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

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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. These equations model microfluidic and electrochemical systems that include the 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. The global mass conservation and electric energy decay of the scheme are also established. Also, we rigorously derive unconditionally optimal error estimates for both the electrostatic potential and ionic concentrations of PNP equations in the L^2 and H^1-norms, as well as for the velocity and pressure of NS equations in the $\mathbf{L}^2$, $\mathbf{H}^1$- 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 are relevant in applications of water desalination.

Keywords Coupled Poisson–Nernst–Planck/Navier–Stokes equations · mixed virtual element method · optimal convergence · charged species transport · electrokinetic instability · water desalination · microfluidic systems.

Mathematics Subject Classification (2010) 65L60 · 82B24.

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., [36]). 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. 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., [15, 16, 20, 33, 37, 43, 44, 52] 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 [35, 45], 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, [34, 48, 49] and the references therein.

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Reliable computational results may also be 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 [39]. Although numerical methods of different types have been used by computational physicists, biophysicists and other practitioners over many decades, the rigorous analysis of numerical schemes is relatively much 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 [17, 18, 25, 26, 30–32, 39, 40, 46, 47, 56].

Since the formulation of FEMs requires explicit knowledge of the basis functions, such 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. As an extension of FEMs onto polygonal/polyhedral meshes, VEMs were introduced in [2]. 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.

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 purpose 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. VEMs for general second-order elliptic problems were presented in [13]. 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 [6]. Other formulations (of mixed, discontinuous, nonconforming, and other types) for NS include [7, 27, 41, 51, 53], whereas for the PNP system a VEM scheme has been recently proposed in [42]. The present method also follows other VEM formulations for Stokes flows from [5, 11, 12, 54]. For a more thorough survey, we refer to [3, 9] 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 VE discretization, introducing the mesh entities, the degrees of freedom, the construction of VE spaces, and establishing properties of the discrete multilinear forms. In Section 4, we obtain two conservative properties global mass conservation and electric (and kinetic) energy conservation of the proposed scheme. In Section 3, 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. Finally, Section 7 has concluding remarks.

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., [21, 28], 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-boundary conditions, and appropriate initial conditions)

$$
\begin{aligned}
\partial_t c_i - \operatorname{div}\left(\kappa_i(\nabla c_i + e_i c_i \nabla\phi)\right) + \operatorname{div}(\mathbf{u} c_i) &= 0, && \text{in } \Omega \times (0, t_F], && \text{(1.1a)}\\
-\operatorname{div}(\epsilon\nabla\phi) &= c_1 - c_2, && \text{in } \Omega \times (0, t_F], && \text{(1.1b)}\\
\partial_t \mathbf{u} - \boldsymbol{\Delta}\mathbf{u} + (\mathbf{u}\cdot\boldsymbol{\nabla})\mathbf{u} + \nabla p = -(c_1 - c_2)\nabla\phi&, && \text{in } \Omega \times (0, t_F], && \text{(1.1c)}\\
\operatorname{div}(\mathbf{u}) &= 0, && \text{in } \Omega \times (0, t_F], && \text{(1.1d)}\\
(\nabla c_i + \mathbf{u} c_i)\cdot\mathbf{n} = \nabla\phi\cdot\mathbf{n} = 0, \quad \mathbf{u} &= \mathbf{0}, && \text{on } \partial\Omega \times (0, t_F], && \text{(1.1e)}
\end{aligned}
$$

$$c_i(\mathbf{x},0) = c_{i,0}(\mathbf{x}), \quad \phi(\mathbf{x},0) = \phi_0(\mathbf{x}), \quad \mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}), \qquad \text{in } \Omega, \tag{1.1f}$$

where $i \in \{1,2\}$, c_1, c_2 are the concentrations of positively and negatively charged ions with valences $e_1 = 1$ and $e_2 = -1$, 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 (assumed a positive constant) and κ_1 and κ_2 are diffusion/mobility coefficients (assumed also constant and positive). 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. According to the homogeneous boundary condition (1.1e), to show the well-posedness of the PNP/NS equations – and in particular, the Poisson equation (1.1b) with pure Neumann boundary conditions– one needs the following initial electroneutrality condition:

$$\int_\Omega (c_1(\mathbf{x},0) - c_2(\mathbf{x},0))\,\mathrm{d}\mathbf{x} = 0. \tag{1.2}$$

