Optimal error estimates of coupled and divergence-free virtual element methods for the Poisson–Nernst–Planck/Navier–Stokes equations

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Abstract

In this article, we propose and analyze a fully coupled, nonlinear, and energy-stable virtual element method (VEM) for solving the coupled Poisson-Nernst-Planck (PNP) and Navier–Stokes (NS) equations modeling microfluidic and electrochemical systems (diffuse transport of charged species within incompressible fluids coupled through electrostatic forces). A mixed VEM is employed to discretize the NS equations whereas classical VEM in primal form is used to discretize the PNP equations. The stability, existence and uniqueness of solution of the associated VEM are proved by fixed point theory. Global mass conservation and electric energy decay of the scheme are also proved. Also, we obtain unconditionally optimal error estimates for both the electrostatic potential and ionic concentrations of PNP equations in the H^1-norm, as well as for the velocity and pressure of NS equations in the $\mathbf{H}^1$- and L^2-norms, respectively. Finally, several numerical experiments are presented to support the theoretical analysis of convergence and to illustrate the satisfactory performance of the method in simulating the onset of electrokinetic instabilities in ionic fluids, and studying how they are influenced by different values of ion concentration and applied voltage. These tests relate to applications in the desalination of water.

Keywords: Coupled Poisson–Nernst–Planck/Navier–Stokes equations, mixed virtual element method, optimal convergence, charged species transport, electrokinetic instability, water desalination.
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1. Introduction and problem statement

1.1. Scope

The coupled Poisson–Nernst–Planck (PNP)/Navier–Stokes (NS) equations (also known as the electron fluid dynamics equations) serve to describe mathematically the dynamical properties of electrically charged fluids, the motion of ions and/or molecules, and to represent the interaction with electric fields and flow patterns of incompressible fluids within cellular environments and occurring at diverse spatial and temporal scales (see, e.g., [30]). Ionic concentrations are described by the Nernst-Planck equations (a convection-diffusion-reaction system), the diffusion of the electrostatic potential is described by a generalized Poisson equation, and the NS equations describe the dynamics of incompressible fluids, neglecting magnetic forces.

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A large number of dedicated applications are possible with this set of equations as for example semiconductors, electrokinetic flows in electrophysiology, drug delivery into biomembranes, and many others (see, e.g., [14, 15, 17, 31, 27, 37, 38, 45] and the references therein).

The mathematical analysis (in particular, existence and uniqueness of solutions) for the coupled PNP/NS equations is a challenging task, due to the coupling of different mechanisms and multiphysics (internal/external charges, convection-diffusion, electro-osmosis, hydrodynamics, and so on) interacting closely. Starting from the early works [29, 39], where one finds the well-posedness analysis and the study of other properties of steady-state PNP equations, a number of contributions have addressed the existence, uniqueness, and regularity of different variants of the coupled PNP/NS equations. See, for instance, [28, 42, 43] and the references therein.

Reliable computational results are also challenging to obtain, again due to the nonlinearities involved, the presence of solution singularities owing to some types of charges, as well as the multiscale nature of the underlying phenomena. Double layers in the electrical fields near the liquid-solid interface are key to capturing the onset of instabilities and fine spatio-temporal resolution is required, whereas the patterns of ionic transport are on a much larger scale [33]. Although numerical methods of different types have been used by computational physicists and biophysicists and other practitioners over many decades, the rigorous analysis of numerical schemes is somewhat more recent. In such a context, the analysis of standard finite element methods (FEMs) as well as of mixed, conservative, discontinuous Galerkin, stabilized, weak Galerkin, and other variants have been established for PNP and coupled PNP/NS equations [19, 20, 24, 25, 26, 33, 34, 40, 41, 49]. Since the formulation of FEMs requires explicit knowledge of the basis functions, these very powerful methods might be often limited (at least in their classical setting) to meshes with simple-geometrical shaped elements, e.g. triangles or quadrilaterals. This constraint is overcome by polytopal element methods such as the VEM, which are designed for providing arbitrary order of accuracy on polygonal/polytopal elements. In the VEM setting, the explicit knowledge of the basis functions is not required, while its practical implementation is based on suitable projection operators which are computable by their degrees of freedom.

One of the main purposes of this paper is to develop efficient numerical schemes, in the framework of VEM to solve the coupled PNP/NS model. By design, the proposed schemes provide the following three desired properties, i.e., (i) accuracy (first order in time); (ii) stability (in the sense that the unconditional energy dissipation law holds); and (iii) simplicity and flexibility to be implemented on general meshes. For this we combine a space discretization by mixed VEM for the NS equations with the usual primal VEM formulation for the PNP system, whereas for the discretization in time we use a classical backward Euler implicit method.

As an extension of FEMs onto polygonal/polyhedral meshes, VEMs were introduced in [1]. In the VEM, the local discrete space on each mesh element consists of polynomials up to a given degree and some additional non-polynomial functions. In order to discretize continuous problems, the VEM only requires the knowledge of the degrees of freedom of the shape functions, such as values at mesh vertices, the moments on mesh edges/faces, or the moments on mesh polygons/polyhedrons, instead of knowing the shape functions explicitly. Moreover, the discrete space can be extended to high order in a straightforward way. VEMs for general second-order elliptic problems were presented in [12]. We also mention that VEMs for the building blocks of the coupled system are already available from the literature. In particular, we employ here the VEM for NS equations introduced in [5]. Other formulations (of mixed, discontinuous, nonconforming, and other types) for NS include [6, 21, 35, 44, 46], whereas for the PNP system a VEM scheme has been recently proposed in [36]. The present method also follows other VEM formulations for Stokes flows from [4, 11, 9, 47]. For a more thorough survey, we refer to [2, 8] and the references therein.

1.2. Outline

The remainder of the paper has been organized in the following manner. In what is left of this Section, we recall the coupled PNP/NS equations in non-dimensional form, we provide notational preliminaries, and introduce the corresponding variational formulation for the system. In Section 2, we present the virtual element discretization, introducing the mesh entities, the degrees of freedom, the construction of VE spaces, and establishing properties of the discrete multilinear forms. In Section 3, we obtain two conservative properties global mass conservation and electric (and kinetic) energy conservation of the proposed scheme. In Section 4, under the assumption of small data, the existence and uniqueness of the discrete problem are proved. In Section 5, we establish error estimates for the velocity, pressure, concentrations and electrostatic potential. A set of numerical tests are reported in Section 6. They allow us to assess the accuracy properties of the method by confirming the experimental rates of convergence predicted by the theory. Examples of applicative interest in the process of water desalination are also included.

1.3. The model problem in non-dimensional form

Consider a spatial bounded domain $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$) with a Lipschitz continuous boundary $\partial\Omega$ with outward-pointing unit normal $\mathbf{n}$, and consider the time interval $t \in [0, t_F]$, with $t_F > 0$ a given final time. We focus on the electro-hydrodynamic model described by the coupled PNP/NS equations following the non-dimensionalization and problem setup from, e.g., [18, 22], and cast in the following strong form (including transport of a dilute 2-component electrolyte, electrostatic equilibrium, momentum balance with body force exerted by the electric field, mass conservation, no-flux and no-slip boundary conditions, and appropriate initial conditions)

$$\begin{cases} c^+_t - \nabla\cdot(D_1(\nabla c^+ + c^+\nabla\phi)) + \nabla\cdot(\mathbf{u}c^+) = 0 & \text{in } \Omega\times(0,t_F], \\ c^-_t - \nabla\cdot(D_2(\nabla c^- - c^-\nabla\phi)) + \nabla\cdot(\mathbf{u}c^-) = 0 & \text{in } \Omega\times(0,t_F], \\ -\nabla\cdot(\epsilon\nabla\phi) = c^+ - c^- & \text{in } \Omega\times(0,t_F], \\ \mathbf{u}_t - \Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = -(c^+ - c^-)\nabla\phi & \text{in } \Omega\times(0,t_F], \\ \nabla\cdot\mathbf{u} = 0 & \text{in } \Omega\times(0,t_F], \\ \dfrac{\partial c^+}{\partial\mathbf{n}} = \dfrac{\partial c^-}{\partial\mathbf{n}} = \dfrac{\partial\phi}{\partial\mathbf{n}} = 0, \quad \mathbf{u} = \mathbf{0} & \text{on } \partial\Omega\times(0,t_F], \\ c^+(\mathbf{x},0) = c^+_0(\mathbf{x}), \quad c^-(\mathbf{x},0) = c^-_0(\mathbf{x}), \quad \phi(\mathbf{x},0) = \phi_0(\mathbf{x}), \quad \mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}) & \text{in } \Omega, \end{cases} \tag{1.1}$$

where c^+, c^- are the concentrations of positively and negatively charged ions, respectively; ϕ is the electrostatic potential, $\mathbf{u}$ and p are the velocity and pressure of the incompressible fluid, respectively; ϵ represents the dielectric coefficient, here assumed heterogeneous, but uniformly bounded $0 < \epsilon_0 \le \epsilon \le \epsilon_1$, and D_1 and D_2 are diffusion/mobility coefficients (heterogeneous and possibly anisotropic, but assumed uniformly positive definite). The boundary conditions considered in (1.1) could be extended to more general scenarios. They are taken as they are for sake of simplicity in the presentation of the analysis.

1.4. Notation and weak formulation

Throughout the paper, let $\mathcal{D}$ be any given open subset of Ω. By $(\cdot,\cdot)$ and $\|\cdot\|_{\mathcal{D}}$ we denote the usual integral inner product and the corresponding norm of $L^2(\mathcal{D})$. For a non-negative integer m, we shall use the common notation for the Sobolev spaces $W^{m,r}(\mathcal{D})$ with the corresponding norm and semi-norm $\|\cdot\|_{m,r,\mathcal{D}}$ and $|\cdot|_{m,r,\mathcal{D}}$, respectively; and if $r = 2$, we set $H^m(\mathcal{D}) := W^{m,2}(\mathcal{D})$, $\|\cdot\|_{m,\mathcal{D}} := \|\cdot\|_{m,2,\mathcal{D}}$ and $|\cdot|_{m,\mathcal{D}} := |\cdot|_{m,2,\mathcal{D}}$. If $\mathcal{D} = \Omega$, the subscript will be omitted.

Let us introduce the following functional spaces for velocity, pressure and electrostatic potential (and concentrations) variables

$$\boldsymbol{X} := \mathbf{H}^1_0(\Omega), \quad Y := L^2_0(\Omega), \quad Z := H^1(\Omega), \quad \widehat{Z} := \{v \in Z : \quad (v,1)_0 = 0\},$$

respectively. We endow $\mathbf{X}$, Y and Z with the following norms

$$\|\boldsymbol{\tau}\|^2_{\mathbf{X}} := \|\boldsymbol{\tau}\|^2_1 := \|\boldsymbol{\tau}\|^2_0 + |\boldsymbol{\tau}|^2_1, \qquad \|q\|^2_Y := \|q\|^2_0, \qquad \|z\|^2_Z := \|z\|^2_1 := \|z\|^2_0 + |z|^2_1, \quad \|z\|^2_{\widehat{Z}} = \|z\|^2_Z,$$

respectively. For functions of both spatial $x \in \Omega$ and temporal variables $t \in J := [0, t_F]$, we will also use the standard function spaces $L^2(J; V)$ whose norms are defined by:

$$\|\boldsymbol{v}\|_{L^2(V)} := \left(\int_0^{t_F} \|v(t)\|^2_V \, \mathrm{d}x \right)^{\frac{1}{2}}, \quad \|v\|_{L^\infty(V)} := \mathrm{ess}_{t\in J} \sup_t \|v(t)\|_V,$$

particularly, V can represent $\mathbf{X}$, Y and Z. Next, and in order to write the variational formulation of problem (1.1), we introduce the following bilinear (and trilinear) forms

$$\mathcal{M}(u,v) := (u,v)_0, \quad \mathcal{A}_i(u,v) := (D_i \nabla u, \nabla v)_0, \quad \mathcal{A}_3(u,v) := (\epsilon \nabla u, \nabla v)_0, \quad \boldsymbol{\mathcal{A}}(\mathbf{u},\mathbf{v}) := (\nabla \mathbf{u}, \nabla \mathbf{v})_0,$$
$$\mathcal{C}(w;u,v) := (w\nabla u, \nabla v)_0, \quad \boldsymbol{\mathcal{M}}(\mathbf{u},\mathbf{v}) := (\mathbf{u},\mathbf{v})_0, \quad \boldsymbol{\mathcal{B}}(p,\mathbf{v}) := (p, \nabla\cdot\mathbf{u})_0.$$

As usual for convective problems, for $\mathbf{u}, \mathbf{v}, \mathbf{w} \in \boldsymbol{X}$ and using the fact that $\nabla\cdot\mathbf{u} = 0$, we utilize equivalent skew-symmetric forms for the terms $(\nabla\cdot(\mathbf{u}p), v)_0$ and $((\mathbf{w}\cdot\nabla)\mathbf{u}, \mathbf{v})_0$, respectively, which are described as

$$\mathcal{D}(\mathbf{w};u,v) := \frac{1}{2}\big[(\mathbf{w}u, \nabla v)_0 - (\mathbf{w}\cdot\nabla u, v)_0\big], \qquad \boldsymbol{\mathcal{C}}(\mathbf{w};\mathbf{u},\mathbf{v}) := \frac{1}{2}\big[(\mathbf{w}\cdot\nabla\mathbf{u}, \mathbf{v})_0 - (\mathbf{w}\cdot\nabla\mathbf{v}, \mathbf{u})_0\big].$$

Now, the variational formulation of (1.1) consists in finding for almost all $t \in J$, $\{c^+(t), c^-(t), \phi(t)\} \in Z \times Z \times \widehat{Z}$ and $\{\mathbf{u}(t), p(t)\} \in \mathbf{X} \times Y$ such that $\partial_t c^+ \in L^2(J; H^{-1}_N)$, $\partial_t c^- \in L^2(J; H^{-1}_N)$, $\partial_t \mathbf{u} \in L^2(J; \mathbf{H}^{-1})$ and such that the following relations hold

$$\begin{cases} \mathcal{M}(c^+_t, z_1) + \mathcal{A}_1(c^+, z_1) + \mathcal{C}(c^+;\phi, z_1) - \mathcal{D}(\mathbf{u}; c^+, z_1) = 0 & \forall z_1 \in Z, \\ \mathcal{M}(c^-_t, z_2) + \mathcal{A}_2(c^-, z_2) - \mathcal{C}(c^-;\phi, z_2) - \mathcal{D}(\mathbf{u}; c^-, z_2) = 0 & \forall z_2 \in Z, \\ \mathcal{A}_3(\phi, z_3) = \mathcal{M}(c^+, z_3) - \mathcal{M}(c^-, z_3) & \forall z_3 \in Z, \\ \boldsymbol{\mathcal{M}}(\mathbf{u}_t, \mathbf{v}) + \boldsymbol{\mathcal{A}}(\mathbf{u},\mathbf{v}) + \boldsymbol{\mathcal{C}}(\mathbf{u};\mathbf{u},\mathbf{v}) - \boldsymbol{\mathcal{B}}(p,\mathbf{v}) = -\left((c^+ - c^-)\nabla\phi, \mathbf{v}\right) & \forall \mathbf{v} \in \mathbf{X}, \\ \boldsymbol{\mathcal{B}}(q,\mathbf{u}) = 0 & \forall q \in Y, \end{cases} \tag{1.2}$$

endowed with initial conditions $c^+(\cdot,0) = c^+_0$, $c^-(\cdot,0) = c^-_0$ and $\mathbf{u}(\cdot,0) = \mathbf{u}^0$. The existence and uniqueness of weak solution to (1.1) has been proved in [43] for the 2D case.

2. Virtual element approximation

The chief target of this section is to present the VE spaces and discrete bilinear (and trilinear) forms that are required for creating a VEM scheme. For simplicity of the presentation we restrict the construction to the 2D case.

2.1. Mesh notation and mesh regularity

By $\{\mathcal{T}_h\}_h$ we will denote a sequence of partitions of the domain Ω into general polygons E (open and simply connected sets whose boundary ∂E is a non-intersecting poly-line consisting of a finite number of straight line segments) having diameter h_E. Let $\mathcal{E}_h$ be the set of edges e of $\{\mathcal{T}_h\}_h$, and let $\mathcal{E}^I_h = \mathcal{E}_h \backslash \partial\Omega$ ($\mathcal{E}^B_h = \mathcal{E}_h \cap \partial\Omega$) be the set of all interior (boundary) edges. By $\mathbf{n}^e_E$, we denote the unit normal (pointing outwards) vector E for any edge $e \in \partial E \cap \mathcal{E}_h$. Following [1, 3, 7, 13], we adopt the following regularity assumption for polygonal meshes

Assumption 1. *([1]) There exist constants ρ_1, $\rho_2 > 0$ such that:*

(1). Every element E is shaped like a star with respect to a ball with radius $\geq \rho_1 h_E$,

(2). In E, the distance between every two vertices is $\geq \rho_2 h_E$.

2.2. Construction of a virtual element space for Z

This subsection is devoted to introducing the VE subspace $Z_h^k \subset Z$. In order to do that, we recall the definition of useful spaces. Given $k \in \mathbb{N}$, $E \in \mathcal{T}_h$ and $e \in \mathcal{E}_h$, we define

- $\mathbb{P}_k(E)$ the set of polynomials of degree at most k on E (with extended notation $\mathbb{P}_{-1}(E) := \emptyset$).
- $\mathbb{P}_k(e)$ the set of polynomials of degree at most k on e (with the extended notation $\mathbb{P}_{-1}(e) := \emptyset$).
- $\mathbb{B}_k(\partial E) := \{v \in C^0(\partial E) : \quad v|_e \in \mathbb{P}_k(e) \quad \textit{for all edges } e \subset \partial E\}$.
- $\widetilde{Z}_k^E := \{z_h \in C^0(E) \cap H^1(E) : \quad z_h|_{\partial E} \in \mathbb{B}_k(E), \quad \Delta z_h \in \mathbb{P}_k(E)\}$.

For $\mathcal{O} \subset \mathbb{R}^2$, we denote by $|O|$ its area, h_O its diameter, and $\mathbf{x}_O$ its barycenter. Given any integer $r \geq 1$, we denote by $\mathcal{M}_r(O)$ the set of scaled monomials

$$\mathcal{M}_r(\mathcal{O}) := \left\{ m : m = \left(\frac{\mathbf{x} - \mathbf{x}_\mathcal{O}}{h_\mathcal{O}} \right)^{\mathbf{s}} \quad \text{for} \quad \mathbf{s} \in \mathbb{N}^2 \quad \text{with} \quad |\mathbf{s}| \leq r \right\},$$

where $\mathbf{s} = (s_1, s_2)$, $|s| = s_1 + s_2$ and $\mathbf{x}^s = x_1^{s_1} x_2^{s_2}$. Besides, we need another set which is as follows

$$\mathcal{M}_r^*(\mathcal{O}) := \left\{ m : m = \left(\frac{\mathbf{x} - \mathbf{x}_\mathcal{O}}{h_\mathcal{O}} \right)^{\mathbf{s}} \quad \text{for} \quad \mathbf{s} \in \mathbb{N}^2 \quad \text{with} \quad |\mathbf{s}| = r \right\}.$$

Further, we recall the helpful polynomial projections $\Pi_k^{0,E}$ and $\Pi_k^{\nabla,E}$ associated with $E \in \mathcal{T}_h$ as follows:

- the L^2-projection $\Pi_k^{0,E} : \widetilde{Z}_k^E \to \mathbb{P}_k(E)$, given by

$$\int_E q_k (z - \Pi_k^{0,E} z) \, \mathrm{d}\mathbf{x} = 0 \quad \forall z \in L^2(E) \quad \text{and} \quad \forall q_k \in \mathbb{P}_k(E),$$

  with obvious extension for vector functions $\mathbf{\Pi}_k^{0,E} : \mathbf{X}|_E \to [\mathbb{P}_k(E)]^2$.

- the H^1-projection $\Pi_k^{\nabla,E} : \widetilde{Z}_k^E \to \mathbb{P}_k(E)$, defined by

$$\begin{cases} \int_E \nabla q_k \cdot \nabla (z - \Pi_k^{\nabla,E} z) \, \mathrm{d}\mathbf{x} = 0, & \forall z \in H^1(E) \quad \text{and } \forall q_k \in \mathbb{P}_k(E), \\ \int_{\partial E} (z - \Pi_k^{\nabla,E} z) \, \mathrm{d}s = 0, & \text{if} \quad k = 1, \\ \int_E (z - \Pi_k^{\nabla,E} z) \, \mathrm{d}\mathbf{x} = 0, & \text{if} \quad k \geq 2. \end{cases}$$

Finally we define a local VE space on each element $E \in \mathcal{T}_h$. Let k be a fixed positive integer. More precisely, we set [16]

$$Z_k^E := \left\{ z_h \in \widetilde{Z}_k^E : \quad (q_h^*, z_h)_E = (q_h^*, \Pi_k^{\nabla,E} z_h)_E \quad \forall q_h^* \in \mathcal{M}_{k-1}^*(E) \cup \mathcal{M}_k^*(E) \right\}.$$

So, the degrees of freedom (guaranteeing unisolvency) for the local VE space V_k^E are stated below [12]:

- (**D1**) The value of z at the i-th vertex of the element E.
- (**D2**) The values of z at $k-1$ distinct points in e, for all $e \subset \partial E$, and for $k \geq 2$.
- (**D2**) The internal moment $\int_E z \, q$, for all $q \in \mathcal{M}_{k-2}(E)$, and $k \geq 2$.

It is noteworthy that $\Pi_k^{0,E}$ and $\Pi_k^{\nabla,E}$ are computable from the knowledge of the degrees of freedom **D1**$-$**D2**. This fact was proved in [12]. Similar to the finite element case, the global VE space can be assembled as:

$$Z_h := \left\{ z_h \in Z : \quad z_h|_E \in Z_k^E \quad \forall E \in \mathcal{T}_h \right\}.$$

Also, we define a VE space on $\mathcal{T}_h$ for the electrostatic potential variable ϕ as follows:

$$\widehat{Z}_h := \{ z_h \in Z_h : \quad (z_h, 1)_{0,\mathcal{T}_h} = 0 \}.$$

Approximation properties in the space Z_k^h. The following estimates (established using Assumption 1) can be obtained for the projection and interpolation operators [1].

(i) there exists a $z_\pi \in \mathbb{P}_k(E)$ such that for $s \in [1, k+1]$ and $z \in H^s(E)$, there holds

$$|z - z_\pi|_{0,E} + h_E\, |z - z_\pi|_{1,E} \leq C h_E^s |z|_{s,E}. \tag{2.1}$$

(ii) there exists a $z_I \in V_k^E$ such that for $s \in [2, k+1]$ and $z \in H^s(E)$, there holds

$$|z - z_I|_{0,E} + h_E\, |z - z_I|_{1,E} \leq C h_E^s |z|_{s,E}. \tag{2.2}$$

2.3. Construction of a virtual element space for $\boldsymbol{X}$

Following [4], for $k \in \mathbb{N}$ let us introduce the spaces

$$\begin{aligned}
\mathcal{G}_k(E) &:= \nabla \mathbb{P}_{k+1}(E) \subset [\mathbb{P}_k(E)]^2, \\
\mathcal{G}_k(E)^\perp &:= \mathbf{x}^\perp [\mathbb{P}_{k-1}(E)] \subset [\mathbb{P}_k(E)]^2 \text{ with } \mathbf{x}^\perp := (x_2, -x_1), \\
\widetilde{\mathbf{X}}_k^E &:= \left\{ \mathbf{v} \in \mathbf{X} \quad \text{s.t } \mathbf{v}\,|_{\partial E} \in [\mathbb{B}_k(\partial E)]^2, \left\{ \begin{array}{l} -\boldsymbol{\Delta} \mathbf{v} - \nabla w \in \mathcal{G}_{k-2}(E)^\perp, \ \forall w \in L^2(E) \setminus \mathbb{R} \\ \operatorname{div} \mathbf{v} \in \mathbb{P}_{k-1}(E), \end{array} \right. \right\}.
\end{aligned}$$

The definition of scaled monomials can be extended to the vectorial case. Let $\boldsymbol{\alpha} := (\alpha_1, \alpha_2)$ and $\boldsymbol{\beta} := (\beta_1, \beta_2)$ be two multi-indexes, then we define a vectorial scaled monomial as

$$\boldsymbol{m}_{\alpha,\beta} := \begin{pmatrix} m_\alpha \\ m_\beta \end{pmatrix}.$$

Also in this case, it is easy to show that the set

$$[\mathcal{M}_r(\mathcal{O})]^2 := \{ \boldsymbol{m}_{\alpha,\emptyset} : 0 \leq |\boldsymbol{\alpha}| \leq r \} \cup \{ \boldsymbol{m}_{\emptyset,\beta} : 0 \leq |\boldsymbol{\beta}| \leq r \} := \{ \boldsymbol{m}_i : 1 \leq i \leq 2\pi_r \},$$

is a basis for the vectorial polynomial space $[\mathbb{P}_r(E)]^2$, where we implicitly use the natural correspondence between one-dimensional indices and double multi-indices.

One core idea in the VEM construction is to define suitable (computable) polynomial projections. The following polynomial projections are presented for each $k \in \mathbb{N}$ and $E \in \mathcal{T}_h$ (see e.g. [9])

- the $\mathbf{L}^2$-projection operator $\boldsymbol{\Pi}_k^{0,E} : \mathbf{X}|_E \to [\mathbb{P}_k(E)]^2$, defined by

$$\int_E (\mathbf{v} - \boldsymbol{\Pi}_k^{0,E} \mathbf{v}) : \mathbf{q}_k \, \mathrm{d}E = 0, \qquad \forall \mathbf{v} \in \mathbf{V},\ \mathbf{q}_k \in [\mathbb{P}_k(E)]^2.$$

- the $\mathbf{H}^1$-projection operator $\boldsymbol{\Pi}_k^{\nabla,E} : \mathbf{X}|_E \to [\mathbb{P}_k(E)]^2$, defined by

$$\left\{ \begin{array}{l} \int_E \boldsymbol{\nabla}(\mathbf{v} - \boldsymbol{\Pi}_k^{\nabla,E} \mathbf{v}) : \ \boldsymbol{\nabla} \mathbf{q}_k \, \mathrm{d}E = 0, \qquad \forall \mathbf{v} \in \mathbf{V}, \quad \mathbf{q}_k \in [\mathbb{P}_k(E)]^2, \\ \boldsymbol{\Pi}_0^{0,E} \left(\boldsymbol{\Pi}_k^{\nabla,E} \mathbf{v} - \mathbf{v} \right) = \mathbf{0}. \end{array} \right.$$

And a VE subspace of $\widetilde{\mathbf{X}}_k^E$ is given by

$$\mathbf{X}_k^E := \left\{ \mathbf{v}_h \in \widetilde{\mathbf{X}}_k^E : \qquad \left(\mathbf{\Pi}_k^{\nabla,E} \mathbf{v}_h - \mathbf{v}_h, \mathbf{g}_k^\perp \right) = 0, \qquad \forall \mathbf{g}_k^\perp \in \mathcal{G}_k^\perp(E)/\mathcal{G}_{k-2}^\perp(E) \right\}.$$

We recall the following properties of the space $\mathbf{X}_k^E$. Also, the corresponding/unisolvent degree of freedoms (Dofs) in $\mathbf{X}_k^E$ can be divided into the following four types (see [4])

- $(\mathbf{D1_v})$: the values of $\mathbf{v}$ at the vertexes of the element E,
- $(\mathbf{D2_v})$: the values of $\mathbf{v}$ at $k-1$ distinct points of any edge $e \subset \partial E$,
- $(\mathbf{D3_v})$: the moments

$$\int_E \mathbf{v} \cdot \mathbf{m}_{\boldsymbol{\alpha}} \, \mathrm{d}E, \qquad \forall \mathbf{m}_{\boldsymbol{\alpha}} \in [\mathcal{M}_{k-2}(E)]^2,$$

- $(\mathbf{D4_v})$: the moments

$$\int_E (\operatorname{div} \mathbf{v}) m_\alpha \, \mathrm{d}E, \qquad \forall m_\alpha \in \mathcal{M}_{k-1}(E)/\mathbb{R}.$$

We observe that the projectors $\mathbf{\Pi}_k^{\nabla,E}$ and $\mathbf{\Pi}_k^{0,E}$ can be computed using only the values $(\mathbf{D1_v})$-$(\mathbf{D4_v})$.

