_0 + \|\mathbf{J}_i^L - \mathbf{J}_{i,h}^L\|_0 + \|\mathbf{J}_i^L - \mathbf{J}_{i,h}^L\|_V \leq M \left(h^{k+1} + \Delta t \right). \end{aligned}$$

Remark 4.1 The error estimate of pressure in Theorem 4.1 is consistent with its continuous form in Theorem 3.4 which bears $L^2(L^2)$ norm. To obtain the same error estimate for pressure in $L^\infty(L^2)$ norm, i.e., $\|p - p_h\|_{L^\infty(L^2)} = O(h^{k+1})$, we need to differentiate (3.26) and (3.27) in time, and choose $\tilde{\mathbf{u}} = \partial_t(\Pi_h \mathbf{u} - \mathbf{u}_h)$ and $\tilde{p} = \partial_t(\Pi_h p - p_h)$, then conduct similar semi-discrete error estimates by means of analogous analysis skills for proving Theorem 3.2. A similar error analysis process can be carried out for the fully discrete scheme to obtain the error estimate of pressure in the discrete $L^\infty(L^2)$ norm, as: $\|p^L - p_h^L\|_{L^2} = O(h^{k+1} + \Delta t)$ for $1 \leq L \leq N$. We thus omit its proof in this paper to avoid the high similarity, on the other hand, it will be numerically validated in Sect. 5.

5 Numerical Experiments

5.1 Example 1: Convergence Test

In this section we apply the fully discrete mixed FEM and the numerical algorithm developed in Sect. 4 to a numerical example defined below, then validate all theoretical results shown in Theorem 4.1. Let

$$\begin{cases} \phi = e^{(x+y)} \sin t, \\ C_1 = \sin(2\pi x) \sin(2\pi y) \sin t, \\ C_2 = \sin(2\pi x) \sin(2\pi y) \sin(2t), \\ \mathbf{u} = (-\cos(\pi x) \sin(\pi y) \sin(3t), \sin(\pi x) \cos(\pi y) \sin(3t))^T, \\ p = (\sin x + \sin y) (1 - e^{-t}) \end{cases} \tag{5.1}$$

be real solutions to the following fourth-order modified PNP/NS problem defined in $\Omega = [0, 1] \times [0, 1]$ and the time interval $[0, 0.25]$:

$$\begin{cases} \Delta^2 \phi - \Delta \phi = C_1 - C_2 + F_3, \\ \partial_t C_i - \nabla \cdot (\nabla C_i + z_i \nabla \phi C_i - \mathbf{u} C_i) = F_i, \quad i = 1, 2, \\ \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} - \Delta \mathbf{u} + \nabla p = -(C_1 - C_2) \nabla \phi + F_4, \\ \nabla \cdot \mathbf{u} = 0, \end{cases} \tag{5.2}$$

by appropriately choosing right hand side functions $F_i \in L^\infty(0, T; L^2(\Omega))$ ($1 \leq i \leq 4$), where all F_i are nonzero functions and do not actually affect our error analyses and theoretical results shown in Sects. 3 and 4 at all. And, all boundary and initial conditions are homogeneous, which matches with the adopted real solutions (5.1) on the boundary $\partial\Omega$ or at $t = 0$.

In the following, we implement Algorithm 4.1 to find discrete solutions of $(\phi, \mathbf{q}, z, C_1, C_2, \mathbf{J}_1, \mathbf{J}_2, \mathbf{u}, p)$ to the fully discrete mixed finite element discretization (4.1)–(4.3), and compute convergence errors in corresponding norms for these variables. To that end, we adopt $\Delta t = 4h^3$ with the grid doubling, i.e., choose mesh sizes $h = 1/4, 1/8, 1/16$ and $1/32$ to form a series of nested uniform grids, on which we define corresponding $P^2 P^1$ (Taylor–Hood) element to discretize (ϕ, \mathbf{q}) , (\mathbf{u}, p) and (\mathbf{J}_i, C_i) ($i = 1, 2$), respectively, and P^1 (linear) element to discretize the variable z by choosing $k = 1$ in (3.1).