Based on (1.1e), the above condition induces the following result

$$\int_\Omega c_1(\mathbf{x},t)\,\mathrm{d}\mathbf{x} \equiv \int_\Omega c_{1,0}(\mathbf{x})\,\mathrm{d}\mathbf{x} = \int_\Omega c_{2,0}(\mathbf{x})\,\mathrm{d}\mathbf{x} \equiv \int_\Omega c_2(\mathbf{x},t)\,\mathrm{d}\mathbf{x}.$$

In addition, since ϕ is unique up to a constant, we consider the zero mean value solution ϕ which satisfies $(\phi,1)_0 = 0$.

1.4 Notation and weak formulation

Throughout the paper, let $\mathcal{D}$ be any given open subset of Ω. By $(\cdot,\cdot)_{0,\mathcal{D}}$ and $\|\cdot\|_{0,\mathcal{D}}$ we denote the usual integral inner product and the corresponding norm of $\mathrm{L}^2(\mathcal{D})$. 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 $\mathrm{H}^m(\mathcal{D}) := W^{m,2}(\mathcal{D})$, $\|\cdot\|_{m,\mathcal{D}} := \|\cdot\|_{m,2,\mathcal{D}}$ and $|\cdot|_{m,\mathcal{D}} := |\cdot|_{m,2,\mathcal{D}}$. If $\mathcal{D} = \Omega$, the subscript will be omitted. By $\mathbf{M}$ we denote the corresponding vectorial counterpart of the generic scalar functional space M. We recall the following well known functional spaces which will be useful in the sequel

$$\mathbf{H}_0^1(\Omega) := \left\{\mathbf{v} \in \mathbf{H}^1(\Omega) : \quad \mathbf{v} = \mathbf{0} \ \text{ on } \partial\Omega\right\},$$
$$\mathring{\mathrm{H}}^1(\Omega) := \left\{v \in \mathrm{H}^1(\Omega) : \quad (v,1)_0 = 0\right\}.$$

Let us introduce the following functional spaces and their corresponding norms for velocity, pressure, and concentrations and electrostatic potential

$$\boldsymbol{X} := \mathbf{H}_0^1(\Omega), \qquad Y := \mathrm{L}_0^2(\Omega), \qquad \mathbf{Z} := Z \times Z, \qquad \mathring{Z} := \mathring{\mathrm{H}}^1(\Omega),$$

respectively, with $Z := \mathrm{H}^1(\Omega)$. For functions of both spatial $\mathbf{x} \in \Omega$ and temporal variables $t \in J := [0, t_F]$, and given a Banach space V endowed with the norm $\|\cdot\|_V$, we will also use the standard function spaces $\mathrm{L}^2(J;V)$ and $\mathrm{L}^\infty(J;V)$ whose norms are defined by:

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

Also, for any vector fields $\mathbf{v} = (v_1, v_2)^{\mathbf{t}}$ and $\mathbf{w} = (w_1, w_2)^{\mathbf{t}}$ we set the gradient, divergence and inner (and tensor) product operators, as

$$\boldsymbol{\nabla}\mathbf{v} := (\nabla v_1, \nabla v_2), \quad \operatorname{div}\mathbf{v} := \partial_x v_1 + \partial_y v_2, \quad \mathbf{v}\cdot\mathbf{w} := v_1 w_1 + v_2 w_2, \quad \mathbf{v}\otimes\mathbf{w} := (w_1\mathbf{v}, w_2\mathbf{v}),$$

respectively. In addition, for any tensor fields $\boldsymbol{\tau} = (\boldsymbol{\tau}_1, \boldsymbol{\tau}_2)$ and $\boldsymbol{\zeta} = (\boldsymbol{\zeta}_1, \boldsymbol{\zeta}_2)$, we write as usual

$$\mathbf{v}\cdot\boldsymbol{\tau} := (\mathbf{v}\cdot\boldsymbol{\tau}_1, \mathbf{v}\cdot\boldsymbol{\tau}_2)^{\mathbf{t}}, \qquad \boldsymbol{\tau} : \boldsymbol{\zeta} := \sum_{i=1}^{2} \boldsymbol{\tau}_i \cdot \boldsymbol{\zeta}_i.$$