Finally, the global finite dimensional space $\mathbf{X}_h$, associated with the partition $\mathcal{T}_h$, is defined such that the restriction of every VE function $\mathbf{v}$ to the mesh element E belongs to $\mathbf{X}_k^E$. On the other hand, the discrete pressure spaces are simply given by piecewise polynomials of degree up to k:

$$Y_h := \left\{ q_h \in Y : \quad q_h|_E \in \mathbb{P}_k(K), \quad \forall E \in \mathcal{T}_h \right\},$$

and we also remark that

$$\operatorname{div} \mathbf{X}_k^h \subseteq Y_k^h. \tag{2.3}$$

Approximation properties associated with the space $\mathbf{X}_k^h$. The following estimates using Assumption 1 can be obtained for the projection and interpolation operators [4]:

(i) there exists a $\mathbf{z}_\pi \in [\mathbb{P}_k(E)]^2$ such that for $s \in [1, k+1]$, $\mathbf{z} \in [H^s(E)]^2$ and $p \in [1, \infty]$ we have

$$|\mathbf{z} - \mathbf{z}_\pi|_{p,E} + h_E \, |\mathbf{z} - \mathbf{z}_\pi|_{1,p,E} \le C h_E^s |\mathbf{z}|_{s,p,E}. \tag{2.4}$$

(ii) there exists a $\mathbf{z}_I \in \mathbf{V}_k^E$ such that for $s \in [2, k+1]$ and $\mathbf{z} \in [H^s(E)]^2$, we have

$$|\mathbf{z} - \mathbf{z}_I|_{p,E} + h_E \, |\mathbf{z} - \mathbf{z}_I|_{1,p,E} \le C h_E^s |\mathbf{z}|_{s,p,E}. \tag{2.5}$$

2.4. The discrete forms and their properties

As usual in the VE literature [1, 2] we define computable discrete bilinear (and trilinear) forms that approximate the exact forms existing in the variational form (1.2) using projections. Similar to the finite element case, we only need to construct the computable local discrete forms, which can be summed up element by element to obtain the corresponding global discrete forms

- Firstly, we define $\mathcal{M}_h^E : Z_k^E \times Z_k^E \to \mathbb{R}$ as
$$\mathcal{M}_h^E(\rho_h,\zeta_h) := \mathcal{M}^E(\Pi_k^{0,E}(\rho_h),\Pi_k^{0,E}(\zeta_h)) + |E|S^E(\rho_h - \Pi_k^{0,E}(\rho_h),\zeta_h - \Pi_k^{0,E}(\zeta_h)), \tag{2.6}$$
where the stabilization $S^E : Z_k^E \times Z_k^E \to \mathbb{R}$ is a symmetric, positive definite, bilinear form such that
$$c_0|\rho_h|_{1,E}^2 \le S^E(\rho_h,\rho_h) \le c_1|\rho_h|_{1,E}^2, \quad \forall \rho_h \in Z_k^E, \quad \text{with } \Pi_k^{0,E}(\rho_h) = 0,$$
for two positive constants c_0, c_1 that are independent of h.

- Secondly, for $i = 1,2,3$ we define $\mathcal{A}_{ih}^E : Z_k^E \times Z_k^E \to \mathbb{R}$ as
$$\mathcal{A}_{ih}^E(\rho_h,\zeta_h) := \mathcal{A}_i^E\left(\Pi_k^{\nabla,E}\rho_h,\Pi_k^{\nabla,E}\zeta_h\right) + |\lambda_i|S^E\left((I-\Pi_k^{\nabla,E})\rho_h,(I-\Pi_k^{\nabla,E})\zeta_h\right), \quad \lambda_i = D_1, D_2, \epsilon.$$

- Moreover, the term $\mathcal{C}(\xi;\rho,\zeta)$ is replaced by
$$\mathcal{C}_h^E(\xi_h;\rho_h,\zeta_h) := \left(\Pi_{k-1}^{0,E}\xi_h\boldsymbol{\Pi}_{k-1}^{0,E}\nabla\rho_h,\boldsymbol{\Pi}_{k-1}^{0,E}\nabla\zeta_h\right)_{0,E} + |\Pi_0^{0,E}\xi_h|S^E\left((I-\Pi_k^{\nabla,E})\rho_h,(I-\Pi_k^{\nabla,E})\zeta_h\right). \tag{2.7}$$

- Also, the discrete local forms $\boldsymbol{\mathcal{M}}_h : \mathbf{X}_k^E \times \mathbf{X}_k^E \to \mathbb{R}$ and $\boldsymbol{\mathcal{A}}_h : \mathbf{X}_k^E \times \mathbf{X}_k^E \to \mathbb{R}$ defined by
$$\boldsymbol{\mathcal{M}}_h^E(\mathbf{u}_h,\mathbf{v}_h) := \boldsymbol{\mathcal{M}}^E(\boldsymbol{\Pi}_k^{0,E}(\mathbf{u}_h),\boldsymbol{\Pi}_k^{0,E}(\mathbf{v}_h)) + |E|\boldsymbol{\mathcal{S}}^E(\mathbf{u}_h - \boldsymbol{\Pi}_k^{0,E}(\mathbf{u}_h),\mathbf{v}_h - \boldsymbol{\Pi}_k^{0,E}(\mathbf{v}_h)),$$
and
$$\boldsymbol{\mathcal{A}}_h^E(\mathbf{u}_h,\mathbf{v}_h) := \boldsymbol{\mathcal{A}}^E(\boldsymbol{\Pi}_k^{\nabla,E}(\mathbf{u}_h),\boldsymbol{\Pi}_k^{\nabla,E}(\mathbf{v}_h)) + \boldsymbol{\mathcal{S}}^E(\mathbf{u}_h - \boldsymbol{\Pi}_k^{\nabla,E}(\mathbf{u}_h),\mathbf{v}_h - \boldsymbol{\Pi}_k^{\nabla,E}(\mathbf{v}_h)),$$
where the stabilizer $\boldsymbol{\mathcal{S}}^E : \mathbf{X}_k^E \times \mathbf{X}_k^E \to \mathbb{R}$ is a symmetric, positive definite, bilinear form such that
$$c_2|\mathbf{z}_h|_{1,E}^2 \le \boldsymbol{\mathcal{S}}^E(\mathbf{z}_h,\mathbf{z}_h) \le c_3|\mathbf{z}_h|_{1,E}^2, \quad \forall \mathbf{z}_h \in \mathbf{X}_k^E, \quad \text{with } \boldsymbol{\Pi}_k^{\nabla,E}(\mathbf{z}_h) = \mathbf{0},$$
for two positive constants c_2, c_3 that are independent of h. Finally, the skew-symmetric trilinear forms $\mathcal{D}(\mathbf{w};\rho,\zeta)$ and $\boldsymbol{\mathcal{C}}(\mathbf{w};\mathbf{u},\mathbf{v})$ are replaced, respectively, by
$$\mathcal{D}_h^E(\mathbf{w}_h;\rho_h,\zeta_h) := \frac{1}{2}\big[(\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\cdot\Pi_k^{0,E}\rho_h,\Pi_{k-1}^{0,E}\nabla\zeta_h)_0 - (\boldsymbol{\Pi}_k^{0,E}\mathbf{w}_h\cdot\Pi_{k-1}^{0,E}\nabla\rho_h,\Pi_k^{0,E}\zeta_h)_0\big],$$
$$\boldsymbol{\mathcal{C}}_h(\mathbf{w}_h;\mathbf{u}_h,\mathbf{v}_h) := \frac{1}{2}\big[(\boldsymbol{\Pi}_k^{0,E}\mathbf{w}_h\cdot\boldsymbol{\Pi}_{k-1}^{0,E}\nabla\mathbf{u}_h,\boldsymbol{\Pi}_k^{0,E}\mathbf{v}_h)_0 - (\boldsymbol{\Pi}_k^{0,E}\mathbf{w}_h\cdot\boldsymbol{\Pi}_{k-1}^{0,E}\nabla\mathbf{v}_h,\boldsymbol{\Pi}_k^{0,E}\mathbf{u}_h)_0\big]. \tag{2.8}$$

Next, we provide the main consistency and stability features of the proposed discrete forms.

Lemma 2.1. *([12]) (**Polynomial consistency**): for every polynomial $q_k \in \mathbb{P}_k(E)$ (and $\boldsymbol{q}_k \in [\mathbb{P}_k(E)]^2$) and every virtual element function $z_h \in Z_k^E$ (and $\boldsymbol{v}_h \in \boldsymbol{X}_k^E$) it holds that*
$$\begin{aligned}
\mathcal{M}_h^E(q_k,z_h) &= \mathcal{M}^E(q_k,z_h), && \forall q_k \in \mathbb{P}_k(E), \forall z_h \in Z_k^E,\\
\mathcal{A}_{ih}^E(q_k,z_h) &= \mathcal{A}_i^E(q_k,z_h), && \forall q_k \in \mathbb{P}_k(E), \forall z_h \in Z_k^E,\\
\boldsymbol{\mathcal{M}}_h^E(\boldsymbol{q}_k,\boldsymbol{v}_h) &= \boldsymbol{\mathcal{M}}^E(\boldsymbol{q}_k,\boldsymbol{v}_h), && \forall \boldsymbol{q}_k \in [\mathbb{P}_k(E)]^2, \forall \boldsymbol{v}_h \in \boldsymbol{X}_k^E,\\
\boldsymbol{\mathcal{A}}_h^E(\boldsymbol{q}_k,\boldsymbol{v}_h) &= \boldsymbol{\mathcal{A}}^E(\boldsymbol{q}_k,\boldsymbol{v}_h), && \forall \boldsymbol{q}_k \in [\mathbb{P}_k(E)]^2, \forall \boldsymbol{v}_h \in \boldsymbol{X}_k^E.
\end{aligned}$$
*(**Stability**): there exist positive constants $\alpha_1,\alpha_2,\beta_{1,i},\beta_{2,i},\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\boldsymbol{\beta}_1,\boldsymbol{\beta}_2$ (independent of E and h) verifying*
$$\begin{aligned}
\mathcal{M}_h^E(\rho_h,\zeta_h) &\le \alpha_2|\rho_h|_{0,E}|\zeta_h|_{0,E}, & \mathcal{A}_{ih}^E(\rho_h,\zeta_h) &\le \beta_{2,i}|\rho_h|_{1,E}|\zeta_h|_{1,E},\\
\boldsymbol{\mathcal{M}}_h^E(\boldsymbol{u}_h,\boldsymbol{v}_h) &\le \boldsymbol{\alpha}_2|\boldsymbol{u}_h|_{0,E}|\boldsymbol{v}_h|_{0,E}, & \boldsymbol{\mathcal{A}}_h^E(\boldsymbol{u}_h,\boldsymbol{v}_h) &\le \boldsymbol{\beta}_2|\boldsymbol{u}_h|_{1,E}|\boldsymbol{v}_h|_{1,E},\\
\mathcal{M}_h^E(\rho_h,\rho_h) &\ge \alpha_1|\rho_h|_{0,E}^2, & \mathcal{A}_{ih}^E(\rho_h,\rho_h) &\ge \beta_{1,i}|\rho_h|_{1,E}^2,\\
\boldsymbol{\mathcal{M}}_h^E(\boldsymbol{u}_h,\boldsymbol{u}_h) &\ge \boldsymbol{\alpha}_1|\boldsymbol{u}_h|_{0,E}^2, & \boldsymbol{\mathcal{A}}_h^E(\boldsymbol{u}_h,\boldsymbol{u}_h) &\ge \boldsymbol{\beta}_1|\boldsymbol{u}_h|_{1,E}^2,
\end{aligned} \tag{2.9}$$
for $i = 1,2,3$, all $\rho_h,\zeta_h \in Z_k^E$ and $\boldsymbol{u}_h,\boldsymbol{v}_h \in \boldsymbol{X}_k^E$.

We now show that the discrete forms $\mathcal{D}_h(\cdot;\cdot,\cdot)$ and $\boldsymbol{\mathcal{C}}_h(\cdot;\cdot,\cdot)$ are continuous on Z_h and $\mathbf{X}_h$, respectively.

Lemma 2.2. *Let*

$$\widehat{C}_{1h} := \sup_{\mathbf{w}_h\in\mathbf{X},\rho_h,\zeta_h\in Z_h} \frac{|\mathcal{D}_h(\mathbf{w}_h;\rho_h,\zeta_h)|}{\|\mathbf{w}_h\|_{\mathbf{X}}\|\rho_h\|_Z\|\zeta_h\|_Z}, \qquad \widehat{C}_{2h} := \sup_{\mathbf{w}_h,\mathbf{u}_h,\mathbf{v}_h\in\mathbf{X}_h} \frac{|\boldsymbol{\mathcal{C}}_h(\mathbf{w}_h;\mathbf{u}_h,\mathbf{v}_h)|}{\|\mathbf{w}_h\|_{\mathbf{X}}\|\mathbf{u}_h\|_{\mathbf{X}}\|\mathbf{v}_h\|_{\mathbf{X}}}.$$

Then the trilinear forms $\mathcal{D}_h(\cdot;\cdot,\cdot)$ and $\boldsymbol{\mathcal{C}}_h(\cdot;\cdot,\cdot)$ are continuous.

Proof. Using definition of discrete form $\mathcal{D}_h$ and the Hölder inequality, we have

$$\begin{aligned}\mathcal{D}_h(\mathbf{w}_h;\rho_h,\zeta_h) &= \frac{1}{2}\big[(\mathbf{\Pi}_k^0\mathbf{w}_h\ \Pi_k^0\rho_h, \Pi_{k-1}^0\nabla\zeta_h)_0 - (\mathbf{\Pi}_k^0\mathbf{w}_h\cdot\Pi_{k-1}^0\nabla\rho_h, \Pi_k^0\zeta_h)_0\big] \\ &\le \|\mathbf{\Pi}_k^0\mathbf{w}_h\|_{0,4}\|\Pi_k^0\rho_h\|_{0,4}\|\Pi_{k-1}^0\nabla\zeta_h\|_0 + \|\mathbf{\Pi}_k^0\mathbf{w}_h\|_{0,4}\|\Pi_{k-1}^0\nabla\rho_h\|_0\|\Pi_k^0\zeta_h\|_{0,4}. \end{aligned} \tag{2.10}$$

Applying the inverse inequality in conjunction with the continuity of the projectors $\mathbf{\Pi}_k^0$ and Π_k^0 (with respect to the L^2-norm), gives the following upper bound for the terms $\|\mathbf{\Pi}_k^0\mathbf{w}_h\|_{0,4}$, $\|\Pi_k^0\rho_h\|_{0,4}$ and $\|\Pi_k^0\zeta_h\|_{0,4}$ on the right-hand side of the above inequality, and for $E\in\mathcal{T}_h$:

$$\|\mathbf{\Pi}_k^{0,E}\mathbf{w}_h\|_{0,4} \le h_E^{-1/2}\|\mathbf{\Pi}_k^{0,E}\mathbf{w}_h\|_{0,E} \le h_E^{-1/2}\|\mathbf{w}_h\|_{0,E} \le C_1\|\mathbf{w}_h\|_{0,4}, \tag{2.11}$$

and similarly

$$\|\Pi_k^0\rho_h\|_{0,4} \le C_2\|\rho_h\|_{0,4}, \quad \|\Pi_k^0\zeta_h\|_{0,4} \le C_3\|\zeta_h\|_{0,4}. \tag{2.12}$$

Combining the above estimates with Eq. (2.10) leads to

$$\mathcal{D}_h(\mathbf{w}_h;\rho_h,\zeta_h) \le \frac{1}{2}\left(C_1C_2 + C_1C_3\right)\|\mathbf{w}_h\|_{\mathbf{X}}\|\rho_h\|_Z\|\zeta_h\|_Z,$$

which confirm the continuity $\mathcal{D}_h(\cdot;\cdot,\cdot)$. The proof of continuity of $\boldsymbol{\mathcal{C}}_h(\cdot;\cdot,\cdot)$ can be find in [5]. □

Lemma 2.3. *[5] (**Discrete inf-sup condition**) Given the VE spaces $\boldsymbol{X}_h$ and Y_h defined in Section 2.3, there exists a positive $\widehat{\beta}$, independent of h, such that:*

$$\sup_{\mathbf{v}_h\in\mathbf{X}_h\mathbf{v}_h\neq\mathbf{0}} \frac{\boldsymbol{\mathcal{B}}\left(\mathbf{v}_h,q_h\right)}{\|\mathbf{v}_h\|_{\mathbf{X}}} \ge \widehat{\beta}\,\|q_h\|_Y \qquad \textit{for all } q_h\in Y_h.$$

Additionally, the discrete inf-sup property together with (2.3) indicate that

$$\operatorname{div}\mathbf{X}_h = Y_h.$$

The following lemma compares $\mathcal{M}^E$, $\mathcal{A}_i^E$, $\boldsymbol{\mathcal{M}}^E$ and $\boldsymbol{\mathcal{A}}^E$ with their computable versions $\mathcal{M}_h^E$, $\mathcal{A}_{ih}^E$, $\boldsymbol{\mathcal{M}}_h^E$ and $\boldsymbol{\mathcal{A}}_h^E$, respectively.

Lemma 2.4. *[16] Let α_2 be the constant from Lemma 2.1. Then for each $E\in\mathcal{T}_h$, there hold*

$$\begin{aligned}|\mathcal{M}^E(\rho,\zeta)-\mathcal{M}_h^E(\rho,\zeta)| &\le \alpha_2\|\rho-\Pi_k^{0,E}(\rho)\|_{0,E}\|\zeta\|_{0,E}, &&\forall\rho,\zeta\in Z_k^E,\\ |\boldsymbol{\mathcal{M}}^E(\boldsymbol{u},\boldsymbol{v})-\boldsymbol{\mathcal{M}}_h^E(\boldsymbol{u},\boldsymbol{v})| &\le \boldsymbol{\alpha}_2\|\boldsymbol{u}-\mathbf{\Pi}_k^{0,E}(\boldsymbol{u})\|_{0,E}\|\boldsymbol{v}\|_{0,E}, &&\forall\boldsymbol{u},\boldsymbol{v}\in\boldsymbol{X}_k^E.\end{aligned}$$

Lemma 2.5. *[16] Let β_2 be the constant from Lemma 2.1. Then for each $E\in\mathcal{T}_h$, there hold*

$$\begin{aligned}|\mathcal{A}_i^E(\rho,\zeta)-\mathcal{A}_{ih}^E(\rho,\zeta)| &\le \beta_{2,i}\|\rho-\Pi_k^{\nabla,E}(\rho)\|_{1,E}\|\zeta\|_{1,E}, &&\forall\rho,\zeta\in Z_k^E,\\ |\boldsymbol{\mathcal{A}}^E(\boldsymbol{u},\boldsymbol{v})-\boldsymbol{\mathcal{A}}_h^E(\boldsymbol{u},\boldsymbol{v})| &\le \boldsymbol{\beta}_2\|\boldsymbol{u}-\mathbf{\Pi}_k^{\nabla,E}(\boldsymbol{u})\|_{1,E}\|\boldsymbol{v}\|_{1,E}, &&\forall\boldsymbol{u},\boldsymbol{v}\in\boldsymbol{X}_k^E.\end{aligned}$$

Lemma 2.6. *Assume that $\boldsymbol{v} \in \boldsymbol{X} \cap [H^{s+1}(\Omega)]^2$ and $s \in [0,k]$. Then, it holds*

$$|\boldsymbol{\mathcal{C}}^E(\boldsymbol{v};\boldsymbol{v},\boldsymbol{w}) - \boldsymbol{\mathcal{C}}_h^E(\boldsymbol{v};\boldsymbol{v},\boldsymbol{w})| \le Ch^s\left(\|\boldsymbol{v}\|_{\boldsymbol{X}} + \|\boldsymbol{v}\|_s + \|\boldsymbol{v}\|_{s+1}\right)\|\boldsymbol{v}\|_{s+1}\|\boldsymbol{w}\|_{\boldsymbol{X}}, \qquad \forall \boldsymbol{w} \in \boldsymbol{X}.$$

Proof. First, by definitions of the trilinear continuous and discrete forms $\boldsymbol{\mathcal{C}}(\cdot;\cdot,\cdot)$ and $\boldsymbol{\mathcal{C}}_h(\cdot;\cdot,\cdot)$, we have

$$\begin{aligned}
\boldsymbol{\mathcal{C}}^E(\mathbf{v};\mathbf{v},\mathbf{w}) - \boldsymbol{\mathcal{C}}_h^E(\mathbf{v};\mathbf{v},\mathbf{w}) &= \frac{1}{2}\left[(\mathbf{v}\cdot\nabla\mathbf{v},\mathbf{w})_0 - (\mathbf{\Pi}_k^{0,E}\mathbf{v}_h\cdot\mathbf{\Pi}_{k-1}^{0,E}\nabla\mathbf{v}_h, \mathbf{\Pi}_k^{0,E}\mathbf{w}_h)_0\right] \\
&+ \frac{1}{2}\left[(\mathbf{v}\cdot\nabla\mathbf{w},\mathbf{v})_0 - (\mathbf{\Pi}_k^{0,E}\mathbf{v}_h\cdot\mathbf{\Pi}_{k-1}^{0,E}\nabla\mathbf{w}_h, \mathbf{\Pi}_k^{0,E}\mathbf{v}_h)_0\right] \\
&:= \frac{1}{2}\left(\boldsymbol{\eta}_1 + \boldsymbol{\eta}_2\right). \qquad (2.13)
\end{aligned}$$

The above terms will now be analyzed. Straightforward computations for $\boldsymbol{\eta}_1$ give

$$\begin{aligned}
\boldsymbol{\eta}_1|_E &= \int_E \Big((\mathbf{v}\cdot\nabla\mathbf{v})\cdot\mathbf{w} - (\mathbf{\Pi}_k^{0,E}\mathbf{v}_h\cdot\mathbf{\Pi}_{k-1}^{0,E}\nabla\mathbf{v}_h)\cdot\mathbf{\Pi}_k^{0,E}\mathbf{w}_h)\Big)dE \\
&= \int_E \Big((\mathbf{v}\cdot\nabla\mathbf{v})\cdot(I-\mathbf{\Pi}_k^{0,E})\mathbf{w} + ((I-\mathbf{\Pi}_k^{0,E})\mathbf{v}\cdot\nabla\mathbf{v})\cdot\mathbf{\Pi}_k^{0,E}\mathbf{w} + (\mathbf{\Pi}_k^{0,E}\mathbf{v}\cdot(I-\mathbf{\Pi}_k^{0,E})\nabla\mathbf{v})\cdot\mathbf{\Pi}_k^{0,E}\mathbf{w}\Big)dE \\
&:= \boldsymbol{\eta}_1^1 + \boldsymbol{\eta}_1^2 + \boldsymbol{\eta}_1^3. \qquad (2.14)
\end{aligned}$$

Now, by definition of L^2-projection $\mathbf{\Pi}_k^{0,E}$, and using estimate (2.1), the Hölder inequality, and Sobolev embedding $H^s \subset W_4^{s-1}$, we have

$$\begin{aligned}
\boldsymbol{\eta}_1^1 &= \int_E \Big((\mathbf{v}\cdot\nabla\mathbf{v})\cdot(I-\mathbf{\Pi}_k^{0,E})\mathbf{w}\Big)\,dE = \int_E \Big((I-\mathbf{\Pi}_{k-2}^{0,E})(\mathbf{v}\cdot\nabla\mathbf{v})\cdot(I-\mathbf{\Pi}_k^{0,E})\mathbf{w}\Big)\,dE \\
&\le \left\|(I-\mathbf{\Pi}_{k-2}^{0,E})(\mathbf{v}\cdot\nabla\mathbf{v})\right\|_{0,E}\left\|(I-\mathbf{\Pi}_k^{0,E})\mathbf{w}\right\|_{0,E} \\
&\le Ch_E^s\|\mathbf{v}\cdot\nabla\mathbf{v}\|_{s-1,E}|\mathbf{w}|_1 \le Ch_E^s\|\mathbf{v}\|_{s-1,4,E}\|\nabla\mathbf{v}\|_{s-1,4,E}|\mathbf{w}|_{1,E} \\
&\le Ch_E^s\|\mathbf{v}\|_{s,E}\|\nabla\mathbf{v}\|_{s,E}|\mathbf{w}|_{1,E}. \qquad (2.15)
\end{aligned}$$

For the term $\boldsymbol{\eta}_1^2$ in (2.14), using the Hölder inequality, the approximation property given in (2.4), and the continuity of $\mathbf{\Pi}_k^{0,E}$ with respect to the L^4-norm, permit us to assert that

$$\begin{aligned}
\boldsymbol{\eta}_1^2 &= \int_E \Big(((I-\mathbf{\Pi}_k^{0,E})\mathbf{v}\cdot\nabla\mathbf{v})\cdot\mathbf{\Pi}_k^{0,E}\mathbf{w}\Big)\,dE \le \|\nabla\mathbf{v}\|_{0,E}\left\|(I-\mathbf{\Pi}_k^{0,E})\mathbf{v}\right\|_{0,4,E}\left\|\mathbf{\Pi}_k^{0,E}\mathbf{w}\right\|_{0,4,E} \\
&\le \|\nabla\mathbf{v}\|_{0,E}\Big(\|\mathbf{v}-\mathbf{v}_\pi\|_{0,4,E} + \|\mathbf{\Pi}_k^{0,E}(\mathbf{v}-\mathbf{v}_\pi)\|_{0,4,E}\Big)\|\mathbf{w}\|_{0,4,E} \\
&\le Ch^s\|\nabla\mathbf{v}\|_{0,E}|\mathbf{v}|_{s,4,E}\|\mathbf{w}\|_{0,4,E} \\
&\le Ch^s\|\mathbf{v}\|_{1,E}\|\mathbf{v}\|_{s+1,E}\|\mathbf{w}\|_{1,E},
\end{aligned}$$

where in the last inequality we have used the Sobolev embeddings $H^1 \subset L^4$ and $H^{s+1} \subset W_4^s$.