Numerical results are reported in Tables 1, 2, and 3 and Figs. 1, 2, and 3, from which we can see all results are at least in accordance with or even better than the theoretical results of optimal error estimates shown in Theorem 4.1. In particular, optimal (second-order) convergence rates are illustrated for approximation errors of all variables in their corresponding energy norm and L^2 norm, except for the velocity’s and the pressure’s

Table 1 Convergence results of the electrostatic potential and relevant vector- and scalar-valued variables

h	1/4	1/8	1/16	1/32
$\ \phi - \phi_h\ _0$	5.37E-03	1.08E-03	2.25E-04	4.93E-05
Order		2.311	2.265	2.193
$\ \mathbf{q} - \mathbf{q}_h\ _0$	3.98E-04	8.46E-05	1.95E-05	4.73E-06
Order		2.234	2.121	2.039
$\ \mathbf{q} - \mathbf{q}_h\ _V$	5.60E-03	1.18E-03	2.67E-04	6.35E-05
Order		2.242	2.149	2.072
$\ z - z_h\ _0$	5.89E-03	1.48E-03	3.70E-04	9.27E-05
Order		1.992	1.999	1.998
$\ z - z_h\ _1$	1.61E-01	8.06E-02	4.03E-02	2.02E-02
Order		0.997	0.999	1.000

Table 2 Convergence results of fluid velocity and pressure

h	1/4	1/8	1/16	1/32
$\ \mathbf{u} - \mathbf{u}_h\ _0$	1.72E-03	2.06E-04	2.54E-05	3.16E-06
Order		3.061	3.021	3.007
$\ \mathbf{u} - \mathbf{u}_h\ _1$	3.44E-02	8.68E-03	2.17E-03	5.44E-04
Order		1.988	1.997	1.999
$\ p - p_h\ _0$	1.64E-02	2.33E-03	3.05E-04	3.99E-05
Order		2.818	2.934	2.936

errors in L^2 norm, i.e., $\|\mathbf{u} - \mathbf{u}_h\|_0$ and $\|p - p_h\|_0$ that even show a third-order spatial convergence rate in Table 2, which is however one order higher than the result demonstrated in our convergence theorem. Due to the nonlinear source term of the momentum equation that involves ionic concentrations and the gradient of electrostatic potential, our proofs for Theorems 3.4 and 4.1 can only show a second-order convergence rate in space for the velocity's error in both H^1 norm and L^2 norm, as well as for the pressure's error in L^2 norm. But, as illustrated by numerical results, it seems that such nonlinear source term does not prevent the mixed FEM for Navier-Stokes equations from achieving an optimal (third-order) convergence rate for $\|\mathbf{u} - \mathbf{u}_h\|_0$ with P^2 element, moreover, a nearly third-order superconvergence property for $\|p - p_h\|_0$ with P^1 element is illustrated as well. Further theoretical studies would be needed in the future to verify both the optimal convergence of velocity and the superconvergence of pressure in L^2 norms, for the fourth-order modified PNP/NS coupling system.

5.2 Example 2: A Practical Problem to Investigate the Force Between Two Charged Particles

To explain why the modified model with a fourth-order elliptic equation for the electrostatic potential is significant and necessary in contrast to the classical Poisson equation, in this section we use both the classical model and the modified model to study a practical example in two dimension for the electrostatic interaction force between two charged particles, and compare numerically obtained forces with experimental results to show that only the modified model can demonstrate a reasonable result that is consistent with experimental phenomena. Figure 4 depicts two spherical particles (represented by Ω_2) that is submerged into an electrolyte (represented by Ω_1) and is surrounded by a uniformly alternating electric current field. Two spherical particles are uniformly charged dielectrics whose electrostatic potentials are defined through either the modified model—the fourth order elliptic equation (1.1) or the classical model—Poisson equation that is reduced from (1.1) by letting $\ell_c = 0$, while the electrolyte, which is an ionic solvent containing ions (cations and anions),