Next, in order to write the variational formulation of problem (1.1), we introduce the following bilinear (and trilinear) forms

$$\begin{aligned}
\mathcal{M}_1(\cdot,\cdot),\ \mathcal{A}_i(\cdot,\cdot),\ \mathcal{A}_3(\cdot,\cdot) : Z \times Z \to \mathbb{R} \qquad & \mathcal{M}_1(\omega,z) := (\omega,z)_0,\ \ \mathcal{A}_i(\omega,z) := (\kappa_i\nabla\omega,\nabla z)_0,\ \ \mathcal{A}_3(\omega,z) := (\epsilon\nabla\omega,\nabla z)_0,\\
\mathcal{M}_2(\cdot,\cdot),\ \mathcal{K}(\cdot,\cdot) : \mathbf{X} \times \mathbf{X} \to \mathbb{R} \qquad & \mathcal{M}_2(\mathbf{w},\mathbf{v}) := (\mathbf{w},\mathbf{v})_0,\ \ \mathcal{K}(\mathbf{w},\mathbf{v}) := (\boldsymbol{\nabla}\mathbf{w},\boldsymbol{\nabla}\mathbf{v})_0,\\
\mathcal{B}(\cdot,\cdot) : Y \times \mathbf{X} \to \mathbb{R} \qquad & \mathcal{B}(q,\mathbf{v}) := (q,\operatorname{div}(\mathbf{v}))_0,\\
\mathcal{C}_i(\cdot;\cdot,\cdot) : Z \times \mathring{Z} \times Z \to \mathbb{R} \qquad & \mathcal{C}_i(\omega;\psi,z) := (\kappa_i\omega\nabla\psi,\nabla z)_0.
\end{aligned}$$

As usual for convective problems, for $\mathbf{u}, \mathbf{v}, \mathbf{w} \in \boldsymbol{X}$ and using that $\mathrm{div}(\mathbf{u}) = 0$, we utilize the following equivalent skew–symmetric forms for the terms $(\mathrm{div}(\mathbf{u}\,\omega), z)_0$ and $((\mathbf{u}\cdot\boldsymbol{\nabla})\mathbf{w}, \mathbf{v})_0$, respectively (see, e.g., [10])

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

The weak formulation of (1.1) consists in finding, for almost all $t \in J$, the functions $\{(c_1(t), c_2(t)), \phi(t)\} \in \mathbf{Z} \times \mathring{Z}$ and $\{\mathbf{u}(t), p(t)\} \in \mathbf{X} \times Y$ such that $\partial_t c_i \in \mathrm{L}^2(J; H^{-1}(\Omega))$, $\partial_t \mathbf{u} \in \mathrm{L}^2(J; \mathbf{H}^{-1}(\Omega))$ and such that for $i \in \{1,2\}$ the following relations hold

$$\mathcal{M}_1(\partial_t c_i, z_i) + \mathcal{A}_i(c_i, z_i) + e_i\mathcal{C}_i(c_i;\phi, z_i) - \mathcal{D}(\mathbf{u}; c_i, z_i) = 0 \qquad \forall z_i \in Z, \tag{1.3a}$$
$$\mathcal{A}_3(\phi,\psi) = \mathcal{M}_1(c_1,\psi) - \mathcal{M}_1(c_2,\psi) \qquad \forall \psi \in \mathring{Z}, \tag{1.3b}$$
$$\mathcal{M}_2(\partial_t \mathbf{u}, \mathbf{v}) + \mathcal{K}(\mathbf{u},\mathbf{v}) + \mathcal{E}(\mathbf{u};\mathbf{u},\mathbf{v}) - \mathcal{B}(p,\mathbf{v}) = -\left((c_1 - c_2)\nabla\phi, \mathbf{v}\right) \qquad \forall \mathbf{v} \in \mathbf{X}, \tag{1.3c}$$
$$\mathcal{B}(q,\mathbf{u}) = 0 \qquad \forall q \in Y, \tag{1.3d}$$

endowed with initial conditions $c_i(\cdot,0) = c_{i,0}$ and $\mathbf{u}(\cdot,0) = \mathbf{u}_0$. The existence and uniqueness of a weak solution to (1.3) has been proved in [49], for the 2D case.