Finally, for the term $\boldsymbol{\eta}_1^3$ in (2.14), using the Hölder inequality, the continuity of $\mathbf{\Pi}_k^{0,E}$ and Sobolev embedding, yields

$$\begin{aligned}
\boldsymbol{\eta}_1^3 &= \int_E \Big((\mathbf{\Pi}_k^{0,E}\mathbf{v}\cdot(I-\mathbf{\Pi}_k^{0,E})\nabla\mathbf{v})\cdot\mathbf{\Pi}_k^{0,E}\mathbf{w}\Big)\,dE \le \left\|\mathbf{\Pi}_k^{0,E}\mathbf{v}\right\|_{0,4,E}\left\|(I-\mathbf{\Pi}_k^{0,E})\nabla\mathbf{v}\right\|_{0,E}\left\|\mathbf{\Pi}_k^{0,E}\mathbf{w}\right\|_{0,4,E} \\
&\le Ch^s\|\nabla\mathbf{v}\|_s\|\mathbf{v}\|_{0,4,E}\|\mathbf{w}\|_{0,4,E} \le Ch^s\|\nabla\mathbf{v}\|_{s,E}\|\mathbf{v}\|_{1,E}\|\mathbf{w}\|_{1,E}. \qquad (2.16)
\end{aligned}$$

Combining Eqs. (2.15)-(2.16) into (2.14) gives

$$\boldsymbol{\eta}_1 \leq Ch^s \left(\|\mathbf{v}\|_{s+1}\|\mathbf{v}\|_s + \|\mathbf{v}\|_{s+1}\|\mathbf{v}\|_1\right)\|\mathbf{w}\|_1. \tag{2.17}$$

A bound for the term $\boldsymbol{\eta}_2$ can be derived using analogous arguments as above

$$\boldsymbol{\eta}_2 \leq Ch^s \left(\|\mathbf{v}\|_{s+1}^2 + \|\mathbf{v}\|_{s+1}\|\mathbf{v}\|_1\right)\|\mathbf{w}\|_1. \tag{2.18}$$

And the rest of the proof can be inferred by combining (2.17) and (2.18) in (2.13). □

Lemma 2.7. *Under the hypothesis of Lemma 2.5, the following error estimate holds*

$$|\mathcal{D}(\boldsymbol{w};\rho,\zeta) - \mathcal{D}_h(\boldsymbol{w};\rho,\zeta)| \leq Ch^s \left(\|\boldsymbol{w}\|_{s+1}(\|\rho\|_{s+1} + \|\rho\|_1) + \|\rho\|_{s+1}(\|\boldsymbol{w}\|_s + \|\boldsymbol{w}\|_1)\right)\|\zeta\|_1.$$

Proof. First, the definitions of the trilinear continuous and discrete forms $\mathcal{D}(\cdot;\cdot,\cdot)$ and $\mathcal{D}_h(\cdot;\cdot,\cdot)$ give

$$\begin{aligned}\mathcal{D}(\mathbf{w};\rho,\zeta) - \mathcal{D}_h(\mathbf{w};\rho,\zeta) &= \frac{1}{2}\left[(\mathbf{w}\rho, \nabla\zeta)_0 - (\boldsymbol{\Pi}_k^0\mathbf{w}\cdot\Pi_k^0\rho, \Pi_{k-1}^0\nabla\zeta)_0\right] \\ &+ \frac{1}{2}\left[(\mathbf{w}\cdot\nabla\rho,\zeta)_0 - (\boldsymbol{\Pi}_k^0\mathbf{w}\cdot\Pi_{k-1}^0\nabla\rho, \Pi_k^0\zeta)_0\right] \\ &= \frac{1}{2}(\eta_1 + \eta_2).\end{aligned} \tag{2.19}$$

We now bound the terms η_1 and η_2. For the first term, elementary calculations show that

$$\begin{aligned}\eta_1|_E &= \int_E \left((\mathbf{w}\rho)\cdot\nabla\zeta - (\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\Pi_k^{0,E}\rho)\cdot\Pi_{k-1}^{0,E}\nabla\zeta\right)dE \\ &= \int_E \left(\mathbf{w}\;\rho\;(I-\Pi_{k-1}^{0,E})\nabla\zeta + (I-\boldsymbol{\Pi}_k^{0,E})\mathbf{w}\;\rho\;\Pi_{k-1}^{0,E}\nabla\zeta + \boldsymbol{\Pi}_k^{0,E}\mathbf{w}(I-\Pi_k^{0,E})\;\rho\;\Pi_{k-1}^{0,E}\nabla\zeta\right)dE.\end{aligned} \tag{2.20}$$

Then, using the Hölder inequality, the continuity of $\boldsymbol{\Pi}_k^{0,E}$ (with respect to the L^4-norm), as well as Sobolev embeddings, we can control the terms on the right-hand side of (2.19) as follows

$$\eta_1 \leq Ch^s \left(\|\mathbf{w}\|_{s+1}(\|\rho\|_{s+1} + \|\rho\|_1) + \|\rho\|_{s+1}\|\mathbf{w}\|_1\right)\|\zeta\|_1, \tag{2.21a}$$
$$\eta_2 \leq Ch^s \left(\|\rho\|_{s+1}(\|\mathbf{w}\|_s + \|\mathbf{w}\|_1) + \|\mathbf{w}\|_{s+1}\|\rho\|_1\right)\|\zeta\|_1. \tag{2.21b}$$

Consequently, the proof follows after putting together (2.21a) and (2.21b) into (2.20). □

Lemma 2.8. *Assume that $\xi \in H^s(\Omega)\cap L^\infty(\Omega)$, $\rho \in H^{s+1}(\Omega)\cap W^{1,\infty}(\Omega)$ and $s \in [0,k]$. Then, it holds*

$$\left|\mathcal{C}(\xi;\rho,\zeta) - \mathcal{C}_h(\xi;\rho,\zeta)\right| \leq C\left(h^k\|\xi\nabla\rho\|_k + \|\xi\|_\infty h^k\|\rho\|_{k+1} + \|\rho\|_{1,\infty}h^k\|\xi\|_k\right)\|\zeta\|_1, \quad \forall\zeta\in Z.$$

Proof. We first write on each element $E \in \mathcal{T}_h$ the following relation

$$\begin{aligned}\mathcal{C}^E(\xi;\rho,\zeta) - \mathcal{C}_h^E(\xi;\rho,\zeta) &= (\xi\nabla\rho,\nabla\zeta)_{0,E} - \left(\Pi_{k-1}^{0,E}\xi\boldsymbol{\Pi}_{k-1}^{0,E}\nabla\rho, \boldsymbol{\Pi}_{k-1}^{0,E}\nabla\zeta\right)_{0,E} \\ &= \left[(\xi\nabla\rho,\nabla\zeta)_{0,E} - (\boldsymbol{\Pi}_{k-1}^{0,E}(\xi\nabla\rho),\nabla\zeta)_{0,E}\right] \\ &+ \left[(\boldsymbol{\Pi}_{k-1}^{0,E}(\xi\nabla\rho),\nabla\zeta)_{0,E} - (\boldsymbol{\Pi}_{k-1}^{0,E}(\xi\boldsymbol{\Pi}_{k-1}^{0,E}\nabla\rho),\nabla\zeta)_{0,E}\right] \\ &+ \left[(\boldsymbol{\Pi}_{k-1}^{0,E}(\xi\boldsymbol{\Pi}_{k-1}^{0,E}\nabla\rho),\nabla\zeta)_{0,E} - (\Pi_{k-1}^{0,E}\xi\boldsymbol{\Pi}_{k-1}^{0,E}\nabla\rho, \boldsymbol{\Pi}_{k-1}^{0,E}\nabla\zeta)_{0,E}\right] \\ &\leq C\left(h^k\|\xi\nabla\rho\|_k + \|\xi\|_\infty h^k\|\rho\|_{k+1} + \|\boldsymbol{\Pi}_{k-1}^{0,E}\nabla\rho\|_\infty h^k\|\xi\|_k\right)\|\zeta\|_1,\end{aligned}$$

where in the last step the approximation properties of the L^2-projectors are used, and the term $\|\boldsymbol{\Pi}_{k-1}^{0,E}\nabla\rho\|_\infty$ is estimated as in (4.3). □

2.5. Semi-discrete and fully-discrete schemes

With the aid of the discrete forms (2.6)-(2.8) we can state the semi-discrete VE scheme as: Find $\{c_h^+(\cdot,t), c_h^-(\cdot,t), \phi_h(\cdot,t)\} \in Z_h \times Z_h \times \widehat{Z}_h$ and $\{\mathbf{u}_h(\cdot,t), p_h(\cdot,t)\} \in \mathbf{X}_h \times Y_h$ such that for nearly all $t \in [0, t_F]$

$$\begin{cases} \mathcal{M}_h(c_{ht}^+, z_1) + \mathcal{A}_{1h}(c_h^+, z_1) + \mathcal{C}_h(c_h^+; \phi_h, z_1) - \mathcal{D}_h(\mathbf{u}_h; c_h^+, z_1) = 0 & \forall z_1 \in Z_h, \\ \mathcal{M}_h(c_{ht}^-, z_2) + \mathcal{A}_{2h}(c_h^-, z_2) - \mathcal{C}_h(c_h^-; \phi_h, z_2) - \mathcal{D}_h(\mathbf{u}_h; c_h^-, z_2) = 0 & \forall z_2 \in Z_h, \\ \mathcal{A}_{3h}(\phi_h, z_3) = \mathcal{M}_h(c_h^+, z_3) - \mathcal{M}_h(c_h^-, z_3) & \forall z_3 \in Z_h, \\ \boldsymbol{\mathcal{M}}_h(\mathbf{u}_{ht}, \mathbf{v}) + \boldsymbol{\mathcal{A}}_h(\mathbf{u}_h, \mathbf{v}) + \boldsymbol{\mathcal{C}}_h(\mathbf{u}_h; \mathbf{u}_h, \mathbf{v}) - \boldsymbol{\mathcal{B}}(p_h, \mathbf{v}) = -\left((c_h^+ - c_h^-)\nabla\phi_h, \mathbf{v}\right)_h & \forall \mathbf{v} \in \mathbf{X}_h, \\ \boldsymbol{\mathcal{B}}(q, \mathbf{u}_h) = 0 & \forall q \in Y_h, \end{cases}$$

where

$$\left((c_h^+ - c_h^-)\nabla\phi_h, \mathbf{v}\right)_h := \sum_{E\in\mathcal{T}_h} \left((\Pi_k^{0,E} c_h^+ - \Pi_k^{0,E} c_h^-)\boldsymbol{\Pi}_{k-1}^{0,E}\nabla\phi_h, \boldsymbol{\Pi}_k^{0,E}\mathbf{v}\right)_{0,E},$$

with initial conditions $c_h^+(\cdot,0) = c_{0,h}^+$, $c_h^-(\cdot,0) = c_{0,h}^-$ and $\mathbf{u}_h(\cdot,0) = \mathbf{u}_{0,h}$ where $c_{0,h}^+(\cdot)$, $c_{0,h}^-(\cdot)$ and $\mathbf{u}_{0,h}(\cdot)$ are proper approximations of c_0^+, c_0^- and $\mathbf{u}_0$, respectively. Next, we discretise in time using the backward Euler method with the constant step size $\Delta t = \frac{t_F}{N}$ and for any function f, denote $f^n = f(\cdot, t_n)$, $\delta_t f^n = \frac{f^n - f^{n-1}}{\Delta t}$.

On the other hand, the fully discrete system in iterative form reads as follows: we solve the PNP/NS equation for $\{(c_h^+)^n, (c_h^-)^n, \phi^n\} \in Z_h \times Z_h \times \widehat{Z}_h$, $\{\mathbf{u}_h^n, p_h^n\} \in \mathbf{X}_h \times Y_h$ and $n = 1, \cdots, N$:

$$\begin{cases} \mathcal{M}_h(\delta_t(c_h^+)^n, z_1) + \mathcal{A}_{1h}((c_h^+)^n, z_1) + \mathcal{C}_h((c_h^+)^n; \phi_h^n, z_1) - \mathcal{D}_h(\mathbf{u}_h^n; (c_h^+)^n, z_1) = 0, \\ \mathcal{M}_h(\delta_t(c_h^-)^n, z_2) + \mathcal{A}_{2h}((c_h^-)^n, z_2) - \mathcal{C}_h((c_h^-)^n; \phi_h^n, z_2) - \mathcal{D}_h(\mathbf{u}_h^n; (c_h^-)^n, z_2) = 0, \\ \mathcal{A}_{3h}(\phi_h^n, z_3) = \mathcal{M}_h((c_h^+)^n, z_3) - \mathcal{M}_h((c_h^-)^n, z_3), \\ \boldsymbol{\mathcal{M}}_h(\delta_t \mathbf{u}_h^n, \mathbf{v}) + \boldsymbol{\mathcal{A}}_h(\mathbf{u}_h^n, \mathbf{v}) + \boldsymbol{\mathcal{C}}_h(\mathbf{u}_h^n; \mathbf{u}_h^n, \mathbf{v}) - \boldsymbol{\mathcal{B}}(p_h^n, \mathbf{v}) = -\left(((c_h^+)^n - (c_h^-)^n)\nabla\phi_h^n, \mathbf{v}\right)_h, \\ \boldsymbol{\mathcal{B}}(q, \mathbf{u}_h^n) = 0. \end{cases} \tag{2.22}$$

for all $\{z_1, z_2, z_3\} \in Z_h \times Z_h \times Z_h$ and $\{\mathbf{v}, q\} \in \mathbf{X}_h \times Y_h$, where $(c_h^+)^0 = c_{0,h}^+$, $(c_h^-)^0 = c_{0,h}^-$, $\mathbf{u}_h^0 = \mathbf{u}_{0,h}$.

Remark 2.1. *The last equation in (2.22) along with the property (2.3), implies that the discrete velocity $\boldsymbol{u}_h^n \in \boldsymbol{X}_k^h$ is exactly divergence-free. More generally, introducing the kernels:*

$$\widetilde{\boldsymbol{X}} = \{\boldsymbol{v} \in \boldsymbol{X} : \quad \boldsymbol{\mathcal{B}}(q, \boldsymbol{v}) = 0, \quad \forall q \in Y\}, \qquad \widetilde{\boldsymbol{X}}_h = \{\boldsymbol{v}_h \in \boldsymbol{X}_h : \quad \boldsymbol{\mathcal{B}}(q_h, \boldsymbol{v}_h) = 0, \quad \forall q_h \in Y_h\},$$

we can readily check that $\widetilde{\boldsymbol{X}}_h \subseteq \widetilde{\boldsymbol{X}}$. Therefore we can consider the following restricted problem, which is equivalent to the variational formulation (2.22): Find $\{(c_h^+)^n, (c_h^-)^n, \phi^n\} \in Z_h \times Z_h \times \widehat{Z}_h$, $\boldsymbol{u}_h^n \in \widetilde{\boldsymbol{X}}_h$ and $n = 1, \cdots, N$ such that

$$\begin{cases} \mathcal{M}_h(\delta_t(c_h^+)^n, z_1) + \mathcal{A}_{1h}((c_h^+)^n, z_1) + \mathcal{C}_h((c_h^+)^n; \phi_h^n, z_1) - \mathcal{D}_h(\boldsymbol{u}_h^n; (c_h^+)^n, z_1) = 0, \\ \mathcal{M}_h(\delta_t(c_h^-)^n, z_2) + \mathcal{A}_{2h}((c_h^-)^n, z_2) - \mathcal{C}_h((c_h^-)^n; \phi_h^n, z_2) - \mathcal{D}_h(\boldsymbol{u}_h^n; (c_h^-)^n, z_2) = 0, \\ \mathcal{A}_{3h}(\phi_h^n, z_3) = \mathcal{M}_h((c_h^+)^n, z_3) - \mathcal{M}_h((c_h^-)^n, z_3), \\ \boldsymbol{\mathcal{M}}_h(\delta_t \boldsymbol{u}_h^n, \boldsymbol{v}) + \boldsymbol{\mathcal{A}}_h(\boldsymbol{u}_h^n, \boldsymbol{v}) + \boldsymbol{\mathcal{C}}_h(\boldsymbol{u}_h^n; \boldsymbol{u}_h^n, \boldsymbol{v}) = -\left(((c_h^+)^n - (c_h^-)^n)\nabla\phi_h^n, \boldsymbol{v}\right)_h. \end{cases} \tag{2.23}$$

3. Discrete mass conservativon and discrete thermal energy decay

This section is devoted to investigate discrete mass conservative and discrete energy decaying properties of the proposed VE scheme (2.23).

Theorem 3.1. ***(Discrete mass conservative)***. *Let $\{((c_h^+)^n, (c_h^-)^n, \phi^n), \boldsymbol{u}_h^n\}_{n=1}^N$ be a solution of VE numerical scheme (2.23). Then the approximation concentrations satisfies*

$$\sum_{E\in\mathcal{T}_h}\int_E (c_h^+)^n \, dE = \sum_{E\in\mathcal{T}_h}\int_E (c_h^+)^0 \, dE, \qquad \sum_{E\in\mathcal{T}_h}\int_E (c_h^-)^n \, dE = \sum_{E\in\mathcal{T}_h}\int_E (c_h^-)^0 \, dE.$$

Proof. The proof is straightforward and obtained by choosing the test functions $(z_1, z_2, z_3) = (1, 1, 0)$. □

We now establish a discrete energy law of our VE numerical scheme, which represents that the total discrete energy is non-increasing regardless of the sizes of h, τ. Analogous to the total free energy [41], we define the discrete total energy:

$$E_h(\phi_h^n, \mathbf{u}_h^n) := \frac{1}{2}\big[\|\phi_h^n\|_Z^2 + \|\mathbf{u}_h^n\|_0^2\big].$$

Theorem 3.2. ***(Discrete energy law)***. *Let the assumption of Theorem 3.1 be satisfied. Then*

$$E_h(\phi_h^j, \boldsymbol{u}_h^j) + \tau\sum_{n=0}^{j}\big[\alpha_1\|(c_h^+)^n - (c_h^-)^n\|_0^2 + \boldsymbol{\alpha_1}\|\boldsymbol{u}_h^n\|_{\mathbf{X}}^2\big] + \frac{\tau}{2}\big[\beta_1\|\delta_t\phi_h^n\|_Z^2 + \boldsymbol{\alpha_1}\|\delta_t\boldsymbol{u}_h^n\|_0^2\big] \le E_h(\phi_h^0, \boldsymbol{u}_h^0). \tag{3.1}$$

Proof. Using test functions $(z_1, z_2, z_3) = (\tau\phi_h^n, \tau\phi_h^n, \tau(c_h^+)^n - \tau(c_h^-)^n)$ and $\mathbf{v} = \tau\mathbf{u}_h^n$ in (2.22) and (2.23) gives

$$\mathcal{M}_h(\delta_t(c_h^+)^n, \tau\phi_h^n) + \mathcal{A}_{1h}((c_h^+)^n, \tau\phi_h^n) + \mathcal{C}_h((c_h^+)^n; \phi_h^n, \tau\phi_h^n) - \mathcal{D}_h(\mathbf{u}_h^n; (c_h^+)^n, \tau\phi_h^n) = 0, \tag{3.2a}$$

$$\mathcal{M}_h(\delta_t(c_h^-)^n, \tau\phi_h^n) + \mathcal{A}_{2h}((c_h^-)^n, \tau\phi_h^n) - \mathcal{C}_h((c_h^-)^n; \phi_h^n, \tau\phi_h^n) - \mathcal{D}_h(\mathbf{u}_h^n; (c_h^-)^n, \tau\phi_h^n) = 0, \tag{3.2b}$$

$$\mathcal{A}_{3h}(\tau\phi_h^n, (c_h^+)^n - (c_h^-)^n) - \tau\mathcal{M}_h((c_h^+)^n - (c_h^-)^n, (c_h^+)^n - (c_h^-)^n) = 0, \tag{3.2c}$$

$$\boldsymbol{\mathcal{M}}_h(\delta_t\mathbf{u}_h^n, \tau\mathbf{u}_h^n) + \boldsymbol{\mathcal{A}}_h(\mathbf{u}_h^n, \tau\mathbf{u}_h^n) + \boldsymbol{\mathcal{C}}_h(\mathbf{u}_h^n; \mathbf{u}_h^n, \tau\mathbf{u}_h^n) + \big(((c_h^+)^n - (c_h^-)^n)\nabla\phi_h^n, \tau\mathbf{u}_h^n\big)_h = 0. \tag{3.2d}$$

Besides, we differentiate the third equation of (2.22) with respect to t,

$$\mathcal{A}_{3h}(\partial_t\phi_h^n, z_h) = \mathcal{M}_h(\partial_t(c_h^+)^n, z_h) - \mathcal{M}_h(\partial_t(c_h^-)^n, z_h), \qquad \forall z_h \in Z_h.$$

Using the backward Euler method to approximate the time derivative in the above equation yields

$$\mathcal{A}_{3h}(\delta_t\phi_h^n, z_h) = \mathcal{M}_h(\delta_t(c_h^+)^n, z_h) - \mathcal{M}_h(\delta_t(c_h^-)^n, z_h), \qquad \forall z_h \in Z_h,$$

then taking $z_h = \tau\phi_h^n$ gives

$$\mathcal{A}_{3h}(\delta_t\phi_h^n, \tau\phi_h^n) = \mathcal{M}_h(\delta_t(c_h^+)^n, \tau\phi_h^n) - \mathcal{M}_h(\delta_t(c_h^-)^n, \tau\phi_h^n). \tag{3.3}$$

Combining (3.2a)-(3.2c) and (3.3) and using the identity

$$\begin{aligned}\mathcal{A}_{3h}(\delta_t\phi_h^n, \tau\phi_h^n) &= \mathcal{A}_{3h}(\phi_h^n - \phi_h^{n-1}, \phi_h^n) = \frac{1}{2}\mathcal{A}_{3h}(\phi_h^n - \phi_h^{n-1}, (\phi_h^n - \phi_h^{n-1}) + (\phi_h^n + \phi_h^{n-1}))\\ &= \frac{\tau^2}{2}\mathcal{A}_{3h}(\delta_t\phi_h^n, \delta_t\phi_h^n) + \frac{\tau}{2}\delta_t\mathcal{A}_{3h}(\phi_h^n, \phi_h^n),\end{aligned} \tag{3.4}$$

we readily conclude that

$$\frac{\tau^2}{2}\mathcal{A}_{3h}(\delta_t\phi_h^n, \delta_t\phi_h^n) + \frac{\tau}{2}\delta_t\mathcal{A}_{3h}(\phi_h^n, \phi_h^n) = -\tau\mathcal{M}_h((c_h^+)^n - (c_h^-)^n, (c_h^+)^n - (c_h^-)^n) - \mathcal{C}_h((c_h^+)^n - (c_h^-)^n; \phi_h^n, \tau\phi_h^n)$$

$$+ \mathcal{D}_h(\mathbf{u}_h^n; (c_h^+)^n - (c_h^-)^n, \tau\phi_h^n).$$

Also applying fact $\boldsymbol{\mathcal{C}}_h(\mathbf{u}_h^n; \mathbf{u}_h^n, \tau\mathbf{u}_h^n) = 0$ and its analogous identity (3.4) in (3.2d), we obtain

$$\frac{\tau^2}{2}\boldsymbol{\mathcal{M}}_h(\delta_t\mathbf{u}_h^n, \delta_t\mathbf{u}_h^n) + \frac{\tau}{2}\delta_t\boldsymbol{\mathcal{M}}_{3h}(\mathbf{u}_h^n, \mathbf{u}_h^n) + \tau\boldsymbol{\mathcal{A}}_h(\mathbf{u}_h^n, \mathbf{u}_h^n) = -\tau\left(((c_h^+)^n - (c_h^-)^n)\nabla\phi_h^n, \mathbf{u}_h^n\right)_h.$$

Summing the two obtained inequalities and employing Lemma 2.1, gives

$$\frac{\tau^2}{2}\left[\beta_{1,3}\|\delta_t\phi_h^n\|_Z^2 + \boldsymbol{\alpha_1}\|\delta_t\mathbf{u}_h^n\|_0^2\right] + \frac{\tau}{2}\left[\beta_{1,3}\delta_t\|\phi_h^n\|_Z^2 + \boldsymbol{\alpha_1}\delta_t\|\mathbf{u}_h^n\|_0^2\right] + \tau\alpha_1\|(c_h^+)^n - (c_h^-)^n\|_0^2$$
$$+ \tau\boldsymbol{\alpha_1}\|\mathbf{u}_h^n\|_{\mathbf{X}}^2 + \|((c_h^+)^n + (c_h^-)^n)^{1/2}\phi_h^n\|_0^2 \le 0.$$

And summing up the above inequality from $n = 0$ to $n = j$ for all $j \ge 0$, leads to (3.1). □

Corollary 1. *Suppose the conditions of Theorem 3.1 hold. Under the assumption $E_h(\phi_h^0, \boldsymbol{u}_h^0) < \infty$, we can obtain the following estimates, some positive constants $C_{\boldsymbol{u}}, C_\phi, C_c$ independent of h and τ*

$$\|\mathbf{u}_h^n\|_0 + \tau\left(\boldsymbol{\alpha_1}\sum_{n=0}^{j}\|\boldsymbol{u}_h^n\|_{\boldsymbol{X}}^2\right)^{1/2} \le C_{\boldsymbol{u}}, \qquad \|\phi_h^n\|_Z \le C_\phi, \qquad \|(c_h^+)^n - (c_h^-)^n\|_0 \le C_c.$$

4. Well-posedness analysis

The following lemma demonstrates the well-posedness of the fully-discrete scheme (2.23).