Table 3 Convergence results of ionic concentrations and relevant vector-valued variables

h	1/4	1/8	1/16	1/32
$\ C_1 - C_{1,h}\ _0$	2.11E-02	4.33E-03	1.02E-03	2.53E-04
Order		2.285	2.080	2.021
$\ J_1 - J_{1,h}\ _0$	1.05E-01	2.36E-02	5.48E-03	1.34E-03
Order		2.154	2.107	2.036
$\ J_1 - J_{1,h}\ _V$	2.02E-01	3.62E-02	7.99E-03	1.93E-03
Order		2.479	2.179	2.049
$\ C_2 - C_{2,h}\ _0$	4.09E-02	8.40E-03	1.99E-03	4.89E-04
Order		2.286	2.080	2.021
$\ J_2 - J_{2,h}\ _0$	2.18E-01	4.97E-02	1.16E-02	2.82E-03
Order		2.131	2.106	2.037
$\ J_2 - J_{2,h}\ _V$	4.43E-01	7.86E-02	1.72E-02	4.13E-03
Order		2.493	2.196	2.055

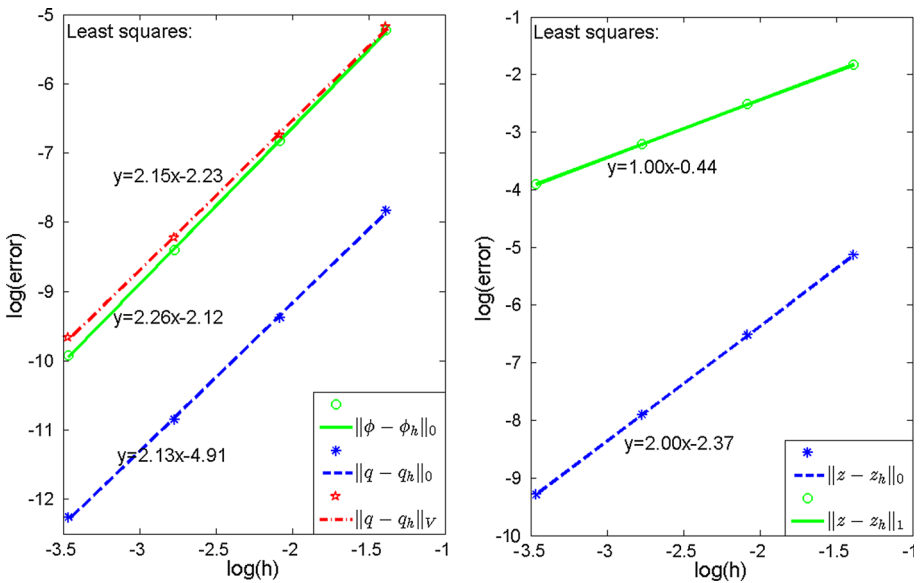


Fig. 1 Linear least squares fitting of convergence trends against mesh size for ϕ , q and z in respective norms

supposes to be modeled by Nernst-Planck equations, as shown in (2.1), for ionic concentrations. But, since in this section we only focus on the comparison between the modified and the classical models of the electrostatic potential, we simply replace Nernst-Planck equations by an empirical function for ionic concentrations that explicitly depends on the electrostatic potential [12]. Such an empirical function is derived based on the Bikerman model [40] for volume constraints only with equal sized cations and anions, as shown below in (5.3).