We end this section with the presentation of the Gagliardo–Nirenberg inequality which will be frequently used in our proofs.

Lemma 1.1 *(**Gagliardo–Nirenberg inequality** [60]) Let j and m be non-negative integers such that $j < m$. Furthermore, let $p, q, r \geq 1$ be real and $a \in [0,1]$ such that*

$$\frac{1}{q} = \frac{j}{d} + a\left(\frac{1}{r} - \frac{m}{d}\right) + (1-a)\frac{1}{p}, \qquad \frac{j}{m} \leq a \leq 1,$$

holds. Then

$$\|D^j v\|_{0,q} \leq \|D^m v\|_{0,r}^a \|v\|_{0,p}^{1-a}.$$

2 Virtual element approximation

The chief target of this section is to present the VE spaces and required discrete bilinear (and trilinear) forms. The presentation is restricted to the 2D case, for which the well-posedness of the continuous problem is available.

2.1 Mesh notation and mesh regularity

By $\{\mathcal{T}_h\}_h$ we will denote a sequence of partitions of 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 $\mathcal{E}_h^I = \mathcal{E}_h \backslash \partial\Omega$ ($\mathcal{E}_h^B = \mathcal{E}_h \cap \partial\Omega$) be the set of all interior edges. By $\mathbf{n}_E^e$, we denote the unit normal (pointing outwards) vector of E for any edge $e \in \partial E \cap \mathcal{E}_h$. Following, for example, [2,4,8,14], we adopt the following regularity assumption

Assumption 2.1 *There exist constants $\rho_1, \rho_2 > 0$ such that:*

- *Every element E is shaped like a star with respect to a ball with radius $\geq \rho_1 h_E$,*
- *In E, the distance between every two vertices is $\geq \rho_2 h_E$.*

The above assumption implies that the following inverse inequality holds:

$$\|\varrho\|_{0,q,E} \leq \mathrm{c_{inv}}\, h_E^{d(\frac{1}{q}-\frac{1}{p})} \|\varrho\|_{0,p,E} \qquad \text{for } 1 \leq p \leq q \leq \infty, \tag{2.1}$$

for all piecewise polynomial functions ϱ, with $\mathrm{c_{inv}}$ independent of h_E.

2.2 Construction of a virtual element space for $\mathbf{Z}$ and $\mathring{Z}$

This subsection is devoted to introducing the VE subspaces $\mathbf{Z}_h \subset \mathbf{Z}$ and $\mathring{Z}_h \subset \mathring{Z}$. In order to do that, we recall the definition of some 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 $\mathbb{P}_{-1}(E) := \{0\}$) with dimension $\pi_k = (k+1)(k+2)/2$.
- $\mathbb{P}_k(e)$ the set of polynomials of degree at most k on e (with the extended notation $\mathbb{P}_{-1}(e) := \{0\}$).
- $\mathbb{B}_k(\partial E) := \{z_h \in C^0(\partial E) : \quad z_h|_e \in \mathbb{P}_k(e) \quad \text{for all edges } e \subset \partial E\}$.
- $\widetilde{Z}_k(E) := \left\{z_h \in C^0(E) \cap \mathrm{H}^1(E) : \quad z_h|_{\partial E} \in \mathbb{B}_k(E), \quad \Delta z_h \in \mathbb{P}_k(E)\right\}$.
- $\mathbb{P}_k(\mathcal{T}_h) := \{q \in \mathrm{L}^2(\Omega) : \quad q|_E \in \mathbb{P}_k(E) \ \text{ for all } E \in \mathcal{T}_h\}$.