Lemma 4.1. *Assume that τ, $C_{\boldsymbol{u}}$ and C_ϕ satisfy $\tau \le h$, $C_{\boldsymbol{u}} + C_\phi \le \frac{\alpha_1}{2}$. Then (2.23) is well-posed for all $n = 0, \cdots, N$, that is, there exists an unique solution $\{((c_h^+)^n, (c_h^-)^n, \phi_h^n), \boldsymbol{u}_h^n\} \in (Z_h \times Z_h \times \widehat{Z}_h) \times \widetilde{\boldsymbol{X}}_h$ to problem (2.23).*

Proof. The proof proceeds with Brouwer's fixed point Theorem. To this end, we will split the proof into 3 steps. First, let $\mathcal{L}$ be a continuous mapping of $\mathcal{K}$ into itself,

$$\mathcal{L} : ((\rho_h, \zeta_h, \xi_h), \mathbf{w}_h) \mapsto \mathcal{L}((\rho_h, \zeta_h, \xi_h), \mathbf{w}_h) = \left(\left((c_h^+)^n, (c_h^-)^n, \phi_h^n\right), \mathbf{u}_h^n\right), \tag{4.1}$$

where the non-empty compact convex set $\mathcal{K}$ is defined as follows:

$$\mathcal{K} := \left\{((z_{1h}, z_{2h}, z_{3h}), \mathbf{v}_h) \in (Z_k^h \times Z_k^h \times \widehat{Z}_k^h) \times \widetilde{\mathbf{X}}_h; \quad \|\mathbf{v}_h\|_0 \le C_{\mathbf{u}}, \quad \|z_{3h}\|_Z \le C_\phi, \quad \|z_{h1} - z_{2h}\|_0 \le C_c\right\},$$

and $\left(\left((c_h^+)^n, (c_h^-)^n, \phi_h^n\right), \mathbf{u}_h^n\right)$ is the solution for the following linearized version of problem (2.23):

$$\begin{cases} \mathcal{M}_h(\delta_t(c_h^+)^n, z_1) + \mathcal{A}_{1h}((c_h^+)^n, z_1) + \mathcal{C}_h((c_h^+)^n; \xi_h, z_1) - \mathcal{D}_h(\mathbf{w}_h; (c_h^+)^n, z_1) = 0, \\ \mathcal{M}_h(\delta_t(c_h^-)^n, z_2) + \mathcal{A}_{2h}((c_h^-)^n, z_2) - \mathcal{C}_h((c_h^-)^n; \xi_h, z_2) - \mathcal{D}_h(\mathbf{w}_h; (c_h^-)^n, z_2) = 0, \\ \mathcal{A}_{3h}(\phi_h^n, z_3) = \mathcal{M}_h((c_h^+)^n, z_3) - \mathcal{M}_h((c_h^-)^n, z_3), \\ \boldsymbol{\mathcal{M}}_h(\delta_t\mathbf{u}_h^n, \mathbf{v}) + \boldsymbol{\mathcal{A}}_h(\mathbf{u}_h^n, \mathbf{v}) + \boldsymbol{\mathcal{C}}_h(\mathbf{w}_h; \mathbf{u}_h^n, \mathbf{v}) = -((\rho_h - \zeta_h)\nabla\phi_h^n, \mathbf{v})_h. \end{cases} \tag{4.2}$$

Step1: $\mathcal{L}$ is well-defined. Regarding (4.2), we firstly rewrite it as

$$\begin{cases} \mathcal{M}_h((c_h^+)^n, z_1) + \tau\mathcal{A}_{1h}((c_h^+)^n, z_1) + \tau\mathcal{C}_h((c_h^+)^n; \xi_h, z_1) - \tau\mathcal{D}_h(\mathbf{w}_h; (c_h^+)^n, z_1) = \mathcal{M}_h((c_h^+)^{n-1}, z_1), \\ \mathcal{M}_h((c_h^-)^n, z_2) + \tau\mathcal{A}_{2h}((c_h^-)^n, z_2) - \tau\mathcal{C}_h((c_h^-)^n; \xi_h, z_2) - \tau\mathcal{D}_h(\mathbf{w}_h; (c_h^-)^n, z_2) = \mathcal{M}_h((c_h^-)^{n-1}, z_2), \\ \mathcal{A}_{3h}(\phi_h^n, z_3) = \mathcal{M}_h((c_h^+)^n, z_3) - \mathcal{M}_h((c_h^-)^n, z_3), \\ \boldsymbol{\mathcal{M}}_h(\mathbf{u}_h^n, \mathbf{v}) + \tau\boldsymbol{\mathcal{A}}_h(\mathbf{u}_h^n, \mathbf{v}) + \tau\boldsymbol{\mathcal{C}}_h(\mathbf{w}_h; \mathbf{u}_h^n, \mathbf{v}) = \boldsymbol{\mathcal{M}}_h(\mathbf{u}_h^{n-1}, \mathbf{v}) - \tau((\rho_h - \zeta_h)\nabla\phi_h^n, \mathbf{v})_h. \end{cases}$$

It can be seen that all terms in the above relation are continuous. More precisely, Lemmas 2.1 and 2.2 confirm the continuity of the discrete forms $\mathcal{M}_h$, $\mathcal{A}_h$, $\boldsymbol{\mathcal{M}}_h$, $\boldsymbol{\mathcal{A}}_h$ and $\mathcal{D}_h$, $\boldsymbol{\mathcal{C}}_h$, $((\rho_h-\zeta_h)\nabla\phi_h^n,\mathbf{v})_h$, respectively, whereas for the term involving $\mathcal{C}_h$ we have the estimate

$$\begin{aligned}\mathcal{C}_h^E((c_h^\pm)^n;\phi_h^n,z_i) &= \left(\Pi_{k-1}^{0,E}(c_h^\pm)^n\mathbf{\Pi}_{k-1}^{0,E}\nabla\phi_h^n,\mathbf{\Pi}_{k-1}^{0,E}\nabla z_i\right)_{0,E} + |\Pi_0^{0,E}\phi_h^n|S^E\left((I-\Pi_k^{\nabla,E})(c_h^\pm)^n,(I-\Pi_k^{\nabla,E})z_i\right)\\ &\le \|\mathbf{\Pi}_{k-1}^{0,E}\nabla\phi_h^n\|_\infty\|\Pi_{k-1}^{0,E}(c_h^\pm)^n\|_{0,E}\|\mathbf{\Pi}_{k-1}^{0,E}\nabla z_i\|_{0,E} + \|\Pi_0^{0,E}\phi_h^n\|_\infty\|(c_h^\pm)^n\|_1\|z_i\|_{1,E}.\end{aligned}$$

Applying the inverse estimate and the continuity of the projector $\mathbf{\Pi}_{k-1}^0$, allows us to assert that

$$\|\mathbf{\Pi}_{k-1}^{0,E}\nabla\phi_h^n\|_{\infty,E}\le h_E^{-1}\|\mathbf{\Pi}_{k-1}^{0,E}\nabla\phi_h^n\|_{0,E}\le h_E^{-1}\|\nabla\phi_h^n\|_{0,E}, \tag{4.3}$$

which, together with $\tau\le h$, implies

$$\tau\mathcal{C}_h^E((c_h^\pm)^n;\phi_h^n,z_i)\le C_\phi\|(c_h^\pm)^n\|_Z\|z_i\|_Z,$$

where Poincaré's inequality and Corollary 1 have been employed. Therefore, according to the Lax–Milgram lemma and the coercivity bound (2.9), problem (4.2) is uniquely solvable, and hence $\mathcal{L}$ is well defined.
Step 2: $\mathcal{L}(\mathcal{K})\subset\mathcal{K}$. To that end, let $((z_{1h},z_{2h},z_{3h}),\mathbf{v}_h)\in\mathcal{K}$ be given, and denote by $\left(\left((c_h^+)^n,(c_h^-)^n,\phi_h^n\right),\mathbf{u}_h^n\right)\in(Z_k^h\times Z_k^h\times\widehat{Z}_k^h)\times\widetilde{\mathbf{X}}_h$ the solution for problem (4.2). We consider the test function as $((z_{1h},z_{2h},z_{3h}),\mathbf{v}_h)=((\phi_h^n,\phi_h^n,(c_h^+)^n-(c_h^-)^n),\mathbf{u}_h^n)$ in Eq. (4.2), from the proof of Theorem 3.2 for $j\ge 0$ we have

$$E_h(\phi_h^n,\mathbf{u}_h^n)+\tau\sum_{n=0}^{j}\left[\alpha_1\|(c_h^+)^n-(c_h^-)^n\|_0^2+\boldsymbol{\alpha_1}\|\mathbf{u}_h^n\|_1^2\right]+\frac{\tau}{2}\left[\beta_1\|\delta_t\phi_h^n\|_1^2+\boldsymbol{\alpha_1}\|\delta_t\mathbf{u}_h^n\|_0^2\right]\le E_h(\phi_h^0,\mathbf{u}_h^0).$$

Using the hypothesis $E_h(\phi_h^0,\mathbf{u}_h^0)<\infty$, we can get

$$\|\mathbf{u}_h^n\|_0\le C_{\mathbf{u}},\quad \|\phi_h^n\|_1\le C_\phi,\quad \|(c_h^+)^n-(c_h^-)^n\|_0\le C_c,$$

with

$$C_u=\left(\frac{E_h(\phi_h^0,\mathbf{u}_h^0)}{2\boldsymbol{\alpha_1}}\right)^{1/2},\quad C_\phi=\left(\frac{E_h(\phi_h^0,\mathbf{u}_h^0)}{2\beta_1}\right)^{1/2},\quad C_c=\frac{\beta_2}{\alpha_1}\left(\frac{E_h(\phi_h^0,\mathbf{u}_h^0)}{2\beta_1}\right)^{1/2}.$$

Hence, we have $\left(\left((c_h^+)^n,(c_h^-)^n,\phi_h^n\right),\mathbf{u}_h^n\right)\in\mathcal{K}$.
Step 3: $\mathcal{L}$ is continuous. Let $\{((\rho_m,\zeta_m,\xi_m),\mathbf{w}_m)\}_{m\in\mathbb{N}}\subset\mathcal{K}$ be a sequence converging to $((\rho,\zeta,\xi),\mathbf{w})\subset\mathcal{K}$, that is

$$\|\mathbf{w}_m-\mathbf{w}\|_0\to 0,\quad \|\xi_m-\xi\|_1\to 0,\quad \|\rho_m-\rho\|_0\to 0,\quad \|\zeta_m-\zeta\|_0\to 0. \tag{4.4}$$

Let $(((c_m^+)^n,(c_m^-)^n,\phi_m^n),\mathbf{u}_m^n)$ and $(((c^+)^n,(c^-)^n,\phi^n),\mathbf{u}^n)$ be given by

$$\left(\left((c_m^+)^n,(c_m^-)^n,\phi_m^n\right),\mathbf{u}_m^n\right)=\mathcal{L}\left((\rho_m,\zeta_m,\xi_m),\mathbf{w}_m\right),\qquad \left(\left((c^+)^n,(c^-)^n,\phi^n\right),\mathbf{u}^n\right)=\mathcal{L}\left((\rho,\zeta,\xi),\mathbf{w}\right).$$

Under the following assumption

$$\left\|\mathbf{u}_m^0-\mathbf{u}^0\right\|_0\to 0,\quad \left\|\phi_m^0-\phi^0\right\|_1\to 0,\quad \left\|(c_m^+)^0-(c^+)^0\right\|_0\to 0,\quad \left\|(c_m^-)^0-(c^-)^0\right\|_0\to 0, \tag{4.5}$$

we prove that

$$\|\mathbf{u}_m^n-\mathbf{u}^n\|_0\to 0,\quad \|\phi_m^n-\phi^n\|_1\to 0,\quad \left\|(c_m^+)^n-(c^+)^n\right\|_0\to 0,\quad \left\|(c_m^-)^n-(c^-)^n\right\|_0\to 0.$$

From the definition of $\mathcal{L}$ stated in (4.1), we observe that there hold

$$\mathcal{M}_h(\delta_t(c_m^+)^n, z_1) + \mathcal{A}_{1h}((c_m^+)^n, z_1) + \mathcal{C}_h((c_m^+)^n; \xi_m, z_1) - \mathcal{D}_h(\mathbf{w}_m; (c_m^+)^n, z_1) = 0, \tag{4.6a}$$

$$\mathcal{M}_h(\delta_t(c_m^-)^n, z_2) + \mathcal{A}_{2h}((c_m^-)^n, z_2) - \mathcal{C}_h((c_m^-)^n; \xi_m, z_2) - \mathcal{D}_h(\mathbf{w}_m; (c_m^-)^n, z_2) = 0, \tag{4.6b}$$

$$\mathcal{A}_{3h}(\phi_m^n, z_3) - \mathcal{M}_h((c_m^+)^n, z_3) + \mathcal{M}_h((c_m^-)^n, z_3) = 0, \tag{4.6c}$$

$$\boldsymbol{\mathcal{M}}_h(\delta_t \mathbf{u}_m^n, \mathbf{v}) + \boldsymbol{\mathcal{A}}_h(\mathbf{u}_m^n, \mathbf{v}) + \boldsymbol{\mathcal{C}}_h(\mathbf{w}_m; \mathbf{u}_m^n, \mathbf{v}) + ((\rho_m - \zeta_m)\nabla\phi_m^n, \mathbf{v})_h = 0. \tag{4.6d}$$

and

$$\mathcal{M}_h(\delta_t(c^+)^n, z_1) + \mathcal{A}_{1h}((c^+)^n, z_1) + \mathcal{C}_h((c^+)^n; \xi, z_1) - \mathcal{D}_h(\mathbf{w}; (c^+)^n, z_1) = 0, \tag{4.7a}$$

$$\mathcal{M}_h(\delta_t(c^-)^n, z_2) + \mathcal{A}_{2h}((c^-)^n, z_2) - \mathcal{C}_h((c^-)^n; \xi, z_2) - \mathcal{D}_h(\mathbf{w}; (c^-)^n, z_2) = 0, \tag{4.7b}$$

$$\mathcal{A}_{3h}(\phi^n, z_3) - \mathcal{M}_h((c^+)^n, z_3) + \mathcal{M}_h((c^-)^n, z_3) = 0, \tag{4.7c}$$

$$\boldsymbol{\mathcal{M}}_h(\delta_t \mathbf{u}^n, \mathbf{v}) + \boldsymbol{\mathcal{A}}_h(\mathbf{u}^n, \mathbf{v}) + \boldsymbol{\mathcal{C}}_h(\mathbf{w}; \mathbf{u}^n, \mathbf{v}) + ((\rho - \zeta)\nabla\phi^n, \mathbf{v})_h = 0, \tag{4.7d}$$

for all $((z_1, z_2, z_3), \mathbf{v}) \in (Z_h \times Z_h \times \widehat{Z}_h) \times \widetilde{\mathbf{X}}_h$. Then, subtracting Eqs. (4.6a)-(4.6d) from Eqs. (4.7a)-(4.7a), respectively, gives

$$\begin{aligned}\mathcal{M}_h(\delta_t((c_m^+)^n - (c^+)^n), z_1) + \mathcal{A}_{1h}((c_m^+)^n - (c^+)^n, z_1) + \big[\mathcal{C}_h((c_m^+)^n; \xi_m, z_1) - \mathcal{C}_h((c^+)^n; \xi, z_1)\big]& \\ -\big[\mathcal{D}_h(\mathbf{w}_m; (c_m^+)^n, z_1) - \mathcal{D}_h(\mathbf{w}; (c^+)^n, z_1)\big] = 0,& \end{aligned} \tag{4.8a}$$

$$\begin{aligned}\mathcal{M}_h(\delta_t((c_m^-)^n - (c^-)^n), z_2) + \mathcal{A}_{2h}((c_m^-)^n - (c^-)^n, z_2) - \big[\mathcal{C}_h((c_m^-)^n; \xi_m, z_2) - \mathcal{C}_h((c^-)^n; \xi, z_2)\big]& \\ -\big[\mathcal{D}_h(\mathbf{w}_m; (c_m^-)^n, z_2) - \mathcal{D}_h(\mathbf{w}; (c^-)^n, z_2)\big] = 0,& \end{aligned} \tag{4.8b}$$

$$\mathcal{A}_{3h}(\phi_m^n - \phi^n, z_3) - \mathcal{M}_h((c_m^+)^n - (c^+)^n, z_3) + \mathcal{M}_h((c_m^-)^n - (c^-)^n, z_3) = 0, \tag{4.8c}$$

$$\begin{aligned}\boldsymbol{\mathcal{M}}_h(\delta_t(\mathbf{u}_m^n - \mathbf{u}^n), \mathbf{v}) + \boldsymbol{\mathcal{A}}_h(\mathbf{u}_m^n - \mathbf{u}^n, \mathbf{v}) + \big[\boldsymbol{\mathcal{C}}_h(\mathbf{w}_m; \mathbf{u}_m^n, \mathbf{v}) - \boldsymbol{\mathcal{C}}_h(\mathbf{w}; \mathbf{u}^n, \mathbf{v})\big] =& \\ -\big[\, ((\rho_m - \zeta_m)\nabla\phi_m^n, \mathbf{v})_h - ((\rho - \zeta)\nabla\phi^n, \mathbf{v})_h \,\big].& \end{aligned} \tag{4.8d}$$

We first consider Eqs. (4.8a)-(4.8b). Adding zero in the forms $\pm\mathcal{C}_h((c^+)^n; \xi_m, z_1)$, $\pm\mathcal{D}_h(\mathbf{w}; (c_m^+)^n, z_1)$ and $\pm\mathcal{C}_h((c^-)^n; \xi_m, z_1)$, $\pm\mathcal{D}_h(\mathbf{w}; (c_m^-)^n, z_1)$ to the left-hand side of Eqs. (4.8a) and (4.8b), respectively, gives

$$\begin{aligned}\mathcal{M}_h(\delta_t((c_m^+)^n - (c^+)^n), z_1) + \mathcal{A}_{1h}((c_m^+)^n - (c^+)^n, z_1) = -\big[\mathcal{C}_h((c_m^+)^n - (c^+)^n; \xi_m, z_1) + \mathcal{C}_h((c^+)^n; \xi_m - \xi, z_1)\big]& \\ + \big[\mathcal{D}_h(\mathbf{w}_m - \mathbf{w}; (c_m^+)^n, z_1) + \mathcal{D}_h(\mathbf{w}; (c_m^+)^n - (c^+)^n, z_1)\big],& \end{aligned} \tag{4.9}$$

and

$$\begin{aligned}\mathcal{M}_h(\delta_t((c_m^-)^n - (c^-)^n), z_2) + \mathcal{A}_{1h}((c_m^-)^n - (c^-)^n, z_2) = \big[\mathcal{C}_h((c_m^-)^n - (c^-)^n; \xi_m, z_2) + \mathcal{C}_h((c^-)^n; \xi_m - \xi, z_2)\big]& \\ + \big[\mathcal{D}_h(\mathbf{w}_m - \mathbf{w}; (c_m^-)^n, z_2) + \mathcal{D}_h(\mathbf{w}; (c_m^-)^n - (c^-)^n, z_2)\big].& \end{aligned} \tag{4.10}$$

Using the inverse estimate, the continuity of Π_k^0 and Π_k^∇ with respect to the L^2 and L^∞-norms (cf. (4.3)), the terms on the right-hand side of Eqs. (4.9) and (4.10), we can derive the following estimates

$$\begin{aligned}\mathcal{C}_h((c_m^*)^n - (c^*)^n; \xi_m, z_i) &\leq \|\Pi_k^\nabla \nabla\xi_m\|_\infty \|\Pi_k^0((c_m^*)^n - (c^*)^n)\|_0 \|\Pi_k^\nabla \nabla z_i\|_0 \\ &\leq \|\xi_m\|_{1,\infty} \|(c_m^*)^n - (c^*)^n\|_0 \|z_i\|_1 \leq h^{-1} C_\phi \|(c_m^*)^n - (c^*)^n\|_0 \|z_i\|_1, \ * = +, -, \ i = 1, 2,\end{aligned} \tag{4.11}$$

$$\mathcal{C}_h((c^*)^n; \xi_m - \xi, z_i) \leq \|\Pi_k^0 (c^*)^n\|_\infty \|\Pi_k^\nabla \nabla(\xi_m - \xi)\|_0 \|\Pi_k^\nabla \nabla z_i\|_0$$

$$\leq \|(c^*)^n\|_\infty \|\xi_m - \xi\|_1 \|z_i\|_1 \leq h^{-1} C_c \|\xi_m - \xi\|_1 \|z_i\|_1, \; * = +, -, \; i = 1, 2, \tag{4.12}$$

$$\mathcal{D}_h(\mathbf{w}_m - \mathbf{w}; (c^*_m)^n, z_i) \leq \|\boldsymbol{\Pi}^0_k(\mathbf{w}_m - \mathbf{w})\|_0 \|\Pi^0_k (c^*_m)^n\|_\infty \|\Pi^\nabla_k \nabla z_i\|_0 \leq h^{-1} C_c \|\mathbf{w}_m - \mathbf{w}\|_0 \|z_i\|_1, \tag{4.13}$$

$$\mathcal{D}_h(\mathbf{w}; (c^*_m)^n - (c^*)^n, z_i) \leq h^{-1} C_{\mathbf{u}} \|(c^*_m)^n - (c^*)^n\|_0 \|z_i\|_1, \; * = +, -, \; i = 1, 2. \tag{4.14}$$

Then, inserting estimates (4.11)-(4.14) into Eqs. (4.9) and (4.10), taking as test functions $z_1 = (c^+_m)^n - (c^+)^n$ and $z_2 = (c^-_m)^n - (c^-)^n$, and applying Lemma 2.1 and assumptions $\tau \leq h$ and (4.4), yields

$$\begin{aligned}
\frac{\alpha_1}{2} \left[\|(c^+_m)^n - (c^+)^n\|_0^2 - \|(c^+_m)^{n-1} - (c^+)^{n-1}\|_0^2 \right] + \tau \beta_1 \|(c^+_m)^n - (c^+)^n\|_1^2 \\
&\leq \Big((C_\phi + C_{\mathbf{u}}) \|(c^*_m)^n - (c^*)^n\|_0 + C_c (\|\xi_m - \xi\|_1 + \|\mathbf{w}_m - \mathbf{w}\|_0) \Big) \|(c^+_m)^n - (c^+)^n\|_1 \\
&\leq (C_\phi + C_{\mathbf{u}}) \|(c^*_m)^n - (c^*)^n\|_0 \|(c^+_m)^n - (c^+)^n\|_1,
\end{aligned}$$

which using assumption $\frac{C_\phi + C_{\mathbf{u}}}{\alpha_1} \leq \frac{1}{2}$ and summing up on n, leads us to

$$\|(c^*_m)^n - (c^*)^n\|_0 \leq \|(c^*_m)^0 - (c^*)^0\|_0, \quad * = +, -,$$

which together with (4.5), yields

$$\lim_{m \to \infty} \|(c^*_m)^n - (c^*)^n\|_0 = 0, \quad * = +, -. \tag{4.15}$$

Regarding Eq. (4.8c), we note that letting $z_3 = \phi^n_m - \phi^n$ yields

$$\mathcal{A}_h(\phi^n_m - \phi^n, \phi^n_m - \phi^n) = \mathcal{M}_h((c^+_m)^n - (c^+)^n, \phi^n_m - \phi^n) + \mathcal{M}_h((c^-_m)^n - (c^-)^n, \phi^n_m - \phi^n).$$

An application of Lemma 2.1, Poincaré inequality and Eq. (4.15) implies that

$$\lim_{m \to \infty} \|\phi^n_m - \phi^n\|_1 = 0. \tag{4.16}$$

With respect to (4.8d), we add and subtract the terms $\boldsymbol{\mathcal{C}}_h(\mathbf{w}_m; \mathbf{u}, \mathbf{v})$ and $((\rho_m - \zeta_m)\nabla\phi^n, \mathbf{v})_h$, to obtain

$$\begin{aligned}
&\boldsymbol{\mathcal{M}}_h(\delta_t(\mathbf{u}^n_m - \mathbf{u}^n), \mathbf{v}) + \boldsymbol{\mathcal{A}}_h(\mathbf{u}^n_m - \mathbf{u}^n, \mathbf{v}) + \boldsymbol{\mathcal{C}}_h(\mathbf{w}_m; \mathbf{u}^n_m - \mathbf{u}^n, \mathbf{v}) = \\
&\quad - \boldsymbol{\mathcal{C}}_h(\mathbf{w}_m - \mathbf{w}; \mathbf{u}^n, \mathbf{v}) - \left[((\rho_m - \zeta_m)(\nabla\phi^n_m - \nabla\phi^n), \mathbf{v})_h - ((\rho - \rho_m + \zeta_m - \zeta)\nabla\phi^n, \mathbf{v})_h \right].
\end{aligned}$$

Letting $\mathbf{v} = \mathbf{u}^n_m - \mathbf{u}^n$ in the above equation and invoking Lemmas 2.1 and 2.2, we readily get

$$\begin{aligned}
\frac{\boldsymbol{\alpha}_1 \tau}{2} \delta_t \|\mathbf{u}^n_m - \mathbf{u}^n\|_0^2 + \boldsymbol{\beta}_1 \|\mathbf{u}^n_m - \mathbf{u}^n\|_1^2 &\leq \Big(\widehat{C}_{2h} \|\mathbf{w}_m - \mathbf{w}\|_0 \|\mathbf{u}^n\|_0 + h^{-1} \|\rho_m - \zeta_m\|_0 \|\phi^n_m - \phi^n\|_1 \\
&\quad + h^{-1} \|\phi^n\|_1 \left(\|\rho - \rho_m\|_0 + \|\zeta_m - \zeta\|_0 \right) \Big) \|\mathbf{u}^n_m - \mathbf{u}^n\|_0,
\end{aligned}$$

which together with (4.4), fact $\boldsymbol{\beta}_1 \|\mathbf{u}^n_m - \mathbf{u}^n\|_1^2 \geq 0$ and assumption $\tau \leq h$, yields

$$\left[\|\mathbf{u}^n_m - \mathbf{u}^n\|_0^2 - \|\mathbf{u}^{n-1}_m - \mathbf{u}^{n-1}\|_0^2 \right] \leq 2\boldsymbol{\alpha}_1^{-1} C_c \|\phi^n_m - \phi^n\|_1 \|\mathbf{u}^n_m - \mathbf{u}^n\|_0 \leq C_\epsilon \|\phi^n_m - \phi^n\|_1^2 + \epsilon \|\mathbf{u}^n_m - \mathbf{u}^n\|_0^2,$$

where ϵ is a sufficiently small positive constant satisfying $\epsilon \leq 1$. Summing up the above inequality from $n = 0$ to $n = j$ for all $j \geq 0$, gives

$$\|\mathbf{u}^n_m - \mathbf{u}^n\|_0 \leq \|\mathbf{u}^0_m - \mathbf{u}^0\|_0 + \left(\sum_{n=0}^{j} \|\phi^n_m - \phi^n\|_1^2 \right)^{1/2},$$

which, alongside (4.16), completes the proof. □

5. Convergence analysis

We split the error analysis in two steps. First one estimates the velocity and pressure discretization errors, $\|\mathbf{u}^n - \mathbf{u}_h^n\|_0$ and $\|p^n - p_h^n\|_0$, respectively; and the second stage corresponds to establishing bounds for the concentrations error $\|(c^+)^n - (c_h^+)^n\|_0$, $\|(c^-)^n - (c_h^-)^n\|_0$ and electrostatic potential error $\|\phi^n - \phi_h^n\|_0$.

5.1. Error bounds: velocity and pressure

We consider the following problem:

$$\boldsymbol{\mathcal{M}}_h(\delta_t \mathbf{u}_h^n, \mathbf{v}) + \boldsymbol{\mathcal{A}}_h(\mathbf{u}_h^n, \mathbf{v}) + \boldsymbol{\mathcal{C}}_h(\mathbf{u}_h^n; \mathbf{u}_h^n, \mathbf{v}) = -\left(((c_h^+)^n - (c_h^-)^n)\nabla\phi_h^n, \mathbf{v}\right)_h, \quad \forall \mathbf{v} \in \widetilde{\mathbf{X}}_h, \tag{5.1}$$

where $\{(c_h^+)^n, (c_h^-)^n, \phi_h^n\}$ is an approximate solution of the PNP system (2.22) and $\mathbf{u}_h^0 = \mathbf{u}_{h,0}$ with $n = 1, \cdots, N$. The aim is to obtain an error bound for $\|\mathbf{u}^n - \mathbf{u}_h^n\|_0$ and $\|p^n - p_h^n\|_0$ dependent on $\|(c^+)^n - (c_h^+)^n\|_0$, $\|(c^-)^n - (c_h^-)^n\|_0$ and $\|\phi^n - \phi_h^n\|_0$.