All necessary physical parameters involved in this section are labeled and explained in Table 4. In particular, we let the charge density $\rho = z_1 e C_1 - z_2 e C_2$ in (1.1), where C_1 and C_2 are concentrations of the ionic species, and, we use ϵ_1 and ϵ_2 to denote the dielectric permittivity in the electrolyte and the particles, respectively, which describes different polarizability of ions. Here we let $\epsilon_1 = \epsilon_0 \epsilon_s$, $\epsilon_2 = \epsilon_0 \epsilon_m$. In addition, we assume a binary $z_1 : z_2$ electrolyte such that the far field concentrations of cations and anions satisfy $z_1 C_\infty^+ = z_2 C_\infty^-$. Following the aforementioned reason, in this section we replace ionic concentration (Nernst-Planck) equations

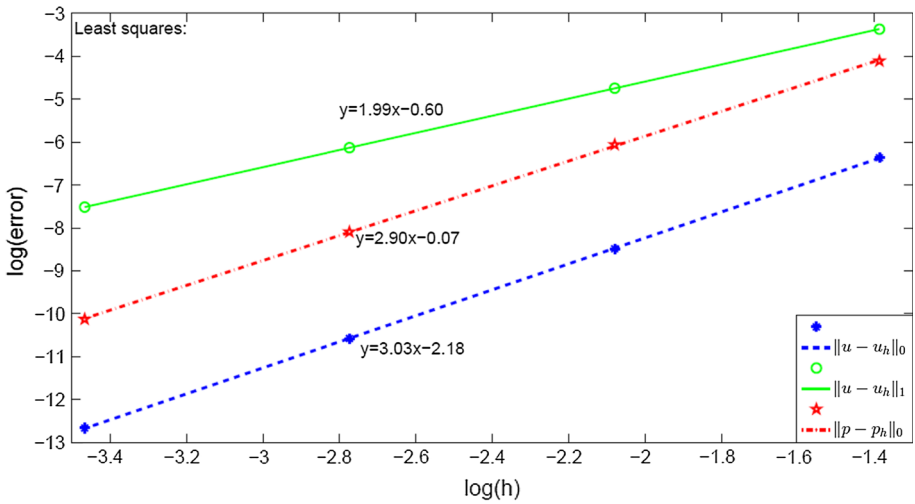


Fig. 2 Linear least squares fitting of convergence trends against mesh size for u and p in respective norms

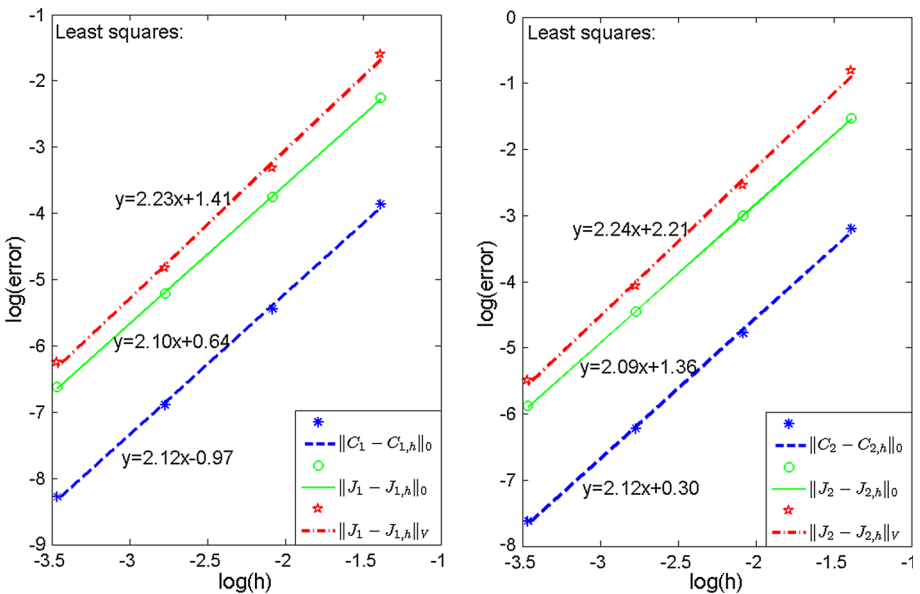


Fig. 3 Linear least squares fitting of convergence trends against mesh size for C_i and J_i in respective norms