Theorem 5.1. *Given $\{(c_h^+)^n, (c_h^-)^n, \phi_h^n\} \in Z_h \times Z_h \times \widehat{Z}_h$, let $\boldsymbol{u}_h^n \in \widetilde{\boldsymbol{X}}_h$ be the solution to (5.1) and $\{(c^+)^n, (c^-)^n, \phi^n\}$, $\{\boldsymbol{u}^n, p^n\}$ be the solution of (1.1) satisfying the following regularity conditions*

$$\left\|\frac{\partial \boldsymbol{u}^n}{\partial t}\right\|_{L^\infty(H^{k+1})} + \|\boldsymbol{u}^n\|_{L^\infty(H^{k+1})} + \left\|\frac{\partial^2 \boldsymbol{u}}{\partial t^2}\right\|_{L^2(L^2)} + \left\|\frac{\partial \boldsymbol{u}}{\partial t}\right\|_{L^2\left(H^{k+1}\right)} + \left(\|\boldsymbol{u}^n\|_k + \|\boldsymbol{u}^n\|_1 + \|\boldsymbol{u}^n\|_{k+1} + \|\boldsymbol{u}_h^n\|_1 + 1\right)\|\boldsymbol{u}^n\|_{k+1} \le C,$$

$$(\|(c^+)^n\|_1 + \|(c^-)^n\|_1)(\|\phi^n\|_2 + \|\phi^n\|_{s+1}) + (\|(c^+)^n\|_{k+1} + \|(c^-)^n\|_{k+1})\|\phi^n\|_1 \le C.$$

Then, for all $k \in \mathbb{N}_0$, the following estimate holds

$$\|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_0^2 + 2\tau\boldsymbol{\beta}_1 \sum_{j=1}^n |\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^j|_1^2 \le C(\tau^2 + h^{2k}) + C\tau \sum_{j=1}^n \left[\|(c^+)^j - (c_h^+)^j\|_1^2 + \|(c^-)^j - (c_h^-)^j\|_1^2 + \|\phi^j - \phi_h^j\|_1^2\right].$$

Proof. The proof is conducted in three steps:

Step 1: evolution equation for the error. Setting $\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n := \mathbf{u}_h^n - \mathbf{u}_I^n$, it holds that $\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n \in \widetilde{\mathbf{X}}_h$. Using Eq. (5.1) and the fourth equation in (1.1) and letting $\mathbf{v} = \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n$, yields

$$\begin{aligned}
&\boldsymbol{\mathcal{M}}_h\Big(\frac{\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n - \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^{n-1}}{\tau}, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\Big) + \boldsymbol{\mathcal{A}}_h(\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n) \\
&= \left[\boldsymbol{\mathcal{M}}_h(\delta_t \mathbf{u}_h^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n) + \boldsymbol{\mathcal{A}}_h(\mathbf{u}_h^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n)\right] - \left[\boldsymbol{\mathcal{M}}_h(\delta_t \mathbf{u}_I^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n) + \boldsymbol{\mathcal{A}}_h(\mathbf{u}_I^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n)\right] \\
&= \boldsymbol{\mathcal{M}}_h(\delta_t(\mathbf{u}^n - \mathbf{u}_I^n), \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n) + \left[\boldsymbol{\mathcal{M}}\Big(\frac{\partial \mathbf{u}^n}{\partial t}, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\Big) - \boldsymbol{\mathcal{M}}_h(\delta_t \mathbf{u}^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n)\right] + \boldsymbol{\mathcal{A}}_h(\mathbf{u}^n - \mathbf{u}_I^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n) \\
&\quad + \left[\boldsymbol{\mathcal{A}}(\mathbf{u}^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n) - \boldsymbol{\mathcal{A}}_h(\mathbf{u}^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n)\right] + \left[\boldsymbol{\mathcal{C}}(\mathbf{u}^n; \mathbf{u}^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n) - \boldsymbol{\mathcal{C}}_h(\mathbf{u}_h^n; \mathbf{u}_h^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n)\right] \\
&\quad + \left[\left(((c^+)^n - (c^-)^n)\nabla\phi^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\right) - \left(((c_h^+)^n - (c_h^-)^n)\nabla\phi_h^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\right)_h\right] \\
&:= \mathbf{R}_1 + \mathbf{R}_2 + \mathbf{R}_3 + \mathbf{R}_4 + \mathbf{R}_5 + \mathbf{R}_6.
\end{aligned} \tag{5.2}$$

Step 2: bounding the error terms $\mathbf{R}_1$-$\mathbf{R}_6$. For $\mathbf{R}_1$ and $\mathbf{R}_3$, an application of Lemma 2.1 (the continuity of $\boldsymbol{\mathcal{M}}_h(\cdot,\cdot)$ and $\boldsymbol{\mathcal{A}}_h(\cdot,\cdot)$) and the approximation properties of the interpolator $\mathbf{u}_I$ given in (2.2), lead to

$$\begin{aligned}
|\mathbf{R}_1| = |\boldsymbol{\mathcal{M}}_h(\delta_t(\mathbf{u}^n - \mathbf{u}_I^n), \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n)| &\le \boldsymbol{\mathcal{M}}_h\left(\delta_t \mathbf{u}^n - \frac{\partial \mathbf{u}^n}{\partial t}, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\right) + \boldsymbol{\mathcal{M}}_h\left(\frac{\partial \mathbf{u}^n}{\partial t} - \delta_t \mathbf{u}_I^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\right) \\
&\le \boldsymbol{\alpha}_2 \left\{2\tau^{1/2}\left\|\frac{\partial^2 \mathbf{u}}{\partial t^2}\right\|_{L^2(L^2)} + \tau^{-1/2}h^{k+1}\left\|\frac{\partial \mathbf{u}}{\partial t}\right\|_{L^2\left(H^{k+1}\right)}\right\}\|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_0,
\end{aligned}$$

and similarly

$$|\mathbf{R}_3| = |\boldsymbol{\mathcal{A}}_h(\mathbf{u}^n - \mathbf{u}_I^n, \boldsymbol{\vartheta_u}^n)| \le Ch^{k+1} \|u^n\|_{L^\infty(H^{k+1})} \, |\boldsymbol{\vartheta_u}^n|_1 \,.$$

For $\mathbf{R}_2$ and $\mathbf{R}_4$ we first notice that, by adding zero in the form $\pm \boldsymbol{\mathcal{M}}_h(\frac{\partial \mathbf{u}^n}{\partial t}, \boldsymbol{\vartheta_u}^n)$, we can obtain

$$\mathbf{R}_2 = \boldsymbol{\mathcal{M}}\left(\frac{\partial \mathbf{u}^n}{\partial t}, \boldsymbol{\vartheta_u}^n\right) - \boldsymbol{\mathcal{M}}_h\left(\delta_t \mathbf{u}^n, \boldsymbol{\vartheta_u}^n\right) = \boldsymbol{\mathcal{M}}(\frac{\partial \mathbf{u}^n}{\partial t}, \boldsymbol{\vartheta_u}^n) - \boldsymbol{\mathcal{M}}_h(\frac{\partial \mathbf{u}^n}{\partial t}, \boldsymbol{\vartheta_u}^n) + \boldsymbol{\mathcal{M}}_h(\frac{\partial \mathbf{u}^n}{\partial t} - \delta_t \mathbf{u}^n, \boldsymbol{\vartheta_u}^n). \quad (5.3)$$

To determine upper bounds for the terms in the right-hand side of (5.3), we use Cauchy-Schwarz's inequality, Lemma 2.4, and the continuity of the L^2-projector Π_k^0. This gives

$$\left|\boldsymbol{\mathcal{M}}(\frac{\partial \mathbf{u}^n}{\partial t}, \boldsymbol{\vartheta_u}^n) - \boldsymbol{\mathcal{M}}_h(\frac{\partial \mathbf{u}^n}{\partial t}, \boldsymbol{\vartheta_u}^n)\right| \le \boldsymbol{\alpha}_2 \|\frac{\partial \mathbf{u}^n}{\partial t} - \boldsymbol{\Pi}_k^0 \frac{\partial \mathbf{u}^n}{\partial t}\|_0 \|\boldsymbol{\vartheta_u}^n\|_0 \le Ch^{k+1} \|\frac{\partial \mathbf{u}^n}{\partial t}\|_{k+1} \|\boldsymbol{\vartheta_u}^n\|_0, \quad (5.4)$$

and

$$\boldsymbol{\mathcal{M}}_h(\frac{\partial \mathbf{u}^n}{\partial t} - \delta_t \mathbf{u}^n, \boldsymbol{\vartheta_u}^n) \le \boldsymbol{\alpha}_2 \tau^{1/2} \|\frac{\partial^2 \mathbf{u}}{\partial t^2}\|_{L^2(L^2)} \|\boldsymbol{\vartheta_u}^n\|_0.$$

After combining this estimate with (5.4) and (5.3), we can conclude that

$$\mathbf{R}_2 \le \left\{ Ch^{k+1} \left\| \frac{\partial \mathbf{u}^n}{\partial t} \right\|_{k+1} + \tau^{1/2} \left\| \frac{\partial^2 \mathbf{u}}{\partial t^2} \right\|_{L^2(L^2)} \right\} \|\boldsymbol{\vartheta_u}^n\|_0 \,,$$

and similarly

$$|\mathbf{R}_4| = \left|\boldsymbol{\mathcal{A}}(\mathbf{u}^n, \boldsymbol{\vartheta_u}^n) - \boldsymbol{\mathcal{A}}_h(\mathbf{u}^n, \boldsymbol{\vartheta_u}^n)\right| \le \boldsymbol{\beta}_2 \|\mathbf{u}^n - \boldsymbol{\Pi}_k^\nabla \mathbf{u}^n\|_0 \|\boldsymbol{\vartheta_u}^n\|_0 \le Ch^k \|\mathbf{u}^n\|_{k+1} |\boldsymbol{\vartheta_u}^n|_1.$$

The term $\mathbf{R}_5$ can be rewritten by adding and subtracting some suitable terms

$$\begin{aligned}
\mathbf{R}_5 &= \boldsymbol{\mathcal{C}}(\mathbf{u}^n; \mathbf{u}^n, \boldsymbol{\vartheta_u}^n) - \boldsymbol{\mathcal{C}}_h(\mathbf{u}_h^n; \mathbf{u}_h^n, \boldsymbol{\vartheta_u}^n) \\
&= \left[\boldsymbol{\mathcal{C}}(\mathbf{u}^n; \mathbf{u}^n, \boldsymbol{\vartheta_u}^n) - \boldsymbol{\mathcal{C}}_h(\mathbf{u}^n; \mathbf{u}^n, \boldsymbol{\vartheta_u}^n)\right] + \left[\boldsymbol{\mathcal{C}}_h(\mathbf{u}^n; \mathbf{u}^n, \boldsymbol{\vartheta_u}^n) - \boldsymbol{\mathcal{C}}_h(\mathbf{u}_h^n; \mathbf{u}_h^n, \boldsymbol{\vartheta_u}^n)\right] \\
&:= \mathbf{R}_5^1 + \mathbf{R}_5^2. \qquad (5.5)
\end{aligned}$$

The first term of the above equation is estimated by Lemma 2.6

$$|\mathbf{R}_5^1| \le Ch^k \left(\|\mathbf{u}^n\|_k + \|\mathbf{u}^n\|_{\mathbf{X}} + \|\mathbf{u}^n\|_{k+1}\right) \|\mathbf{u}^n\|_{k+1} \|\boldsymbol{\vartheta_u}^n\|_{\mathbf{X}},$$

while for the second term we perform simple computations, we use the skew-symmetry of $\boldsymbol{\mathcal{C}}$ and $\boldsymbol{\mathcal{C}}_h$, and we recall that $\boldsymbol{\vartheta_u}^n = \mathbf{u}_h^n - \mathbf{u}_I^n$

$$\begin{aligned}
\mathbf{R}_5^2 &= \boldsymbol{\mathcal{C}}_h(\mathbf{u}^n; \mathbf{u}^n - \mathbf{u}_h^n, \boldsymbol{\vartheta_u}^n) + \boldsymbol{\mathcal{C}}_h(\mathbf{u}^n - \mathbf{u}_h; \mathbf{u}_h^n, \boldsymbol{\vartheta_u}^n) \\
&= \boldsymbol{\mathcal{C}}_h(\mathbf{u}^n; \mathbf{u}^n - \mathbf{u}_h^n + \boldsymbol{\vartheta_u}^n, \boldsymbol{\vartheta_u}^n) + \boldsymbol{\mathcal{C}}_h(\mathbf{u}^n - \mathbf{u}_h + \boldsymbol{\vartheta_u}^n; \mathbf{u}_h^n, \boldsymbol{\vartheta_u}^n) - \boldsymbol{\mathcal{C}}_h(\boldsymbol{\vartheta_u}^n; \mathbf{u}_h^n, \boldsymbol{\vartheta_u}^n) \\
&\le \widehat{C}_{2h}\Big(\|\mathbf{u}^n - \mathbf{u}_h^n + \boldsymbol{\vartheta_u}^n\|_1 (\|\mathbf{u}^n\|_1 + \|\mathbf{u}_h^n\|_1) + \|\mathbf{u}_h^n\|_1 \|\boldsymbol{\vartheta_u}^n\|_1\Big) \|\boldsymbol{\vartheta_u}^n\|_1 \\
&\le \widehat{C}_{2h}\Big(\|\mathbf{u}^n - \mathbf{u}_I^n\|_1 (\|\mathbf{u}^n\|_1 + \|\mathbf{u}_h^n\|_1) + \|\mathbf{u}_h^n\|_1 \|\boldsymbol{\vartheta_u}^n\|_1\Big) \|\boldsymbol{\vartheta_u}^n\|_1 \\
&\le \widehat{C}_{2h}\Big(h^k \|\mathbf{u}^n\|_{k+1} (\|\mathbf{u}^n\|_1 + \|\mathbf{u}_h^n\|_1) + \|\mathbf{u}_h^n\|_1 \|\boldsymbol{\vartheta_u}^n\|_1\Big) \|\boldsymbol{\vartheta_u}^n\|_1.
\end{aligned}$$

Substituting these expressions into (5.5) and rearranging terms, implies that

$$|\mathbf{R}_5| \leq \left(Ch^k \left(\|\mathbf{u}^n\|_k + \|\mathbf{u}^n\|_1 + \|\mathbf{u}^n\|_{k+1} + \|\mathbf{u}_h^n\|_1 \right) \|\mathbf{u}^n\|_{k+1} + \|\mathbf{u}_h^n\|_1 \|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_1 \right) \|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_1.$$

Finally, the term $\mathbf{R}_6$ is rewritten as

$$\begin{aligned}\mathbf{R}_6 &= \left[\left((c^+)^n \nabla\phi^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\right) - \left((c^+)^n \nabla\phi^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\right)_h \right] + \left[\left((c^+)^n \nabla\phi^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\right)_h - \left((c_h^+)^n \nabla\phi_h^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\right)_h \right] \\ &+ \left[\left((c^-)^n \nabla\phi^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\right) - \left((c^-)^n \nabla\phi^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\right)_h \right] + \left[\left((c^-)^n \nabla\phi^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\right)_h - \left((c_h^-)^n \nabla\phi_h^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\right)_h \right] \\ &= \mathbf{R}_6^1 + \mathbf{R}_6^2 + \mathbf{R}_6^3 + \mathbf{R}_6^4. \end{aligned} \tag{5.6}$$

Recalling the definition of the discrete inner product $(\cdot;\cdot,\cdot)_h$ we add and subtract suitable terms to have

$$\begin{aligned}\mathbf{R}_6^1 &= \sum_{E\in\mathcal{T}_h} \int_E \left(((c^+)^n \nabla\phi^n) \cdot \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n - (\Pi_k^0 (c^+)^n \mathbf{\Pi}_{k-1}^0 \nabla\phi^n) \cdot \mathbf{\Pi}_k^0 \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n \right) dE \\ &= \sum_{E\in\mathcal{T}_h} \int_E \Bigg(((c^+)^n \nabla\phi^n) \cdot (I - \mathbf{\Pi}_k^0) \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n + (I - \Pi_k^{0,E})(c^+)^n \nabla\phi^n \cdot \mathbf{\Pi}_k^0 \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n \\ &+ \Pi_k^{0,E} (c^+)^n (I - \mathbf{\Pi}_{k-1}^0) \nabla\phi^n \cdot \mathbf{\Pi}_k^0 \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n \Bigg) dE. \end{aligned} \tag{5.7}$$

The definition of the L^2-projection $\mathbf{\Pi}_k^{0,E}$, estimate (2.1), the Hölder inequality and Sobolev embedding $H^k \subset W_4^{k-1}$ lead to

$$\begin{aligned}\int_E \left(((c^+)^n \nabla\phi^n) \cdot (I - \mathbf{\Pi}_k^0) \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n \right) dE &= \int_E \left((I - \mathbf{\Pi}_{k-1}^0)((c^+)^n \nabla\phi^n) \cdot (I - \mathbf{\Pi}_k^0) \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n \right) dE \\ &\leq \|(I - \mathbf{\Pi}_{k-1}^0)((c^+)^n \nabla\phi^n)\|_{0,E} \|(I - \mathbf{\Pi}_k^0) \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_{0,E} \\ &\leq Ch_E^k \|(c^+)^n \nabla\phi^n\|_{k-1,E} \|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_{1,E} \\ &\leq Ch_E^k \|(c^+)^n\|_{k-1,4,E} \|\nabla\phi^n\|_{k-1,4,E} \|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_{1,E} \\ &\leq Ch_E^k \|(c^+)^n\|_{1,E} \|\nabla\phi^n\|_{1,E} \|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_{1,E}. \end{aligned}$$

Also, the Hölder inequality, the approximation property (2.1), and the continuity of $\mathbf{\Pi}_k^{0,E}$, gives

$$\begin{aligned}\int_E \left((I - \Pi_k^{0,E})(c^+)^n \nabla\phi^n \cdot \mathbf{\Pi}_k^0 \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n \right) dE &\leq \|(I - \Pi_k^{0,E})(c^+)^n\|_{0,4,E} \|\nabla\phi^n\|_{0,E} \|\mathbf{\Pi}_k^0 \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_{0,4,E} \\ &\leq \left(\|(c^+)^n - (c_\pi^+)^n\|_{0,4,E} + \|\Pi_k^{0,E}((c^+)^n - (c_\pi^+)^n)\|_{0,4,E} \right) \|\nabla\phi^n\|_{0,E} \|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_{0,4,E} \\ &\leq Ch_E^k \|(c^+)^n\|_{k,4,E} \|\phi^n\|_{1,E} \|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_{1,E} \\ &\leq Ch_E^k \|(c^+)^n\|_{k+1,E} \|\phi^n\|_{1,E} \|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_{1,E}, \end{aligned}$$

and

$$\begin{aligned}\int_E \left(\Pi_k^{0,E} (c^+)^n (I - \mathbf{\Pi}_{k-1}^0) \nabla\phi^n \cdot \mathbf{\Pi}_k^0 \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n \right) dE &\leq \|\Pi_k^{0,E} (c^+)^n\|_{0,4,E} \|(I - \mathbf{\Pi}_{k-1}^0) \nabla\phi^n\|_{0,E} \|\mathbf{\Pi}_k^0 \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_{0,4,E} \\ &\leq Ch_E^k \|(c^+)^n\|_{1,E} \|\phi^n\|_{k+1} \|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_{1,E}. \end{aligned}$$

Substituting this expression into (5.7) and rearranging terms, leads to

$$|\mathbf{R}_6^1| \leq Ch^k\bigg(\|(c^+)^n\|_1(\|\phi^n\|_2 + \|\phi^n\|_{k+1}) + \|(c^+)^n\|_{k+1}\|\phi^n\|_1\bigg)\|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_1. \tag{5.8}$$

The second term appearing on Eq. (5.6) can be easily estimated by the Hölder inequality, Sobolev embedding $H^k \subset W_4^{k-1}$ and the continuity of $\mathbf{\Pi}_k^{0,E}$ with respect to the L^4-norm as

$$\begin{aligned}
\mathbf{R}_6^2 &= \big((c^+)^n\nabla\phi^n - (c_h^+)^n\nabla\phi_h^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\big)_h \\
&= \big((c^+)^n(\phi^n - \phi_h^n), \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\big)_h + \big(((c^+)^n - (c_h^+)^n)(\phi^n - \phi_h^n), \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\big)_h + \big(((c^+)^n - (c_h^+)^n)\phi^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\big)_h \\
&\leq \bigg(\|\Pi_k^0(c^+)^n\|_{0,4}\|\mathbf{\Pi}_{k-1}^0\nabla(\phi^n - \phi_h^n)\|_0 + \|\Pi_k^0((c^+)^n - (c_h^+)^n)\|_{0,4}\|\mathbf{\Pi}_{k-1}^0\nabla(\phi^n - \phi_h^n)\|_0 \\
&\quad + \|\Pi_k^0((c^+)^n - (c_h^+)^n)\|_0\|\mathbf{\Pi}_{k-1}^0\nabla\phi^n\|_{0,4}\bigg)\|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_{0,4} \\
&\leq \bigg((\|(c^+)^n\|_1 + \|(c^+)^n - (c_h^+)^n\|_1)\|\phi^n - \phi_h^n\|_1 + \|(c^+)^n - (c_h^+)^n\|_0\|\phi^n\|_2\bigg)\|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_1.
\end{aligned}$$

Proceeding in a similar manner as above, we have

$$\mathbf{R}_6^3 \leq Ch^k\bigg(\|(c^-)^n\|_1(\|\phi^n\|_2 + \|\phi^n\|_{k+1}) + \|(c^-)^n\|_{k+1}\|\phi^n\|_1\bigg)\|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_1,$$

and

$$\mathbf{R}_6^4 \leq \bigg((\|(c^-)^n\|_1 + \|(c^-)^n - (c_h^-)^n\|_1)\|\phi^n - \phi_h^n\|_1 + \|(c^-)^n - (c_h^-)^n\|_0\|\phi^n\|_2\bigg)\|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_1. \tag{5.9}$$

Substituting Eqs. (5.8)-(5.9) in (5.6), gives

$$\begin{aligned}
\mathbf{R}_6 &\leq Ch^k\bigg((\|(c^+)^n\|_1 + \|(c^-)^n\|_1)(\|\phi^n\|_2 + \|\phi^n\|_{k+1}) + (\|(c^+)^n\|_{s+1} + \|(c^-)^n\|_{k+1})\|\phi^n\|_1\bigg)\|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_1 \\
&\quad + \bigg((\|(c^+)^n\|_1 + \|(c^+)^n - (c_h^+)^n\|_1 + \|(c^-)^n\|_1 + \|(c^-)^n - (c^-)^n\|_1)\|\phi^n - \phi_h^n\|_1 \\
&\quad + (\|(c^+)^n - (c_h^+)^n\|_0 + \|(c^-)^n - (c_h^-)^n\|_0)\|\phi^n\|_2\bigg)\|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_1.
\end{aligned}$$

Step 3: error estimate at the n-th time step. Inserting the bounds on $\mathbf{R}_1$-$\mathbf{R}_6$ into (5.2), yields

$$\begin{aligned}
\boldsymbol{\mathcal{M}}_h\Big(\frac{\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n - \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^{n-1}}{\tau}, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\Big) + \boldsymbol{\mathcal{A}}_h(\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n, \boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n) &\leq \big[\boldsymbol{\varpi}_1^n + \|\mathbf{u}_h^n\|_1\,|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n|_1 + (\|(c^+)^n - (c_h^+)^n\|_0 \\
&\quad + \|(c^-)^n - (c_h^-)^n\|_0)\|\phi^n\|_2 + \big(\boldsymbol{\varpi}_2^n + \|(c^+)^n - (c_h^+)^n\|_1 + \|(c^-)^n - (c_h^-)^n\|_1\big)\,\|\phi^n - \phi_h^n\|_1\big]\,\|\boldsymbol{\vartheta}_{\boldsymbol{u}}{}^n\|_1\,,
\end{aligned}$$

with positive scalars

$$\boldsymbol{\varpi}_1^n \leq \overline{C}_1h^{k+1} + \overline{C}_2h^k + \tau^{1/2}O_1^n + \tau^{-1/2}h^{k+1}O_2^n, \quad \boldsymbol{\varpi}_2^n \leq \|(c^+)^n\|_1 + \|(c^-)^n\|_1, \tag{5.10}$$

and where

$$\overline{C}_1 \leq \left\|\frac{\partial\mathbf{u}^n}{\partial t}\right\|_{L^\infty(H^{k+1})} + \|\mathbf{u}^n\|_{L^\infty(H^{k+1})}, \quad O_1 \leq \left\|\frac{\partial^2\mathbf{u}}{\partial t^2}\right\|_{L^2(L^2)}, \quad O_2 \leq \left\|\frac{\partial\mathbf{u}}{\partial t}\right\|_{L^2\left(H^{k+1}\right)},$$

$$C_2 \leq (\|\mathbf{u}^n\|_k + \|\mathbf{u}^n\|_1 + \|\mathbf{u}^n\|_{k+1} + \|\mathbf{u}_h^n\|_1 + 1)\,\|\mathbf{u}^n\|_{k+1} + (\|(c^+)^n\|_1 + \|(c^-)^n\|_1)(\|\phi^n\|_2 + \|\phi^n\|_{k+1}) + (\|(c^+)^n\|_{k+1} + \|(c^-)^n\|_{k+1})\|\phi^n\|_1.$$

It is not difficult to verify that

$$\boldsymbol{\mathcal{M}}_h(\frac{\boldsymbol{\vartheta_u}^n - \boldsymbol{\vartheta_u}^{n-1}}{\tau}, \boldsymbol{\vartheta_u}^n) \geq \frac{1}{2\tau}\left(\boldsymbol{\alpha}_1\|\boldsymbol{\vartheta_u}^n\|_0^2 - \boldsymbol{\alpha}_2\|\boldsymbol{\vartheta_u}^{n-1}\|_0^2\right), \qquad \boldsymbol{\mathcal{A}}_h(\boldsymbol{\vartheta_u}^n, \boldsymbol{\vartheta_u}^n) \geq \boldsymbol{\beta}_1|\boldsymbol{\vartheta_u}^n|_1^2.$$

Employing the last inequalities gives

$$\frac{1}{2\tau}\left(\|\boldsymbol{\vartheta_u}^n\|_0^2 - \|\boldsymbol{\vartheta_u}^{n-1}\|_0^2\right) + \boldsymbol{\beta}_1|\boldsymbol{\vartheta_u}^n|_1^2 \leq \|\mathbf{u}_h^n\|_1\,|\boldsymbol{\vartheta_u}^n|_1^2 + \big[\boldsymbol{\varpi}_1^n + (\|(c^+)^n - (c_h^+)^n\|_0 + \|(c^-)^n - (c_h^-)^n\|_0)\|\phi^n\|_2 + \left(\boldsymbol{\varpi}_2^n + \|(c^+)^n - (c_h^+)^n\|_1 + \|(c^-)^n - (c_h^-)^n\|_1\right)\|\phi^n - \phi_h^n\|_1\big]^2 + \frac{\boldsymbol{\beta}_1}{4}\|\boldsymbol{\vartheta_u}^n\|_1^2. \tag{5.11}$$

Next, using Corollary 1, and invoking a smallness assumption on the term $\|\mathbf{u}_h^n\|_1$ such that it holds

$$\|\mathbf{u}_h^n\|_1 \leq \frac{\boldsymbol{\beta}_1}{4},$$

we have, from (5.11), the bound

$$\|\boldsymbol{\vartheta_u}^n\|_0^2 + 2\tau\boldsymbol{\beta}_1|\boldsymbol{\vartheta_u}^n|_1^2 \leq \|\boldsymbol{\vartheta_u}^{n-1}\|_0^2 + 2\tau\big[\boldsymbol{\varpi}_1^n + (\|(c^+)^n - (c_h^+)^n\|_0 + \|(c^-)^n - (c_h^-)^n\|_0)\|\phi^n\|_2 + \left(\boldsymbol{\varpi}_2^n + \|(c^+)^n - (c_h^+)^n\|_1 + \|(c^-)^n - (c_h^-)^n\|_1\right)\|\phi^n - \phi_h^n\|_1\big]^2.$$

Summing up the above inequality over $j = 1, \cdots, n$, $n \leq N$, gives

$$\|\boldsymbol{\vartheta_u}^n\|_0^2 + 2\tau\boldsymbol{\beta}_1\sum_{j=1}^n|\boldsymbol{\vartheta_u}^j|_1^2 \leq \|\boldsymbol{\vartheta_u}^0\|_0^2 + \tau\sum_{j=1}^n\big[\boldsymbol{\varpi}_1^j + (\|(c^+)^j - (c_h^+)^j\|_0 + \|(c^-)^j - (c_h^-)^j\|_0)\|\phi^j\|_2 + \left(\boldsymbol{\varpi}_2^j + \|(c^+)^j - (c_h^+)^j\|_1 + \|(c^-)^j - (c_h^-)^j\|_1\right)\|\phi^j - \phi_h^j\|_1\big]^2. \tag{5.12}$$

Since $\sum_{j=1}^n \tau \leq t_F$, and using definitions of ϖ_1^n and ϖ_2^n in (5.10), we obtain

$$\begin{aligned}
\tau\sum_{j=1}^n\left((\varpi_1^j)^2 + (\varpi_2^j)^2 + (\varpi_3^j)^2\right) &\leq \sum_{j=1}^n\tau\left(\overline{C}_1h^{k+1} + \overline{C}_2h^k + \tau^{1/2}O_1^n + \tau^{-1/2}h^{k+1}O_2^n\right)^2 \\
&+ \sum_{j=1}^n\tau\left(\overline{C}_3h^{k+1} + \overline{C}_4h^k + \tau^{1/2}O_3^n + \tau^{-1/2}h^{k+1}O_4^n\right)^2 \\
&+ \sum_{j=1}^n\tau\left(\overline{C}_5h^{k+1} + \overline{C}_6h^k + \tau^{1/2}O_5^n + \tau^{-1/2}h^{k+1}O_6^n\right)^2 \\
&\leq \left[h^{2(k+1)}(\overline{C}_1^2 + \overline{C}_3^2 + \overline{C}_5^2) + h^{2(k)}(\overline{C}_2^2 + \overline{C}_4^2 + \overline{C}_6^2)\right]\sum_{j=1}^n\tau \\
&+ \tau^2\sum_{j=1}^n\left((O_1^n)^2 + (O_3^n)^2 + (O_5^n)^2\right) + h^{2(k+1)}\sum_{j=1}^n\left((O_2^n)^2 + (O_4^n)^2 + (O_6^n)^2\right) \\
&\leq C(h^{2k} + \tau^2),
\end{aligned}$$

which, together with (5.12), completes the proof. □

5.2. Error bounds: concentrations and electrostatic potential

We consider the following problem:

$$\begin{cases} \mathcal{M}_h(\delta_t(c_h^+)^n, z_1) + \mathcal{A}_{1h}((c_h^+)^n, z_1) + \mathcal{C}_h((c_h^+)^n; \phi_h^n, z_1) + \mathcal{D}_h(\mathbf{u}_h^n; (c_h^+)^n, z_1) = 0, \\ \mathcal{M}_h(\delta_t(c_h^-)^n, z_2) + \mathcal{A}_{2h}((c_h^-)^n, z_2) - \mathcal{C}_h((c_h^-)^n; \phi_h^n, z_2) + \mathcal{D}_h(\mathbf{u}_h^n; (c_h^-)^n, z_2) = 0, \\ \mathcal{A}_{3h}(\phi_h^n, z_3) = \mathcal{M}_h((c_h^+)^n, z_3) - \mathcal{M}_h((c_h^-)^n, z_3), \end{cases} \tag{5.13}$$

where $\mathbf{u}_h^n \in \widetilde{\mathbf{X}}_h$ is the solution from (2.23) for $n = 1, \cdots, N$. Next, we define discrete projection operators which will be utilized to derive error estimates for concentrations and electrostatic potential.

5.2.1. Electrostatic potential

We now derive an upper bound for $\|\phi^n - \phi_h^n\|_1$ in terms of the concentration errors for $n = 1, \cdots, N$. For any $t \in [0, t_F]$, we define the energy projection $\mathcal{P}_h : H^1(\Omega) \cap H^{k+1}(\Omega) \to Z_h$ as the solution of

$$\mathcal{A}_{3h}(\mathcal{P}_h\phi(t), z_3) = \mathcal{A}_3(\phi(t), z_3), \qquad \forall z_3 \in Z_h. \tag{5.14}$$

Using the interpolation property (2.5), we recall the following approximation properties of $\mathcal{P}_h$.

Lemma 5.2. *Assume that $z \in H^{k+1}(\Omega) \cap H^1(\Omega)$. Then, there exists a unique $\mathcal{P}_h z \in Z_h$ solution of (5.14) satisfying*

$$\|z - \mathcal{P}_h z\|_0 + h|z - \mathcal{P}_h z|_1 \leq C h^{k+1} \|z\|_{k+1}, \tag{5.15}$$

and

$$\|z - \mathcal{P}_h z\|_{1,\infty} \leq C h^k \|z\|_{k+1,\infty}.$$

In the next result we state an optimal error estimate for $\mathcal{P}_h\phi - \phi_h$.

Lemma 5.3. *Let $\{c^+, c^-, \phi\}$ and $\{(c_h^+)^n, (c_h^-)^n, \phi_h^n\}$ be solutions to (1.1) and (5.13), respectively. Then for $n = 1, \cdots, N$ we have*

$$\|\phi^n - \phi_h^n\|_1 \leq C\left(\|(c^+)^n - (c_h^+)^n\|_0 + \|(c^-)^n - (c_h^-)^n\|_0 + h^{k+1}(\|(c^+)^n\|_{k+1} + \|(c^-)^n\|_{k+1})\right).$$

Proof. Setting $\vartheta^n = \phi_h^n - \mathcal{P}_h\phi^n$, it holds that $\vartheta^n \in Z_h$. Using the third equation of (5.13) and Eq. (5.14) and letting $z_3 = \vartheta^n$, yields

$$\begin{aligned} \beta_1|\vartheta^n|_1^2 \leq \mathcal{A}_{3h}(\vartheta^n, \vartheta^n) &= \mathcal{A}_{3h}(\phi_h^n, \vartheta^n) - \mathcal{A}_{3h}(\mathcal{P}_h\phi^n, \vartheta^n) \\ &= \left[\mathcal{M}_h((c_h^+)^n, \vartheta^n) - \mathcal{M}((c^+)^n, \vartheta^n)\right] - \left[\mathcal{M}_h((c_h^-)^n, z_3) - \mathcal{M}((c^-)^n, \vartheta^n)\right] \\ &= \mathcal{M}_h((c_h^+)^n - (c^+)^n, \vartheta^n) - \mathcal{M}_h((c_h^-)^n - (c^-)^n, \vartheta^n) \\ &\quad + \left[\mathcal{M}_h((c^+)^n, \vartheta^n) - \mathcal{M}((c^+)^n, \vartheta^n)\right] - \left[\mathcal{M}_h((c^-)^n, z_3) - \mathcal{M}((c^-)^n, \vartheta^n)\right]. \end{aligned}$$

The continuity of $\mathcal{M}_h(\cdot,\cdot)$ given in Lemma 2.1 and the error estimate from Lemma 2.4, confirm that

$$\beta_1|\vartheta^n|_1^2 \leq \left(\alpha_2(\|(c^+)^n - (c_h^+)^n\|_0 + \|(c^-)^n - (c_h^-)^n\|_0) + Ch^{k+1}(\|(c^+)^n\|_{k+1} + \|(c^-)^n\|_{k+1})\right)\|\vartheta^n\|_0,$$

which, by Poincaré inequality, implies that

$$|\vartheta^n|_1 \leq C_P\beta_1^{-1}\left(\alpha_2(\|(c^+)^n - (c_h^+)^n\|_0 + \|(c^-)^n - (c_h^-)^n\|_0) + Ch^{k+1}(\|(c^+)^n\|_{k+1} + \|(c^-)^n\|_{k+1})\right). \tag{5.16}$$

Next, a duality argument for nonlinear elliptic equations [10], gives the following L^2 error estimate

$$\|\vartheta^n\|_0 \leq Ch|\vartheta^n|_1 + C_P\beta_1^{-1}\left(\alpha_2(\|(c^+)^n - (c_h^+)^n\|_0 + \|(c^-)^n - (c_h^-)^n\|_0) + Ch^{k+1}(\|(c^+)^n\|_{k+1} + \|(c^-)^n\|_{k+1})\right). \tag{5.17}$$

And combining (5.16), (5.17), the triangle inequality, and estimate (5.15), the desired result follows. □

5.2.2. Concentrations

The aim of this part is to attain an upper bound for $\|(c^+)^n - (c_h^+)^n\|_0$ and $\|(c^-)^n - (c_h^-)^n\|_0$. For this purpose, we define a discrete projection operator $\mathcal{P}_h : Z \to Z_h$, for fixed $\mathbf{u}(t) \in \mathbf{X}$, $\phi(t) \in Z$ and $t \in J$ by

$$\begin{cases} \mathcal{L}_{1h}(\mathbf{u}(t), \phi(t); \mathcal{P}_h c^+, z_1) = \mathcal{L}_1(\mathbf{u}(t), \phi(t); c^+, z_1), & \forall z_1 \in Z_h \\ \mathcal{L}_{2h}(\mathbf{u}(t), \phi(t); \mathcal{P}_h c^-, z_2) = \mathcal{L}_2(\mathbf{u}(t), \phi(t); c^-, z_2), & \forall z_2 \in Z_h, \end{cases} \tag{5.18}$$

where

$$\mathcal{L}_{1h}(\mathbf{u}(t), \phi; c^+, z_1) = \mathcal{A}_{1h}(c^+, z_1) + \mathcal{C}_h(c^+; \phi, z_1) - \mathcal{D}_h(\mathbf{u}(t); c^+, z_1) + (c^+, z_1)_h, \tag{5.19a}$$
$$\mathcal{L}_{1}(\mathbf{u}(t), \phi; c^+, z_1) = \mathcal{A}_{1}(c^+, z_1) + \mathcal{C}(c^+; \phi, z_1) - \mathcal{D}(\mathbf{u}(t); c^+, z_1) + (c^+, z_1)_0, \tag{5.19b}$$
$$\mathcal{L}_{2h}(\mathbf{u}(t), \phi; c^-, z_2) = \mathcal{A}_{2h}(c^-, z_2) + \mathcal{C}_h(c^-; \phi, z_2) - \mathcal{D}_h(\mathbf{u}(t); c^-, z_2) + (c^-, z_2)_h, \tag{5.19c}$$
$$\mathcal{L}_{2}(\mathbf{u}(t), \phi; c^-, z_2) = \mathcal{A}_{2}(c^-, z_2) + \mathcal{C}(c^-; \phi, z_2) - \mathcal{D}(\mathbf{u}(t); c^-, z_2) + (c^-, z_2)_0. \tag{5.19d}$$

Lemma 5.4. *Assume that $\boldsymbol{u} \in [L^\infty(\Omega)]^2$ and $\phi \in W^{1,\infty}(\Omega)$ for all $t \in (0, t_F]$. Then, the operator $\mathcal{P}_h : Z \to Z_h$ in (5.18) is well-defined.*

Proof. We proceed by the Lax–Milgram lemma and the proof is divided into two steps. The first step establishes that the bilinear form on the left-hand side of (5.18) is continuous and coercive on $V_h \times V_h$, whereas the second step proves that the right-hand side functional is bounded over V_h. Continuity of $\mathcal{L}_1$ and $\mathcal{L}_2$ is achieved by the continuity of the forms $(\cdot,\cdot)_0$ and $\mathcal{A}(\cdot,\cdot)$, and Poincaré inequality with

$$\mathcal{C}(c^+; \phi, z_1) = (c^+\nabla\phi, \nabla z_1)_0 \le \|\phi\|_{1,\infty}|c^+|_1|z_1|_1, \quad \mathcal{C}(c^-; \phi, z_2) = (c^-\nabla\phi, \nabla z_2)_0 \le \|\phi\|_{1,\infty}|c^-|_1|z_2|_1,$$

and

$$\mathcal{D}(\mathbf{u}(t); c^+, z_1) \le \frac{1}{2}\|\mathbf{u}\|_{0,4}\left(\|c^+\|_{0,4}\|z_1\|_1 + \|c^+\|_1\|z_1\|_{0,4}\right) \le C\|\mathbf{u}\|_{\mathbf{X}}\|c^+\|_Z\|z_1\|_Z,$$
$$\mathcal{D}(\mathbf{u}(t); c^-, z_2) \le \frac{1}{2}\|\mathbf{u}\|_{0,4}\left(\|c^-\|_{0,4}\|z_2\|_1 + \|c^-\|_1\|z_2\|_{0,4}\right) \le C\|\mathbf{u}\|_{\mathbf{X}}\|c^-\|_Z\|z_2\|_Z.$$

The continuity of $\mathcal{L}_{1h}$ and $\mathcal{L}_{2h}$ can be handled using Lemmas 2.1 and 2.2. In turn, to derive the coercivity of $\mathcal{L}_{1h}$ and $\mathcal{L}_{2h}$, we have

$$\mathcal{D}_h^E(\mathbf{u}; c^+, c^+) = \frac{1}{2}\left[(\boldsymbol{\Pi}_k^{0,E}\mathbf{u}\cdot\Pi_k^{0,E}c^+, \Pi_{k-1}^{0,E}\nabla c^+)_0 - (\boldsymbol{\Pi}_k^{0,E}\mathbf{u}\cdot\Pi_{k-1}^{0,E}\nabla c^+, \Pi_k^{0,E}c^+)_0\right] = 0.$$

Then, combining this result with (2.9) completes the proof. □

Now we derive the error estimates of $(c^+)^n - \mathcal{P}_h(c^+)^n$ and $(c^-)^n - \mathcal{P}_h(c^-)^n$ in the L^2-norm.

Lemma 5.5. *Assume that $\{c^+, c^-, \phi\}$ is the solution of (1.1) satisfing the regularity assumptions*

$$\begin{aligned} C(\|\boldsymbol{u}\|_{\boldsymbol{X}}, \|\phi\|_{1,\infty})\|(c^+)^n\|_{k+1} &+ \|(c^+)^n\nabla\phi^n\|_k + \|(c^+)^n\|_\infty\|\phi^n\|_{k+1} + \|\phi^n\|_{1,\infty}\|(c^+)^n\|_k \\ &+ \|\boldsymbol{u}\|_{k+1}(\|(c^+)^n\|_{k+1} + \|(c^+)^n\|_1) + \|(c^+)^n\|_{k+1}(\|\boldsymbol{u}\|_k + \|\boldsymbol{u}\|_1) \le C, \\ C(\|\boldsymbol{u}\|_{\boldsymbol{X}}, \|\phi\|_{1,\infty})\|(c^-)^n\|_{k+1} &+ \|(c^-)^n\nabla\phi^n\|_k + \|(c^-)^n\|_\infty\|\phi^n\|_{k+1} + \|\phi^n\|_{1,\infty}\|(c^-)^n\|_k \\ &+ \|\boldsymbol{u}\|_{k+1}(\|(c^-)^n\|_{k+1} + \|(c^-)^n\|_1) + \|(c^-)^n\|_{k+1}(\|\boldsymbol{u}\|_k + \|\boldsymbol{u}\|_1) \le C, \end{aligned}$$

and $\mathcal{P}_h$ is defined as in (5.18). Then for $n = 1, \cdots, N$, we have the following error estimates

$$\|(c^+)^n - \mathcal{P}_h(c^+)^n\|_0 + h|(c^+)^n - \mathcal{P}_h(c^+)^n|_1 \le Ch^{k+1},$$
$$\|(c^-)^n - \mathcal{P}_h(c^-)^n\|_0 + h|(c^-)^n - \mathcal{P}_h(c^-)^n|_1 \le Ch^{k+1}.$$

Proof. We first bound the term $(c^+)^n - \mathcal{P}_h(c^+)^n$ and $(c^-)^n - \mathcal{P}_h(c^-)^n$ in the H^1-norm for any $n = 1, \cdots, N$. To this end, for $\{(c^+)^n, (c^-)^n\} \in H^{k+1}(\Omega) \times H^{k+1}(\Omega)$ we recall the estimate of its interpolant $\{(c_I^+)^n, (c_I^-)^n\}$ given in (2.5). Let $\theta_{c^+}^n := \mathcal{P}_h(c^+)^n - (c_I^+)^n$ and $\theta_{c^-}^n := \mathcal{P}_h(c^-)^n - (c_I^-)^n$ be elements of V_h. Employing the discrete coercivity of $\mathcal{L}_{1h}$ and $\mathcal{L}_{2h}$ (cf. proof of Lemma 5.4) and Eq. (5.18), yields

$$\begin{aligned}
\hat{C}|\theta_{c^+}^n|_1^2 &\le \mathcal{L}_{1h}(\mathbf{u}(t), \phi; \theta_{c^+}^n, \theta_{c^+}^n) = \mathcal{L}_{1h}(\mathbf{u}(t), \phi; \mathcal{P}_h(c^+)^n, \theta_{c^+}^n) - \mathcal{L}_{1h}(\mathbf{u}(t), \phi; (c_I^+)^n, \theta_{c^+}^n) \\
&= \left[\mathcal{L}_1(\mathbf{u}(t), \phi; (c^+)^n, \theta_{c^+}^n) - \mathcal{L}_{1h}(\mathbf{u}(t), \phi; (c^+)^n, \theta_{c^+}^n)\right] + \mathcal{L}_{1h}(\mathbf{u}(t), \phi; (c^+)^n - (c_I^+)^n, \theta_{c^+}^n) \\
&:= L_1 + L_2.
\end{aligned} \tag{5.20}$$

Using the definitions of $\mathcal{L}_1$ and $\mathcal{L}_{1h}$ given in (5.19a) and (5.19b), respectively, splits the term L_1 as follows:

$$\begin{aligned}
L_1 &= \left[\mathcal{A}_1((c^+)^n, \theta_{c^+}^n) - \mathcal{A}_{1h}((c^+)^n, \theta_{c^+}^n)\right] + \left[\mathcal{C}((c^+)^n; \phi^n, \theta_{c^+}^n) - \mathcal{C}_h((c^+)^n; \phi, \theta_{c^+}^n)\right] \\
&\quad + \left[\mathcal{D}(\mathbf{u}^n; (c^+)^n, \theta_{c^+}^n) - \mathcal{D}_h(\mathbf{u}^n; (c^+)^n, \theta_{c^+}^n)\right] + \left[((c^+)^n, \theta_{c^+}^n)_0 - ((c^+)^n, \theta_{c^+}^n)_h\right] \\
&\quad := L_1^{(1)} + L_1^{(2)} + L_1^{(3)} + L_1^{(4)}.
\end{aligned}$$

Next, we will bound each of the terms $L_1^{(i)}$, with $i = 1, 2, 3, 4$ in the above decomposition. This is achieved by Lemmas 2.5, 2.8, 2.7 and 2.4, respectively, as

$$L_1^{(1)} \le Ch^k \|(c^+)^n\|_{k+1} |\theta_{c^+}^n|_1, \quad L_1^{(2)} \le C\Big(h^k \|(c^+)^n \nabla\phi^n\|_k + \|(c^+)^n\|_\infty h^k \|\phi^n\|_{k+1} + \|\phi^n\|_{1,\infty} h^k \|(c^+)^n\|_k\Big) |\theta_{c^+}^n|_1,$$
$$L_1^{(3)} \le Ch^k \left(\|\mathbf{u}\|_{k+1}(\|(c^+)^n\|_{k+1} + \|(c^+)^n\|_1) + \|(c^+)^n\|_{k+1}(\|\mathbf{u}\|_k + \|\mathbf{u}\|_1)\right) \|\theta_{c^+}^n\|_1,$$
$$L_1^{(4)} \le Ch^{k+1} \|(c^+)^n\|_{k+1} \|\theta_{c^+}^n\|_0.$$

Next, to estimate L_2, we apply the continuity of $\mathcal{L}_{1h}$ (cf. Lemma 5.4) and the interpolation error estimate (2.2), to find that

$$L_2 = \mathcal{L}_{1h}(\mathbf{u}(t), \phi; (c^+)^n - (c_I^+)^n, \theta_{c^+}^n) \le C(\|\mathbf{u}\|_{\mathbf{X}}, \|\phi\|_{1,\infty}) h^k \|(c^+)^n\|_{k+1} |\theta_{c^+}^n|_1.$$

Thus, the H^1-seminorm estimate is derived by inserting all bounds $L_1^{(i)}$ for $i = 1, \cdots, 4$ into L_1 and then substituting the obtained estimates for L_1 and L_2 in (5.20). Note that an estimate in the L^2-norm is obtained by combining the arguments in above with a standard duality approach. That is omitted here. □

Finally, we state an error estimate for $(c^+)^n - (c_h^+)^n$, $(c^-)^n - (c_h^-)^n$ and $\phi^n - \phi_h^n$ in the L^2-norm valid for the scheme (2.23).

Theorem 5.6. *Let $\{(c^+)^n, (c^-)^n, \phi^n\}$ be the solution of (1.1) satisfying the regularity assumptions presented in Lemma 5.5 and $\{(c_h^+)^n, (c_h^-)^n, \phi_h^n\}$ be the solution of (5.13). Moreover, we assume that $k \ge d-1$. Then, the following error estimation holds for $n = 1, \cdots, N$,*

$$\|(c^+)^n - (c_h^+)^n\|_0 + \|(c^-)^n - (c_h^-)^n\|_0 + \tau \sum_{j=1}^n \left(|(c^+)^n - (c_h^+)^n|_1 + |(c^-)^n - (c_h^-)^n|_1\right) \le C(\tau + h^k).$$

Proof. We divide the proof into three steps.

Step 1: discrete evolution equation for the error. First, we split the concentration errors as follows

$$\begin{aligned}
(c^+)^n - (c_h^+)^n &= (c^+)^n - \mathcal{P}_h(c^+)^n + \mathcal{P}_h(c^+)^n - (c_h^+)^n := \vartheta_{c^+}^n + \rho_{c^+}^n, \\
(c^-)^n - (c_h^-)^n &= (c^-)^n - \mathcal{P}_h(c^-)^n + \mathcal{P}_h(c^-)^n - (c_h^-)^n := \vartheta_{c^-}^n + \rho_{c^-}^n,
\end{aligned}$$

where $\rho^n_{c^+}$ and $\rho^n_{c^-}$ are estimated in Lemma 5.5. Now we estimate $\vartheta^n_{c^+}$ and $\vartheta^n_{c^-}$. An application of Eqs. (1.2) and (5.13) with $z_1 = \vartheta^n_{c^+}$ and $z_2 = \vartheta^n_{c^-}$ and the definition of the projector $\mathcal{P}_h$ given in (5.18) imply

$$
\begin{aligned}
&\mathcal{M}_h(\frac{\vartheta^n_{c^+} - \vartheta^n_{c^+}}{\tau}, \vartheta^n_{c^+}) + \mathcal{A}_h(\vartheta^n_{c^+}, \vartheta^n_{c^+}) \\
&= \big[\mathcal{M}(\frac{\partial (c^+)^n}{\partial t}, \vartheta^n_{c^+}) - \mathcal{M}_h(\delta_t \mathcal{P}_h (c^+)^n, \vartheta^n_{c^+})\big] + \big[\mathcal{C}_h(\mathcal{P}_h(c^+)^n; \phi^n, \vartheta^n_{c^+}) - \mathcal{C}_h((c^+_h)^n; \phi^n_h, \vartheta^n_{c^+})\big] \\
&+ \big[\mathcal{D}_h(\mathbf{u}^n; \mathcal{P}_h(c^+)^n, \vartheta^n_{c^+}) - \mathcal{D}_h(\mathbf{u}^n_h; (c^+_h)^n, \vartheta^n_{c^+})\big] + \big[(\mathcal{P}_h(c^+)^n, \vartheta^n_{c^+})_h - ((c^+)^n, \vartheta^n_{c^+})_0\big] \\
&:= R_1 + R_2 + R_3 + R_4,
\end{aligned} \tag{5.21}
$$

and

$$
\begin{aligned}
&\mathcal{M}_h(\frac{\vartheta^n_{c^-} - \vartheta^{n-1}_{c^-}}{\tau}, \vartheta^n_{c^-}) + \mathcal{A}_h(\vartheta^n_{c^-}, \vartheta^n_{c^-}) \\
&= \big[\mathcal{M}(\frac{\partial (c^-)^n}{\partial t}, \vartheta^n_{c^-}) - \mathcal{M}_h(\delta_t \mathcal{P}_h (c^-)^n, \vartheta^n_{c^-})\big] - \big[\mathcal{C}_h(\mathcal{P}_h(c^-)^n; \phi^n, \vartheta^n_{c^-}) - \mathcal{C}_h((c^-_h)^n; \phi^n_h, \vartheta^n_{c^-})\big] \\
&+ \big[\mathcal{D}_h(\mathbf{u}^n; \mathcal{P}_h(c^-)^n, \vartheta^n_{c^-}) - \mathcal{D}_h(\mathbf{u}^n_h; (c^-_h)^n, \vartheta^n_{c^-})\big] \ + \big[(\mathcal{P}_h(c^-)^n, \vartheta^n_{c^-})_h - ((c^-)^n, \vartheta^n_{c^-})_0\big] \\
&:= Q_1 + Q_2 + Q_3 + Q_4.
\end{aligned} \tag{5.22}
$$

And owing to the coercivity of $\mathcal{A}_h$, we have

$$
\mathcal{A}_h(\vartheta^n_{c^+}, \vartheta^n_{c^+}) \geq \beta_1 |\vartheta^n_{c^+}|^2_1, \quad \text{and} \quad \mathcal{A}_h(\vartheta^n_{c^-}, \vartheta^n_{c^-}) \geq \beta_1 |\vartheta^n_{c^-}|^2_1.
$$

Step 2: bounding the error terms R_1-R_4 and Q_1-Q_4. For the terms R_1 and Q_1 we first notice that by adding zero in the form $\pm\mathcal{M}_h(\frac{\partial (c^+)^n}{\partial t}, \vartheta^n_{c^+})$ and $\pm\mathcal{M}_h(\frac{\partial (c^-)^n}{\partial t}, \vartheta^n_{c^-})$, we can obtain

$$
\begin{aligned}
R_1 &= \mathcal{M}(\frac{\partial (c^+)^n}{\partial t}, \vartheta^n_{c^+}) - \mathcal{M}_h(\delta_t \mathcal{P}_h(c^+)^n, \vartheta^n_{c^+}) \\
&= \big[\mathcal{M}(\frac{\partial (c^+)^n}{\partial t}, \vartheta^n_{c^+}) - \mathcal{M}_h(\frac{\partial (c^+)^n}{\partial t}, \vartheta^n_{c^+})\big] + \mathcal{M}_h(\frac{\partial (c^+)^n}{\partial t} - \delta_t \mathcal{P}_h(c^+)^n, \vartheta^n_{c^+}), \\
Q_1 &= \mathcal{M}(\frac{\partial (c^-)^n}{\partial t}, \vartheta^n_{c^-}) - \mathcal{M}_h(\delta_t \mathcal{P}_h(c^-)^n, \vartheta^n_{c^-}) \\
&= \big[\mathcal{M}(\frac{\partial (c^-)^n}{\partial t}, \vartheta^n_{c^-}) - \mathcal{M}_h(\frac{\partial (c^-)^n}{\partial t}, \vartheta^n_{c^-})\big] + \mathcal{M}_h(\frac{\partial (c^-)^n}{\partial t} - \delta_t \mathcal{P}_h(c^-)^n, \vartheta^n_{c^-}).
\end{aligned}
$$