by two empirical functions at equilibrium which are explicit functions of the electrostatic potential, defined by [12]

$$\begin{cases} C_1 = C_\infty^+ e^{-z_1 \frac{e}{\kappa_B T} \phi}, \\ C_2 = \frac{z_1}{z_2} C_\infty^+ e^{z_2 \frac{e}{\kappa_B T} \phi}, \end{cases} \quad (5.3)$$

where the far field concentration, C_∞^+ (in the SI unit of $1/m^3$), describes the degree of concentration of cations in physical spaces, while $c_0 = \frac{C_\infty^+}{N_A}$, is often adopted to change the unit of the far field cationic concentration

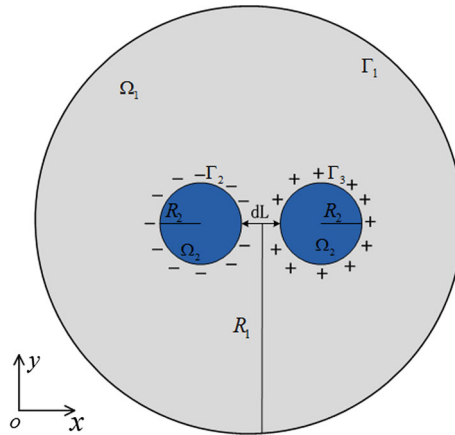


Fig. 4 The schematics of the submerged particles in an electrolyte

Table 4 Notations and physical constants

Symbol	Physical parameter	Value	Unit
R_1	Radius of the spherical electrolyte field	5000	nm
R_2	Radius of spherical particles	1000	nm
e	Charge of one electron	1.6×10^{-19}	C
$K_B T$	Boltzmann energy	4.14×10^{-21}	J (or N m)
ϵ_0	Permittivity of vacuum	8.85×10^{-12}	$C^2/(N m^2)$
ϵ_s	Dielectric constant of electrolyte	80	
ϵ_m	Dielectric constant of particle	2	
z_1	Valence number of cation	3	
z_2	Valence number of anion	1	
ℓ_c	Electrostatic correlation length	1	nm
N_A	Avogadro constant	6.02×10^{23}	mol^{-1}

to the most commonly used molar concentration unit: mol/m^3 [12]. Moreover, to compute the interactional force between two particles, we need to introduce the expression of the Maxwell stress tensor, τ , for a fluid (that is the electrolyte in this example) with a non-local permittivity ϵ , defined as [13],

$$\tau = \epsilon q q^T - \frac{1}{2} \epsilon q \cdot q I + \epsilon \ell_c^2 \left[q \cdot (\nabla (\nabla \cdot q)) I - q (\nabla (\nabla \cdot q))^T - (\nabla (\nabla \cdot q)) q^T + \frac{1}{2} (\nabla \cdot q)^2 I \right],$$

where $q = -\nabla\phi$ is the electric current field. Then the total electrostatic force, F , acting on the surface of the particle, e.g., the surface of the right spherical particle, Γ_3 (see Fig. 4), can be calculated by $F = \int_{\Gamma_3} \tau n ds$. Since the vertical component of this total force does not contribute to the interaction between two charged particles that lie along a horizontal direction (as shown in Fig. 4), in what follows, we only take the horizontal component of this total force to investigate the interaction effect between them.