To determine upper bounds of the right-hand side terms above, we will use Cauchy-Schwarz's inequality, Lemma 2.4, and the continuity of the L^2-projector Π^0_k. This gives

$$
\begin{aligned}
|R_1| &\leq \left(Ch^{k+1} \|\frac{\partial (c^+)^n}{\partial t}\|_{k+1} + \alpha_2 \tau^{1/2} \|\frac{\partial^2 c^+}{\partial t^2}\|_{L^2(L^2)} \right) \|\vartheta^n_{c^+}\|_0, \\
|Q_1| &\leq \left(Ch^{k+1} \|\frac{\partial (c^-)^n}{\partial t}\|_{k+1} + \alpha_2 \tau^{1/2} \|\frac{\partial^2 c^-}{\partial t^2}\|_{L^2(L^2)} \right) \|\vartheta^n_{c^-}\|_0.
\end{aligned}
$$

For the terms R_2 and Q_2, note that from the definition of $\mathcal{C}_h(\cdot;\cdot,\cdot)$ in (2.7), it holds

$$
\begin{aligned}
R_2 = \mathcal{C}_h(\mathcal{P}_h(c^+)^n; \phi^n, \vartheta^n_{c^+}) - \mathcal{C}_h((c^+_h)^n; \phi^n_h, \vartheta^n_{c^+}) = (\mathcal{P}_h(c^+)^n \nabla \phi^n, \nabla \vartheta^n_{c^+})_h - ((c^+_h)^n \nabla \phi^n_h, \nabla \vartheta^n_{c^+})_h, \\
Q_2 = \mathcal{C}_h(\mathcal{P}_h(c^-)^n; \phi^n, \vartheta^n_{c^-}) - \mathcal{C}_h((c^-_h)^n; \phi^n_h, \vartheta^n_{c^-}) = (\mathcal{P}_h(c^-)^n \nabla \phi^n, \nabla \vartheta^n_{c^-})_h - ((c^-_h)^n \nabla \phi^n_h, \nabla \vartheta^n_{c^-})_h.
\end{aligned}
$$

Note that, after adding some suitable zeros, we can rewrite

$$\begin{aligned}R_2 &= \big((\mathcal{P}_h(c^+)^n - (c_h^+)^n)\nabla\phi^n, \nabla\vartheta_{c^+}^n\big)_h - \big(((c^+)^n - (c_h^+)^n)\nabla(\phi^n - \phi_h^n), \nabla\vartheta_{c^+}^n\big)_h \\ &\quad + \big((c^+)^n\nabla(\phi^n - \phi_h^n), \nabla\vartheta_{c^+}^n\big)_h \\ &\quad := R_2^1 + R_2^2 + R_2^3,\end{aligned}$$

and

$$\begin{aligned}Q_2 &= \big((\mathcal{P}_h(c^-)^n - (c_h^-)^n)\nabla\phi^n, \nabla\vartheta_{c^-}^n\big)_h - \big(((c^-)^n - (c_h^-)^n)\nabla(\phi^n - \phi_h^n), \nabla\vartheta_{c^-}^n\big)_h \\ &\quad + \big((c^-)^n\nabla(\phi^n - \phi_h^n), \nabla\vartheta_{c^-}^n\big)_h \\ &\quad := Q_2^1 + Q_2^2 + Q_2^3. \end{aligned} \tag{5.23}$$

For R_2^1 and Q_2^1, using the Hölder inequality and the continuity of Π_{k-1}^0 and $\mathbf{\Pi}_{k-1}^{0,E}$ we can write

$$\begin{aligned}R_2^1 &= \left| \big((\mathcal{P}_h(c^+)^n - (c_h^+)^n)\nabla\phi^n, \nabla\vartheta_{c^+}^n\big)_h \right| \leq \|\mathbf{\Pi}_{k-1}^0\nabla\phi^n\|_\infty \|\Pi_{k-1}^0\vartheta_{c^+}^n\|_0 \|\mathbf{\Pi}_{k-1}^0\nabla\vartheta_{c^+}^n\|_0 \\ &\leq C\|\phi^n\|_{1,\infty}\|\vartheta_{c^+}^n\|_0|\vartheta_{c^+}^n|_1, \qquad (5.24a)\\ Q_2^1 &= \left| \big((\mathcal{P}_h(c^-)^n - (c_h^-)^n)\nabla\phi^n, \nabla\vartheta_{c^-}^n\big)_h \right| \leq \|\mathbf{\Pi}_{k-1}^0\nabla\phi^n\|_\infty \|\Pi_{k-1}^0\vartheta_{c^-}^n\|_0 \|\mathbf{\Pi}_{k-1}^0\nabla\vartheta_{c^-}^n\|_0 \\ &\leq C\|\phi^n\|_{1,\infty}\|\vartheta_{c^-}^n\|_0|\vartheta_{c^-}^n|_1. \qquad (5.24b)\end{aligned}$$

For the terms R_2^2 and Q_2^2, Hölder inequality together with Lemmas 5.2 and 5.5, gives

$$\begin{aligned}|R_2^2| &= \left| \big(((c^+)^n - (c_h^+)^n)\nabla(\phi^n - \phi_h^n), \nabla\vartheta_{c^+}^n\big)_h \right| \leq \|(c^+)^n - (c_h^+)^n\|_0 \|\phi^n - \phi_h^n\|_{1,\infty}|\vartheta_{c^+}^n|_1 \\ &\leq \|(c^+)^n - (c_h^+)^n\|_0 \left(\|\phi^n - \mathcal{P}_1\phi^n\|_{1,\infty} + \|\mathcal{P}_1\phi^n - \phi_h^n\|_{1,\infty}\right)|\vartheta_{c^+}^n|_1 \\ &\leq \left(\tau h^k\|\phi^n\|_{k+1,\infty}\left\|\frac{\partial c^+}{\partial t}\right\|_{L^\infty(L^2)} + h^{2k+1}\|(c^+)^{n-1}\|_{k+1}\|\phi^n\|_{k+1,\infty} + h^k\|\phi^n\|_{k+1,\infty}\|\vartheta_{c^+}^{n-1}\|_0\right)|\vartheta_{c^+}^n|_1 \\ &\quad + \left(h^{k+1}\|(c^+)^{n-1}\|_{k+1} + \|\vartheta_{c^+}^{n-1}\|_0\right)\|\mathcal{P}_1\phi^n - \phi_h^n\|_{1,\infty}|\vartheta_{c^+}^n|_1. \end{aligned}\tag{5.25}$$

Then we employ an inverse inequality and Lemma 5.3, and consider $d \leq 2$, to arrive at

$$\begin{aligned}\|\mathcal{P}_1\phi^n - \phi_h^n\|_{1,\infty} &\leq Ch^{-\frac{d}{2}}\|\mathcal{P}_1\phi^n - \phi_h^n\|_{1,0} \leq Ch^{-\frac{d}{2}}\left(\|(c^+)^n - (c_h^+)^n\|_0 + \|(c^-)^n - (c_h^-)^n\|_0\right) \\ &\leq Ch^{k+1-\frac{d}{2}}(\|(c^+)^n\|_{k+1} + \|(c^-)^n\|_{k+1}) + h^{-\frac{d}{2}}\left(\|\vartheta_{c^+}^n\|_0 + \|\vartheta_{c^-}^n\|_0\right) \\ &\leq Ch^k(\|(c^+)^n\|_{k+1} + \|(c^-)^n\|_{k+1}) + h^{-\frac{d}{2}}\left(\|\vartheta_{c^+}^n\|_0 + \|\vartheta_{c^-}^n\|_0\right).\end{aligned}$$

Combining this estimate with (5.25), readily gives

$$\begin{aligned}|R_2^2| &\leq C\left(\tau h^k + h^{2k+1} + h^k\|\vartheta_{c^+}^{n-1}\|_0\right)|\vartheta_{c^+}^n|_1 + \left(\tau + h^{k+1} + \|\vartheta_{c^+}^{n-1}\|_0\right)\left(h^k + h^{-\frac{d}{2}}(\|\vartheta_{c^+}^n\|_0 + \|\vartheta_{c^-}^n\|_0)\right)|\vartheta_{c^+}^n|_1, \\ |Q_2^2| &\leq C\left(\tau h^k + h^{2k+1} + h^k\|\vartheta_{c^-}^{n-1}\|_0\right)|\vartheta_{c^-}^n|_1 + \left(\tau + h^{k+1} + \|\vartheta_{c^-}^{n-1}\|_0\right)\left(h^k + h^{-\frac{d}{2}}(\|\vartheta_{c^+}^n\|_0 + \|\vartheta_{c^-}^n\|_0)\right)|\vartheta_{c^-}^n|_1.\end{aligned}$$

Next we proceed by induction and consider the following hypothesis

$$h^{-\frac{d}{2}}\left(\|\vartheta_{c^+}^r\|_0 + \|\vartheta_{c^-}^r\|_0\right) \leq M, \qquad r = 1, \cdots, N-1. \tag{5.26}$$

Then for h and τ sufficiently small satisfying $\tau \leq h$ and $k + 1 \geq \frac{d}{2}$ we obtain

$$|R_2^2| \leq M\left(h^{k+\frac{d}{2}} + \|\vartheta_{c^+}^n\|_0 + \|\vartheta_{c^-}^n\|_0\right)|\vartheta_{c^+}^n|_1, \quad \text{and} \quad |Q_2^2| \leq M\left(h^{k+\frac{d}{2}} + \|\vartheta_{c^+}^n\|_0 + \|\vartheta_{c^-}^n\|_0\right)|\vartheta_{c^-}^n|_1. \tag{5.27}$$

Regarding the terms R_2^3 and Q_2^3, we have

$$
\begin{aligned}
R_2^3 &= \left| \left((c^+)^n \nabla(\phi^n - \phi_h^n), \nabla \vartheta_{c^+}^n\right)_h \right| \leq \|(c^+)^n\|_\infty \left(Ch^k + \|(c^+)^n - (c_h^+)^n\|_0 + \|(c^-)^n - (c_h^-)^n\|_0\right) |\vartheta_{c^+}^n|_1 \\
&\leq Ch^k |\vartheta_{c^+}^n|_1 + \left(\|\vartheta_{c^+}^n\|_0 + \|\vartheta_{c^-}^n\|_0\right) |\vartheta_{c^+}^n|_1, \qquad (5.28a) \\
Q_2^3 &= \left| \left((c^-)^n \nabla(\phi^n - \phi_h^n), \nabla \vartheta_{c^-}^n\right)_h \right| \leq \|(c^-)^n\|_\infty \left(Ch^k + \|(c^+)^n - (c_h^+)^n\|_0 + \|(c^-)^n - (c_h^-)^n\|_0\right) |\vartheta_{c^-}^n|_1 \\
&\leq Ch^k |\vartheta_{c^-}^n|_1 + \left(\|\vartheta_{c^+}^n\|_0 + \|\vartheta_{c^-}^n\|_0\right) |\vartheta_{c^-}^n|_1. \qquad (5.28b)
\end{aligned}
$$

Substituting Eqs. (5.24a), (5.27), (5.28a) and (5.24b), (5.27), (5.28b) into (5.23), respectively and rearranging terms, yields the following bounds

$$
|R_2| \leq M \left(h^{k+\frac{d}{2}} + \|\vartheta_{c^+}^n\|_0 + \|\vartheta_{c^-}^n\|_0\right) |\vartheta_{c^+}^n|_1, \quad \text{and} \quad |Q_2| \leq M \left(h^{k+\frac{d}{2}} + \|\vartheta_{c^+}^n\|_0 + \|\vartheta_{c^-}^n\|_0\right) |\vartheta_{c^-}^n|_1.
$$

For the terms R_3 and Q_3, we note that the definition of $\mathcal{D}_h(\cdot;\cdot,\cdot)$ implies

$$
\begin{aligned}
R_3 &= \mathcal{D}_h(\mathbf{u}^n; \mathcal{P}_h(c^+)^n, \vartheta_{c^+}^n) - \mathcal{D}_h(\mathbf{u}_h^n; (c_h^+)^n, \vartheta_{c^+}^n) = \frac{1}{2}\left[\left(\mathbf{u}^n \mathcal{P}_h(c^+)^n, \nabla \vartheta_{c^+}^n\right)_h - \left(\mathbf{u}_h^n (c_h^+)^n, \nabla \vartheta_{c^+}^n\right)_h \right] \\
&\quad - \frac{1}{2}\left[\left(\mathbf{u}^n \cdot \nabla \mathcal{P}_h(c^+)^n, \vartheta_{c^+}^n\right)_h - \left(\mathbf{u}_h^n \cdot \nabla (c_h^+)^n, \vartheta_{c^+}^n\right)_h \right].
\end{aligned}
$$

We note that the above equation, after adding zero as

$$
\begin{aligned}
0 &= (\mathbf{u}_h^n \cdot \nabla \vartheta_{c^+}^n, \vartheta_{c^+}^n)_h - (\mathbf{u}_h^n \cdot \nabla \vartheta_{c^+}^n, \vartheta_{c^+}^n)_h \\
&= \left(\mathbf{u}_h^n \cdot \nabla \vartheta_{c^+}^n, (c_h^+)^n\right)_h - \left(\mathbf{u}_h^n \cdot \nabla \vartheta_{c^+}^n, \mathcal{P}_h(c^+)^n\right)_h - \left(\mathbf{u}_h^n \nabla (c_h^+)^n, \vartheta_{c^+}^n\right)_h + \left(\mathbf{u}_h^n \nabla \mathcal{P}_h(c^+)^n, \vartheta_{c^+}^n\right)_h,
\end{aligned}
$$

can be bounded as follows

$$
|R_3| \leq \frac{1}{2}\left[\left((\mathbf{u}^n - \mathbf{u}_h^n)\mathcal{P}_h(c^+)^n, \nabla \vartheta_{c^+}^n\right)_h - \left((\mathbf{u}^n - \mathbf{u}_h^n) \cdot \nabla \mathcal{P}_h(c^+)^n, \vartheta_{c^+}^n\right)_h \right] := R_3^1 + R_3^2.
$$

For R_3^1, applying the Hölder inequality and the continuity of the projectors $\mathbf{\Pi}_k^0$ with respect to the L^2 and L^4-norms we estimate

$$
\begin{aligned}
|R_3^2| = \left| \left((\mathbf{u}^n - \mathbf{u}_h^n) \cdot \nabla \mathcal{P}_h(c^+)^n, \vartheta_{c^+}^n\right)_h \right| &\leq \|\mathbf{\Pi}_k^0(\mathbf{u}^n - \mathbf{u}_h^n)\|_{0,4} \|\mathbf{\Pi}_{k-1}^0 \nabla \mathcal{P}_h(c^+)^n\|_0 \|\Pi_k^0 \vartheta_{c^+}^n\|_{0,4} \\
&\leq \|\mathbf{u}^n - \mathbf{u}_h^n\|_{0,4} \|\nabla \mathcal{P}_h(c^+)^n\|_0 \|\vartheta_{c^+}^n\|_{0,4}.
\end{aligned}
$$

Using the triangle inequality and Lemma 5.5, we end up with the following upper bound for the second term on the right-hand side of the above inequality and $E \in \mathcal{T}_h$

$$
\|\nabla \mathcal{P}_h(c^+)^n\|_0 \leq \|\nabla (c^+)^n\|_0 + \|\nabla(\mathcal{P}_h(c^+)^n - (c^+)^n)\|_0 \leq \|(c^+)^n\|_1,
$$

which together with the Sobolev embeddings $H^1 \subset L^4$ in turn implies

$$
|R_3^2| \leq \|\mathbf{u}^n - \mathbf{u}_h^n\|_{\mathbf{X}} \|(c^+)^n\|_1 \|\vartheta_{c^+}^n\|_1.
$$

Bounding the term R_3^1 analogously to R_3^2, we can confirm that

$$
R_3^1 \leq \|\mathbf{u}^n - \mathbf{u}_h^n\|_{\mathbf{X}} \|(c^+)^n\|_1 \|\vartheta_{c^+}^n\|_1.
$$

Thus we arrive at the bounds

$$R_3 \le \|\mathbf{u}^n - \mathbf{u}_h^n\|_{\mathbf{X}} \|(c^+)^n\|_1 \|\vartheta_{c^+}^n\|_1, \quad Q_3 \le \|\mathbf{u}^n - \mathbf{u}_h^n\|_{\mathbf{X}} \|(c^-)^n\|_1 \|\vartheta_{c^-}^n\|_1.$$

Step 3: error estimate at a generic n-th time step. We now insert the bounds on $R_1 - R_3$ and $Q_1 - Q_3$ into (5.21) and (5.22), respectively. This yields

$$\begin{aligned}\frac{1}{2\tau}\left(\|\vartheta_{c^+}^n\|_0^2 - \|\vartheta_{c^+}^{n-1}\|_0^2\right) + \beta_1 |\vartheta_{c^+}^n|_1^2 &\le \varpi_1 \|\vartheta_{c^+}^n\|_0 + \left[\varpi_2 + \|\mathbf{u}^n - \mathbf{u}_h^n\|_{\mathbf{X}} + \|\vartheta_{c^+}^n\|_0 + \|\vartheta_{c^-}^n\|_0\right] |\vartheta_{c^+}^n|_1 \\ &\le \frac{1}{2}\left[\varpi_1^2 + \|\vartheta_{c^+}^n\|_0^2\right] + \epsilon |\vartheta_{c^+}^n|_1^2 + \left[\varpi_2 + \|\vartheta_{c^+}^n\|_0 + \|\vartheta_{c^-}^n\|_0\right]^2, \qquad (5.29)\end{aligned}$$

and

$$\begin{aligned}\frac{1}{2\tau}\left(\|\vartheta_{c^-}^n\|_0^2 - \|\vartheta_{c^-}^{n-1}\|_0^2\right) + \beta_1 |\vartheta_{c^-}^n|_1^2 &\le \varpi_3 \|\vartheta_{c^-}^n\|_0 + \left[\varpi_2 + \|\mathbf{u}^n - \mathbf{u}_h^n\|_{\mathbf{X}} + \|\vartheta_{c^+}^n\|_0 + \|\vartheta_{c^-}^n\|_0\right] |\vartheta_{c^-}^n|_1 \\ &\le \frac{1}{2}\left[\varpi_3^2 + \|\vartheta_{c^-}^n\|_0^2\right] + \epsilon |\vartheta_{c^-}^n|_1^2 + \left[\varpi_2 + \|\vartheta_{c^+}^n\|_0 + \|\vartheta_{c^-}^n\|_0\right]^2, \qquad (5.30)\end{aligned}$$

with positive scalars

$$\varpi_1 \le Ch^{k+1} \|\frac{\partial (c^+)^n}{\partial t}\|_{k+1} + \alpha_2 \tau^{1/2} \|\frac{\partial^2 c^+}{\partial t^2}\|_{L^2(L^2)}, \ \varpi_3 \le Ch^{k+1} \|\frac{\partial (c^-)^n}{\partial t}\|_{k+1} + \alpha_2 \tau^{1/2} \|\frac{\partial^2 (c^-)^n}{\partial t^2}\|_{L^2(L^2)},$$
$$\varpi_2 \le Mh^{k+\frac{d}{2}},$$

Summing on n from 0 to j on both sides of (5.29) and (5.30), where $0 \le j \le N$, allow us to obtain

$$\begin{aligned}\frac{1}{2\tau}\left(\|\vartheta_{c^+}^j\|_0^2 - \|\vartheta_{c^+}^0\|_0^2\right) + \sum_{n=0}^{j} |\vartheta_{c^+}^n|_1^2 \le \sum_{n=0}^{j}\left(\varpi_1^2 + \varpi_2^2\right) + \sum_{n=0}^{j}\left(\|\vartheta_{c^+}^n\|_0^2 + \|\vartheta_{c^-}^n\|_0^2 + \|\mathbf{u}^n - \mathbf{u}_h^n\|_{\mathbf{X}}^2\right), \\ \frac{1}{2\tau}\left(\|\vartheta_{c^-}^j\|_0^2 - \|\vartheta_{c^-}^0\|_0^2\right) + \sum_{n=0}^{j} |\vartheta_{c^-}^n|_1^2 \le \sum_{n=0}^{j}\left(\varpi_3^2 + \varpi_2^2\right) + \sum_{n=0}^{j}\left(\|\vartheta_{c^+}^n\|_0^2 + \|\vartheta_{c^-}^n\|_0^2 + \|\mathbf{u}^n - \mathbf{u}_h^n\|_{\mathbf{X}}^2\right).\end{aligned}$$

Summing up these inequalities and employing Theorem 5.1 and Gronwall's inequality, it finally gives

$$\|\vartheta_{c^+}^j\|_0^2 + \|\vartheta_{c^-}^j\|_0^2 + \tau \sum_{n=0}^{j}\left(|\vartheta_{c^+}^n|_1^2 + |\vartheta_{c^-}^n|_1^2\right) \le \tau \sum_{n=0}^{j}\left(\varpi_1^2 + \varpi_2^2 + \varpi_3^2 + \varpi_2^2\right).$$

By following similar processes in Theorem 5.1 and employing Lemma 5.5, the desired result is obtained. □

6. Numerical Results

In this section, we provide numerical experiments to show the performance of linearized, decoupled and conservative VEM for coupled PNP/NS equations. In all examples, we use space V_1^h for approximation concentrations and electrostatic potential variables, and the pair space $(\mathbf{V}_1^h, Q_1^h)$ for the mixed NS problem (velocity and pressure) unless otherwise stated.

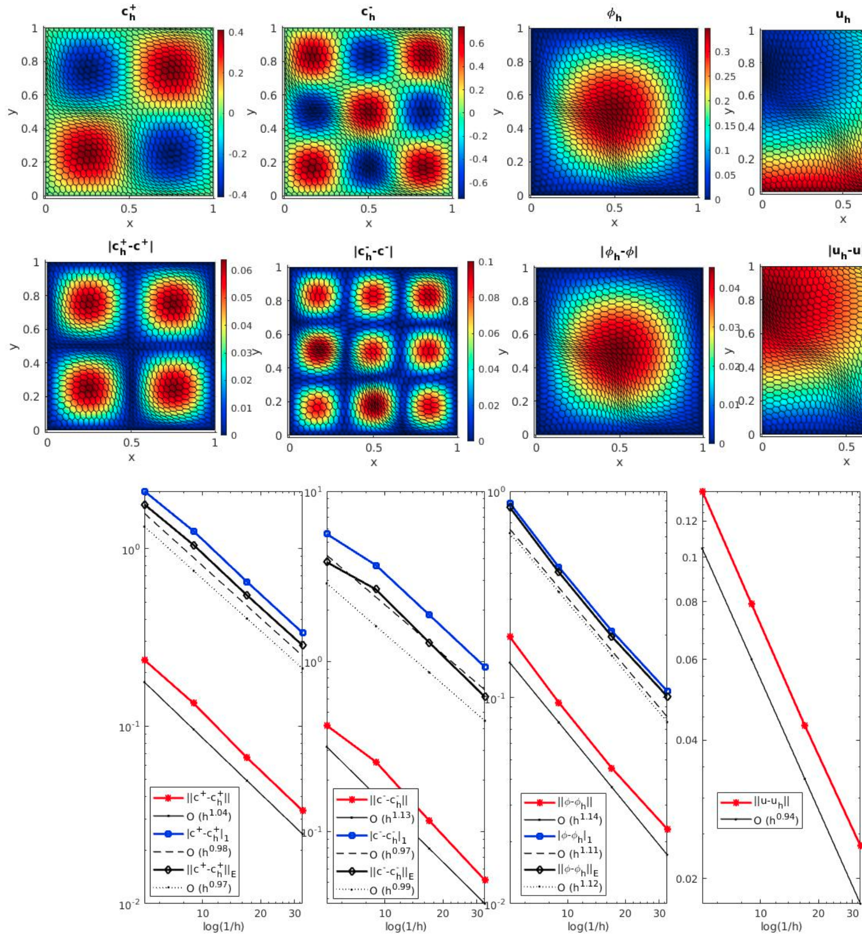

Figure 6.1: Example 1. Snapshots of numerical solutions $\{c_h^+, c_h^-, \phi_h, \mathbf{u}_h\}$ and its absolute error (top) and error history for the verification of convergence (bottom).

6.1. Example 1: Accuracy assessment

In this section we apply the fully discrete VEM and the numerical algorithm developed in Sect. 2 to a numerical example defined below, then validate all theoretical convergence results shown in Theorems 5.1 and 5.6. For this we consider the following closed-form exact solutions to the coupled PNP/NS problem

$$\begin{cases} c^+(x,y,t) = \sin(2\pi x)\sin(2\pi y)\sin(t), \qquad c^-(x,y,t) = \sin(3\pi x)\sin(3\pi y)\sin(2t), \\ \phi(x,y,t) = \sin(\pi x)\sin(\pi y)(1-\exp(-t)), \\ \mathbf{u}(x,y,t) = \begin{pmatrix} -0.5\exp(t)\cos(x)^2\cos(y)\sin(y) \\ 0.5\exp(t)\cos(y)^2\cos(x)\sin(x) \end{pmatrix}, \quad p(x,y,t) = \exp(t)(\sin(x)-\sin(y)), \end{cases} \tag{6.1}$$

defined over the computational domain $\Omega = (0,1)^2$ and the time interval $[0, 0.5]$. The exact velocity is divergence-free and the problem is modified including non-homogeneous forcing and source terms on the momentum and concentration equations constructed using the manufactured solutions (6.1). Moreover, the model parameters for this test are $D_1, D_2, \epsilon = 1$. Approximate errors (computed with the aid of suitable projections) and the associated convergence rates (setting $\tau = h$) generated on a sequence of successively refined grids (uniform hexagon meshes) are displayed in Fig. 6.1 (bottom). One can see the second-order convergence for the total errors of all individual variables in the L^2-norm, and the first-order convergence for errors of concentrations and potential in the H^1-seminorm, which are in agreement with the theoretical analysis. The top panels of the Figure show samples of coarse-mesh approximate solutions together with absolute errors.

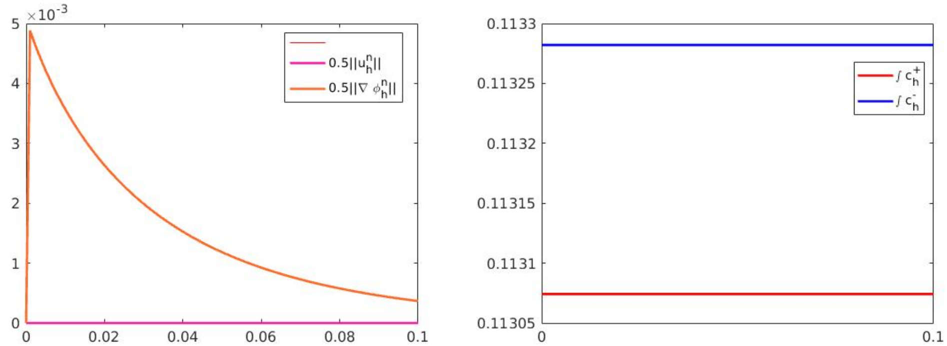

Figure 6.2: Example 2. Evolution of electric (and kinetic) energy (left) and global masses (right) with τ = 1e-3.