Specifically in this example, we set two charged particles to carry opposite charges, as shown in Fig. 4. Then due to the Coulomb’s law, their interaction force in between shall be anti-proportional to (the square of) the distance between them. On the other hand, the classical electromagnetism theory tells that two opposite electric charges attract each other, which however no longer holds for the experimental setup in this example when ionic concentrations in the electrolyte increase to a certain extent, i.e., under that circumstance two oppositely charged particles turns out to repel each other instead. It is the most significant phenomenon that only the BSK theory can explain but classical theories cannot. A physically experimental study in [41] fully supports

Table 5 Horizontal forces (nN) acting on the right particle (see Fig. 4) by two models

dL (nm)	$c_0=1.585E-3 \text{ mol/m}^3$		$c_0 = 0.1585 \text{ mol/m}^3$		$c_0 = 253.6 \text{ mol/m}^3$		$c_0 = 1014.4 \text{ mol/m}^3$	
	Model I	Model II	Model I	Model II	Model I	Model II	Model I	Model II
8	-1.6750	-1.7315	-0.0908	-0.0969	3.29E-3	-1.66E-4	4.18E-3	-6.45E-7
16	-1.3217	-1.3718	-0.0544	-0.0569	3.16E-3	-1.63E-4	3.98E-3	-6.09E-7
24	-0.9524	-0.9915	-0.0440	-0.0427	3.17E-3	-1.60E-4	3.97E-3	-6.42E-7
32	-0.7434	-0.7687	-0.0426	-0.0408	3.17E-3	-1.63E-4	3.87E-3	-6.27E-7
40	-0.6034	-0.6188	-0.0403	-0.0391	3.07E-3	-1.58E-4	3.64E-3	-6.30E-7

this interesting force reversing phenomenon, and we will essentially validate it in our numerical experiment using the modified fourth-order electrostatic potential model that is derived from the BSK theory, i.e., we still expect from our numerical results that the horizontal force between two oppositely charged particles will decrease along the increase of the distance between them, simultaneously, we will see that their interaction force is gradually reversed from the attractive force to the repulsive force, e.g., the sign of the horizontal force acting on the right particle shown in Fig. 4) will be gradually changed from negative to positive along with the increase of ionic concentrations, which means that its horizontal force is eventually reversed from the left (attractive) direction to the right (repulsive) direction.

After applying the developed mixed finite element method to the fourth-order electrostatic potential equation, which is defined in the domain shown in Fig. 4 and involves with simplified ionic concentration functions defined in (5.3), then numerically computing the Maxwell stress tensor τ as well as the total electrostatic force F , we obtain horizontal forces in the unit of Nanonewton (nN) acting on the surface of the right particle with respect to the distance from the left particle, dL, and with respect to the far field ionic concentration, c_0 , as shown in Table 5, where Model I represents the modified model with a fourth-order elliptic equation, and Model II represents the classical model with Poisson equation, both are solved for the electrostatic potential. From Table 5 and Fig. 5 we can see that both models show that the magnitude of horizontal forces decreases along with the increase of the distance between two particles, which is consistent with the trend of experimental results shown in [41, Figure 1]. On the other hand, when c_0 increases, the direction of horizontal forces computed by Model I are eventually reversed from negative to positive, which is still consistent with the pattern of change of experimental results shown in [41, Figure 2]. Nevertheless, such a phenomenon of reversing the interaction force is not observed in numerical results of Model II due to the lacking of considering the ion-ion electrostatic correlation, which is however fully reflected by the modified Model I.

Thus, we can conclude that the modified model for the electrostatic potential characterized as a fourth-order elliptic equation is superior to the classical Poisson equation in terms of the applicability, the accuracy and the practicality.