6.2. Example 2: Dynamics of the PNP/NS equations with initial discontinuous concentrations

In this example, we investigate the dynamics of the PNP equation on the unit square with an initial value as follows (see [40, 19, 20])

$$c_0^+ = \begin{cases} 1 & (0,1)^2 \backslash \{(0,0.75)\times(0,1) \cup (0.75,1)\times(0,\frac{11}{20})\}, \\ \text{1e-06} & \text{otherwise}, \end{cases}$$

$$c_0^- = \begin{cases} 1 & (0,1)^2 \backslash \{(0,0.75)\times(0,1) \cup (0.75,1)\times(\frac{9}{20},1)\}, \\ \text{1e-06} & \text{otherwise}. \end{cases}$$

and $\mathbf{u}_0 = \mathbf{0}$. The discontinuity of the initial concentrations represents an interface between the the electrolyte and the solid surfaces, and the phenomenon of electrosmosis (transport of ions from the electrolyte towards the solid surface) is expected to arise. We consider a fixed time step of τ =1e-03 and a coarse polygonal mesh with mesh size $h = 1/64$. We show snapshots of the numerical solutions (concentrations and electrostatic potential) at times t_F =2e-03, t_F =2e-02 and t_F =0.1 in Fig 6.3. All plots confirm that the obtained results qualitatively match with those obtained in, e.g., [40, 19, 20] (which use similar decoupling schemes). Moreover, Fig. 6.2 shows that the total discrete energy is decreasing and the numerical solution is mass preserving during the evolution, which verifies numerically our findings from Theorems 3.1 and 3.2.

6.3. Example 3: Application to water desalination

The desalination of alternative waters, such as brackish and seawater, municipal wastewater, and industrial wastewater, has become an increasingly important strategy for addressing water shortages and expanding traditional water supplies. Electrodialysis (ED) is a membrane desalination technology that uses semi-permeable ion-exchange membranes (IEMs) to selectively separate salt ions in water under the influence of an electric field [48]. An ED structure consists of pairs of cation-exchange membranes (CEMs) and anion-exchange membranes (ARMs), alternately arranged between a cathode and an anode (Figure 6.4, left). The driving force of ion transfer in the electrodialysis process is the electrical potential difference's applied between an anode and a cathode which causes ions to be transferred out of the aquatic environment and water purification. When an electric field is applied by the electrodes, the appearing charge at the anode surface becomes positive (and at the cathode surface becomes negative). The applied electric field causes positive ions (cations) to migrate to the cathode and negative ions (anions) to the anode. During the migration process, anions pass through anion-selective membranes but are returned by cation-selective membranes. A similar process occurs for cations in the presence of cationic and anionic membranes. As a result of these events, the ion concentration in different parts intermittently decreases and increases. Finally, an ion-free dilute solution and a concentrated solution as saline or concentrated

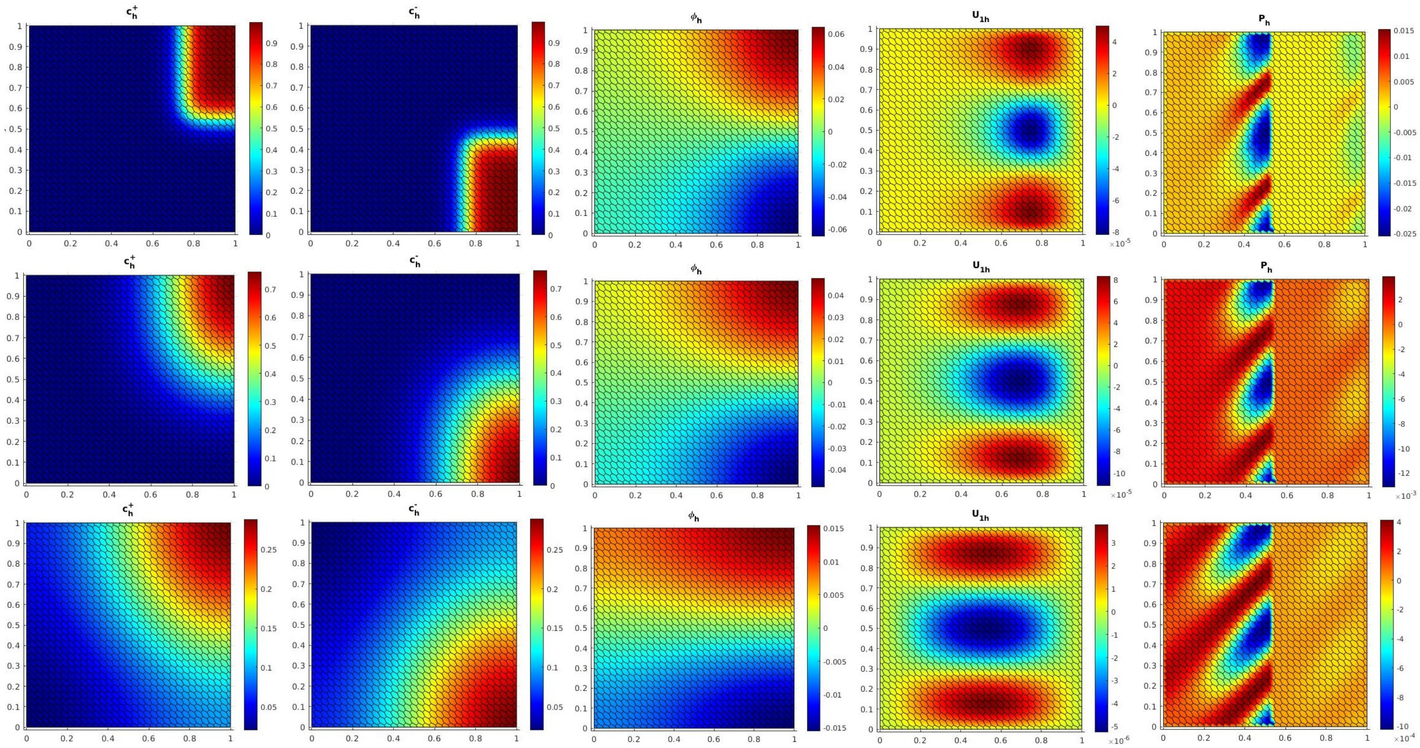

Figure 6.3: Example 2. Snapshots of the approximate solutions $\{c_h^+, c_h^-, \phi_h, \mathbf{u}_h, p_h\}$ obtained with the proposed VEM, and shown at times t_F =2e-03 (top row), t_F =2e-02 (middle) and t_F =1e-01 (bottom).

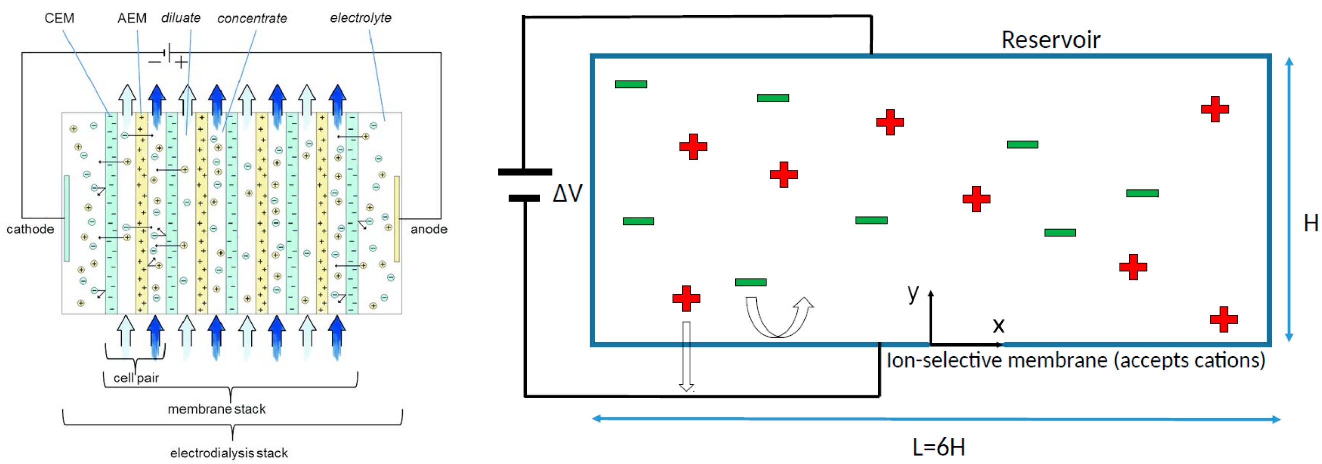

Figure 6.4: Example 3. Schematic of an electrodialysis stack [23] (left) and simplified configuration of a 2D problem with ion-selective membrane from [18] (right).

water are out of the system. In what follows we investigate the effects of the applied voltage and salt concentration on electrokinetic instability appearing in ED processes. For this purpose, simulations of a binary electrolyte solution near a CEM are conducted. Since CEMs and AEMs have similar hydrodynamics and ion transport, the present findings can be applied to AEMs.

The simulations presented here are based on the 2D configuration by [18] (see also [32, 45]). This problem consists of a reservoir on top and a CEM at the bottom that allows cationic species to pass-through (Fig. 6.4, right). An electric field, i.e., $E = \frac{\Delta V}{H}$, is applied in the orientation perpendicular to the membrane and the reservoir. Here, we set the 2D computational domain as $\Omega = [0, 4] \times [0, 1]$ and consider

Case	α	β	Number of elements	Time step
3A: Baseline	1	$30, 40, 120$	32×32	1e-06
3B: Low	10	120	400×100	1e-07
3C: Medium	100	120	400×100	1e-08

Table 6.1: Example 3. Model and discretization parameters to be varied according to each simulated case.

the NS momentum balance equation using the following non-dimensionalization

$$\frac{1}{S_c}\left(\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) - \Delta\mathbf{u} + \nabla p + \frac{\kappa}{\epsilon}(c^+ - c^-)\nabla\phi = \mathbf{0}.$$

The model parameters common to all considered cases are the Schmidt number S_c =1e-03, the rescaled Debye length ϵ =2e-03, and the electrodynamics coupling constant $\kappa = 0.5$. The initial velocity is zero, and the initial concentrations are determined by the randomly perturbed fields, that is:

$$c_0^+(x,y,0) = \alpha\ \mathrm{rand}(x,y)(2-y), \qquad c_0^-(x,y,0) = \alpha\ \mathrm{rand}(x,y)y,$$

where $\mathrm{rand}(x,y)$ is a uniform random perturbation between 0.98 and 1. Mixed boundary conditions are set at the top $\partial\Omega_{top}$ and bottom Ω_{bot} segments of the boundary, and periodic boundary conditions on the vertical walls $\partial\Omega_{lr}$

$$\begin{cases} c^+ = \alpha, \quad c^- = \alpha, \quad \phi = \beta, \quad \mathbf{u} = \mathbf{0}, & \text{on } \partial\Omega_{top}, \\ c^+ = 2\alpha, \quad \nabla c^- \cdot \mathbf{n} = 0, \quad \phi = 0, \quad \mathbf{u} = \mathbf{0}, & \text{on } \partial\Omega_{bot}, \\ u(4,y,t) = u(0,y,t), \quad \forall u \in \{c^+, c^-, \phi, \mathbf{u}\}, & \text{on } \partial\Omega_{lr}. \end{cases}$$

where α and β assume different values in the different simulation cases (see Table 6.1). We utilize triangular meshes which are sufficiently refined towards the ion-selective membrane (i.e., $y = 0$). The number of cells and the computational time step are listed in Table 6.1, right columns.

Example 3A: Effect of the applied voltage. Figs. 6.5 and 6.6 show images of the anion concentration, velocity, and electric potential for $V = 30$ and $V = 40$, representative of the 2D baseline simulation. One can see, in the beginning, at times t =3e-03 for $V = 30$ (and t =8e-04 for $V = 40$), the solutions are still quite similar to the initial condition. As time progresses, electrokinetic instabilities (EKI) appear near the surface of the membrane. As a consequence of the EKI, the contours of vertical velocity show that disturbances are increasing. Higher voltages cause the instability to set in earlier. A periodic structure above the membrane can be observed after the disturbance amplitudes are high enough. Structures are seen at more anion concentrations than electrical potentials. The disturbances at times t =2e-02 ($V = 30$) and 7e-03 ($v = 40$) are strong enough, which cause a significant distortion in the electrical potential. The merging of neighboring structures leads to the formation of larger structures, as evidenced in the snapshot at 5e-02 for $V = 40$.

As it can be seen from Fig. 6.7, by increasing the voltage to $V = 120$ the instability becomes stronger, the disturbances grow faster, and the structures appear earlier. Smaller structures have coalesced into bigger ones at time t =3.3e-03. Such a behavior is consistent with the results in [32, 33] and it is fact similar to the encountered in fluid mechanics vortex fusion.

Example 3B: Effect of salt concentration. Finally, we considered a fixed applied voltage of $V = 120$. A NaCl concentration of 10 was simulated for slightly brackish water and also increasing that concentration to 100 for moderately brackish water. By increasing the concentration, the structures reveal themselves earlier and their size decreases (see Fig. 6.8, left). In the second case, structures appeared much sooner (and were much smaller). For the 100 concentration case, similar findings can be obtained (see Fig. 6.8, right column). Based on this, it can be concluded that the start of the instability depends also on the ion concentration, in addition to voltage.

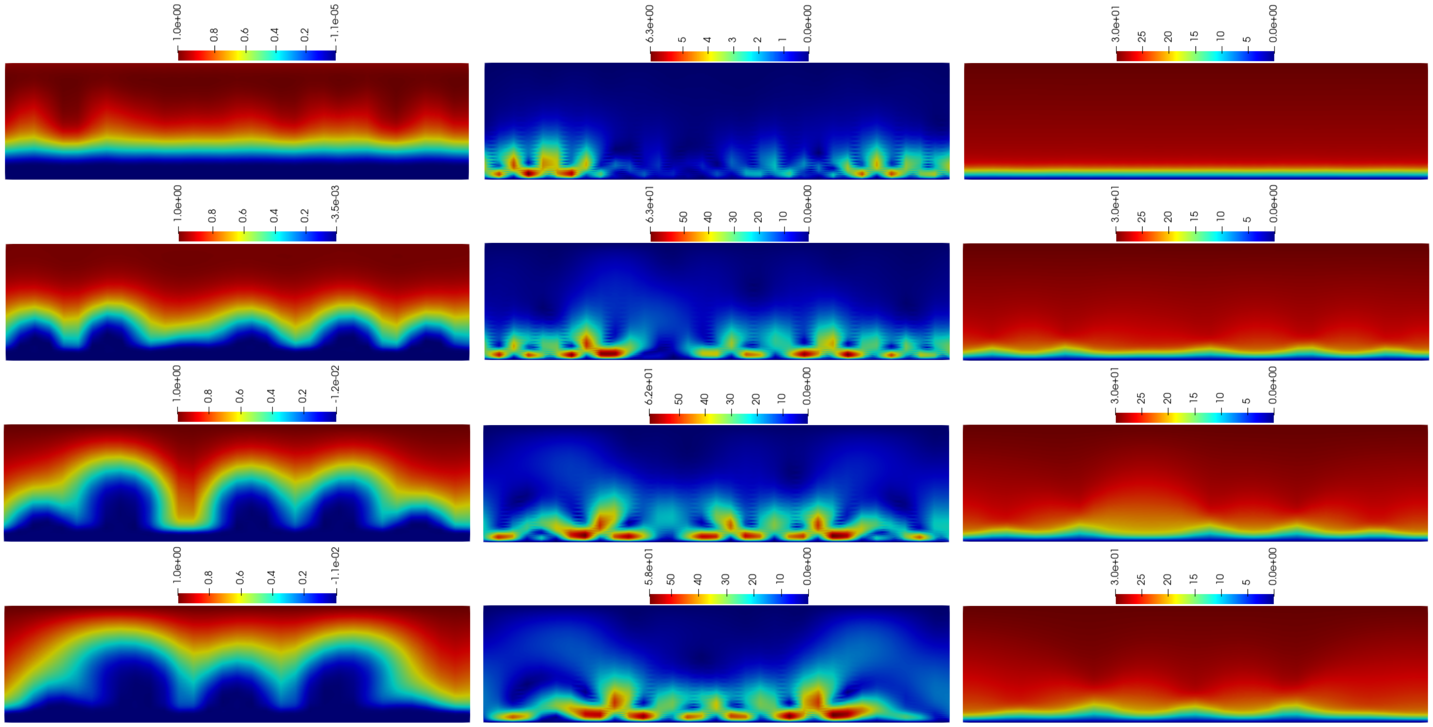

Figure 6.5: Example 3A. Snapshots of numerical solutions c_h^- (left), $\mathbf{u}_h$ (middle) and ϕ_h (right) using the VEM at times t_F =3e-03, t_F =2e-02, t_F =5e-02 and t_F =8e-02 with voltage $V = 30$.

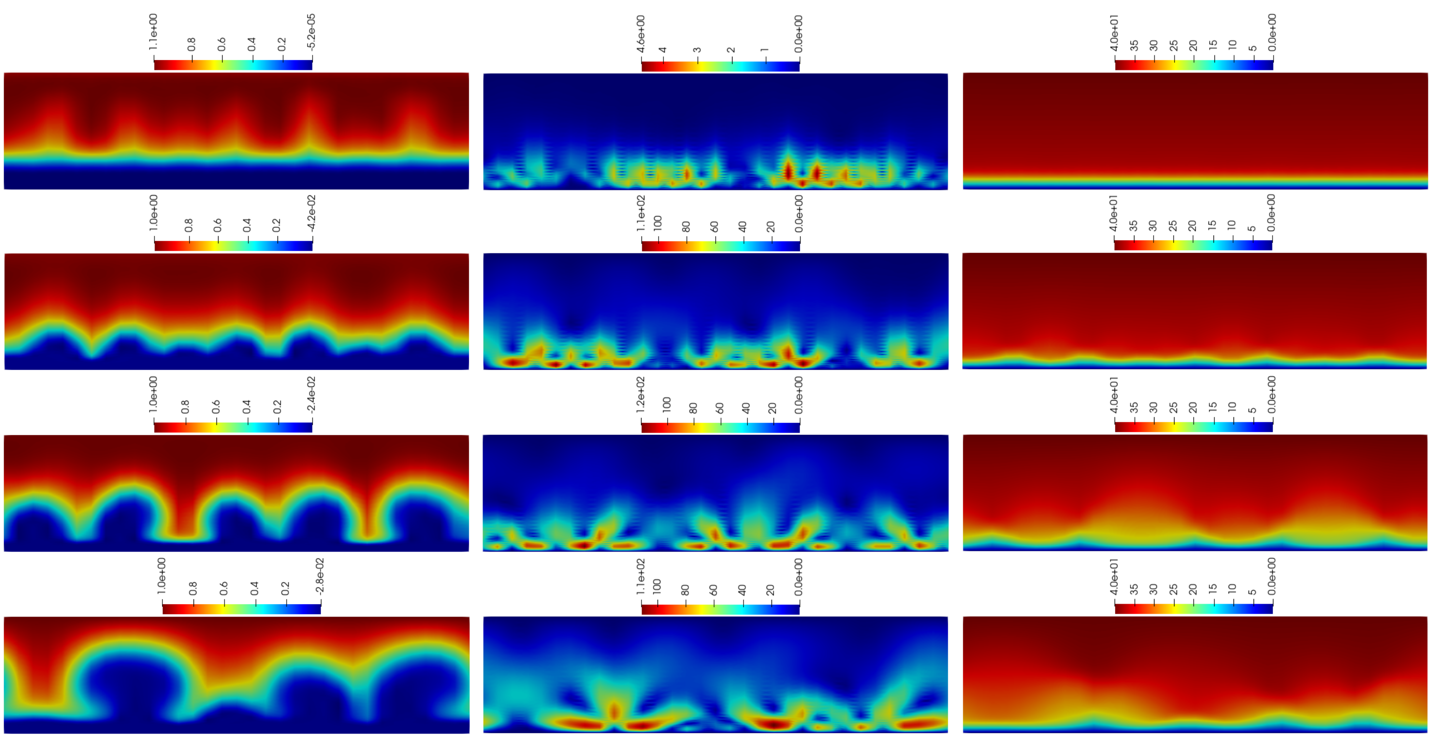

Figure 6.6: Example 3A. Snapshots of numerical solutions c_h^- (left), $\mathbf{u}_h$ (middle) and ϕ_h (right) using the VEM at times t_F =3e-03, t_F =2e-02, t_F =5e-02 and t_F =8e-02 with voltage $V = 40$.

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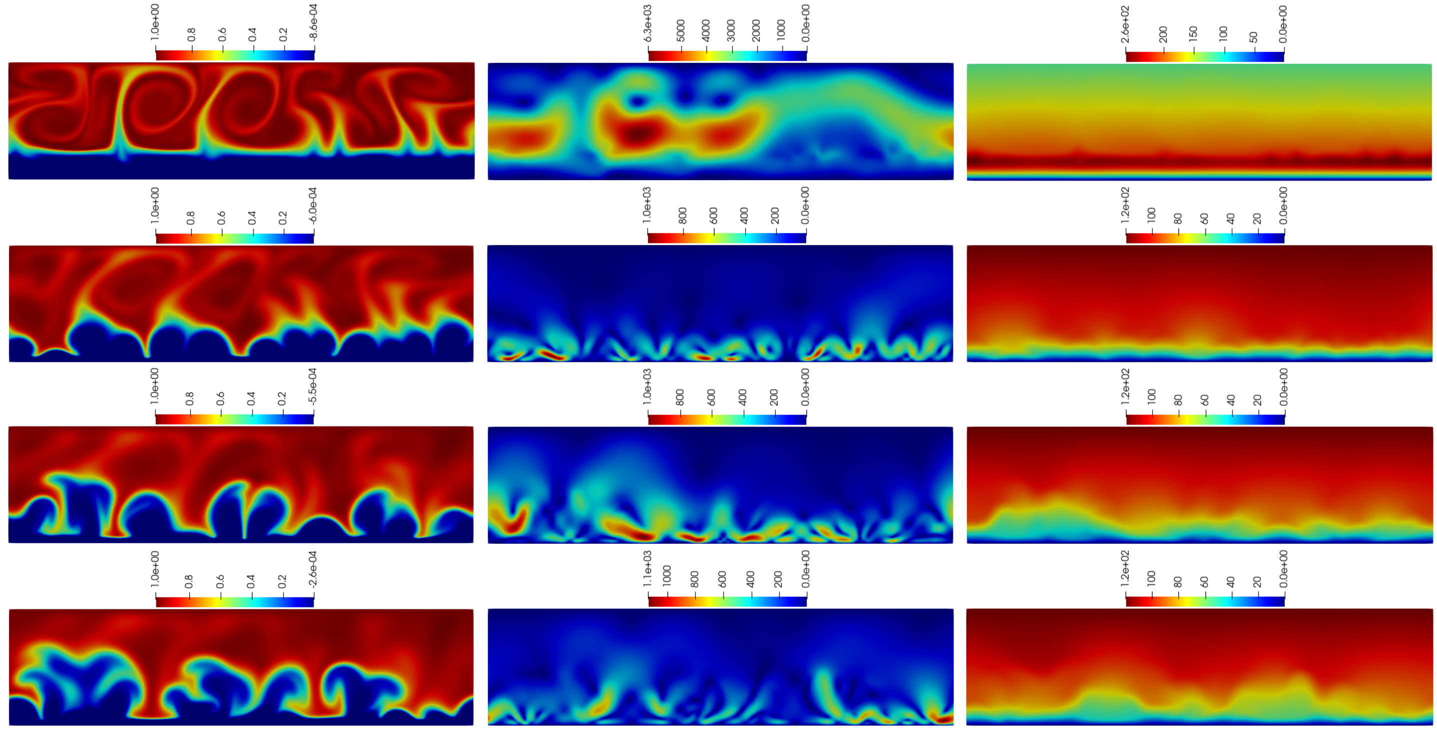

Figure 6.7: Example 3A. Snapshots of numerical solutions c_h^- (left), $\mathbf{u}_h$ (middle) and ϕ_h (right) using the VEM at times t_F =3e-03, t_F =2e-02, t_F =5e-02 and t_F =8e-02 with voltage $V = 120$.

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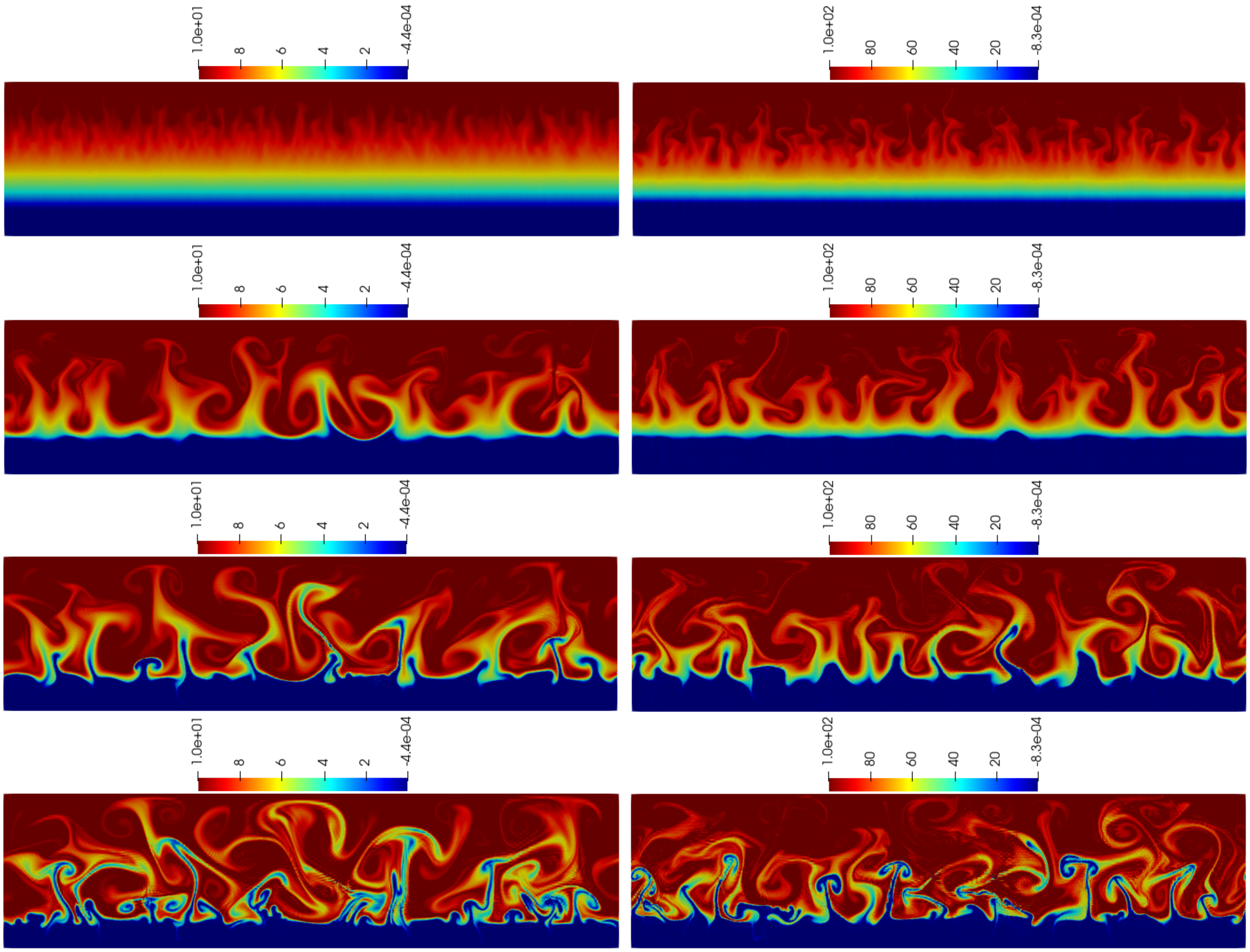

Figure 6.8: Example 3B. Snapshots of numerical solutions c_h^- with voltage $V = 120$, for NaCl=10 at times t_F =5e-07, t_F =2e-06, t_F =3e-06 and t_F =5e-06 (left); and for NaCl = 100 t_F =5e-07, t_F =1e-06, t_F =1.5e-06 and t_F =2e-06 (right).

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