6 Conclusion and Future Work

In this paper, we analyze error estimates of a fully mixed finite element approximation to a recently founded new electrohydrodynamical (Bazant–Storey–Kornyshev) theory driven model — a coupled fourth-order modified Poisson–Nernst–Planck/Navier–Stokes equations. Both semi- and fully discrete Stokes-type mixed finite element methods are developed and are analyzed for a stabilized mixed weak formulation of PNP/NS coupling system, and optimal error estimates are obtained for all primary variables and their vector-valued gradient variables in corresponding energy norms, that is, if Taylor–Hood $P^{k+1}P^k$ element is employed, then we can obtain optimal error estimates for the electrostatic potential flux $q = \nabla\phi$ and ionic mass fluxes $J_j = \nabla C_j - z_j q C_j - u C_j$ in $L^\infty(H(\text{div}))$ norm, for the electrostatic potential ϕ , ionic concentrations C_j and the fluid pressure p in $L^\infty(L^2)$ norm, and for the fluid velocity u in $L^\infty(H^1)$ norm. To the authors’ best knowledge, this seems to be the first time to apply a fully mixed FEM with $P^{k+1}P^k$ element to a time-dependent, coupled fourth-order modified PNP/NS equations and obtain optimal convergence rates for all primary variables and their vector-values variables in respective energy norms. In particular, due to the nonlinear coupling effect of PNP/NS system, the fluid velocity’s error in L^2 norm reaches a suboptimal (second-order) convergence rate in the convergence theorem, which is however illustrated as an optimal (third-order) convergence behavior in numerical experiments and thus may be considered as a superconvergence property. The same

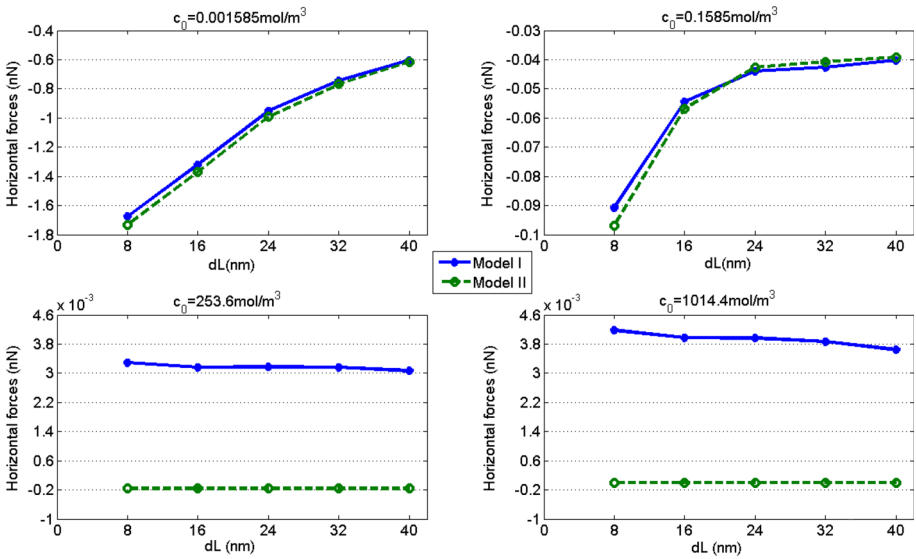


Fig. 5 Horizontal forces (nN) acting on the right particle versus distances and ionic concentrations by two models

superconvergence behavior is also observed in numerical experiments for the pressure’s convergence rate in L^2 norm as well. In addition, we also numerically study a practical example to validate the necessity of introducing the modified electrostatic potential equation characterized as a fourth-order elliptic equation by comparing with the classical Poisson equation. We observe that numerical trends obtained from the modified model are all consistent with experimental results shown in [41], which however cannot be predicted by the classical model.

On the other hand, numerical methodology and analysis tools developed in this paper for the mixed FEM is not limited to the presented fourth-order modified PNP/NS equations with unit constant coefficients, which is the case we study in this paper though, all developed numerical techniques can be easily extended to other kinds of PNP/NS system with more complicated physical coefficients as long as all coefficients are sufficiently differentiable and necessarily bounded. Our future work will be dedicated to applying the newly developed mixed FEM to a physically realistic fourth-order modified PNP/NS problem which could reflect the case of small Debye length and boundary layer effects, etc.

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Data Availability Data sharing not applicable to this article as no datasets were generated or analyzed during the current study.

Declarations

Conflict of interest The authors declare that they have no conflict of interest that are relevant to the content of this article.

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