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 $\Pi_k^{0,E} : \mathrm{L}^2(E) \to \mathbb{P}_k(E)$, given by

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

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

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

Finally, let k be a fixed positive integer and consider the following local VE space on each $E \in \mathcal{T}_h$ (see. [1])

$$Z_k(E) := \left\{ z_h \in \widetilde{Z}_k(E) : \quad (\Pi_k^{\nabla,E} z_h - z_h, q_k^*)_{0,E} = 0 \qquad \forall q_k^* \in \mathcal{M}^*_{k-1}(E) \cup \mathcal{M}^*_k(E) \right\},$$

and a subspace of $Z_k(E)$ by

$$\mathring{Z}_k(E) := \{ z_h \in Z_k(E) : \quad (z_h, 1)_{0,E} = 0 \}.$$

And its degrees of freedom (guaranteeing unisolvency) are as follows (see, e.g., [13]):

- (**D1**) The value of z_h at the i-th vertex of the element E.
- (**D2**) The values of z_h at $k-1$ distinct points in e, for all $e \subset \partial E$, and for $k \geq 2$.
- (**D3**) The internal moment $(z_h, q_{k-2})_{0,E}$, for all $q_{k-2} \in \mathcal{M}_{k-2}(E)$, and $k \geq 2$.

It is noteworthy that for any $z_h \in Z_k(E)$ projections $\Pi_k^{0,E} z_h$ and $\Pi_k^{\nabla,E} z_h$ are computable from knowing (**D1**) – (**D3**) (see, e.g., [13]). Similarly to the FE case, the global VE space can be assembled as:

$$Z_h := \{ z_h \in Z : \quad z_h|_E \in Z_k(E) \quad \forall E \in \mathcal{T}_h \}, \quad \text{and} \quad \mathring{Z}_h := \{ z_h \in Z : \quad z_h|_E \in \mathring{Z}_k(E) \quad \forall E \in \mathcal{T}_h \},$$

Finally, we define a VE space on $\mathcal{T}_h$ for the concentrations as follows:

$$\mathbf{Z}_h := Z_h \times Z_h.$$

Also, for any element $E \in \mathcal{T}_h$ and $z_h \in Z_h$, the global projection operators Π_k^0 and Π_k^∇ on space Z_h are defined as follow

$$\Pi_k^0(z_h)|_E = \Pi_k^{0,E}(z_h|_E), \qquad \text{and} \qquad \Pi_k^\nabla(z_h)|_E = \Pi_k^{\nabla,E}(z_h|_E).$$

Approximation properties in the local space $Z_k(E)$. The following estimates (established using Assumption 2.1) can be obtained for the projection and interpolation operators [2].

- For any $z \in \mathrm{H}^s(E)$ with $s \in [1, k+1]$ there exists $z_\pi \in \mathbb{P}_k(E)$ such that

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

- For any $z \in \mathrm{H}^s(E)$ with $s \in [2, k+1]$ there exists $z_I \in Z_k(E)$ such that

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

2.3 Construction of a VE space approximating $\mathbf{X}$

Following [5], for $k \geq 2$ let us introduce the spaces

$$\mathcal{G}_k(E) := \nabla \mathbb{P}_{k+1}(E) \subset [\mathbb{P}_k(E)]^2, \qquad \mathcal{G}_k(E)^{\perp} := \mathbf{x}^{\perp}[\mathbb{P}_{k-1}(E)] \subset [\mathbb{P}_k(E)]^2 \text{ with } \mathbf{x}^{\perp} := (x_2, -x_1),$$

$$\widetilde{\mathbf{X}}_k(E) := \Big\{ \mathbf{v} \in [\mathrm{H}^1(E)]^2 \quad \text{s.t } \mathbf{v}\,|_{\partial E} \in [\mathbb{B}_k(\partial E)]^2 \quad \begin{array}{l} \text{(i) } \operatorname{div} \mathbf{v} \in \mathbb{P}_{k-1}(E), \\ \text{(ii) } -\boldsymbol{\Delta} \mathbf{v} - \nabla w \in \mathcal{G}_k(E)^{\perp},\ \forall w \in \mathrm{L}^2(E) \setminus \mathbb{R} \end{array} \Big\}.$$

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

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

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

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

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. Polynomial projections can be extended to the vector and tensor cases (see, e.g., [11]): the $\mathbf{L}^2$-projection $\boldsymbol{\Pi}_k^{0,E}$, the $\mathbf{H}^1$-projection $\boldsymbol{\Pi}_k^{\nabla,E}$ and the $\mathbb{L}^2$-projection $\widehat{\boldsymbol{\Pi}}_k^{0,E}$, respectively, similarly as in the scalar case. And a VE subspace of $\widetilde{\mathbf{X}}_k(E)$ is given by

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

We recall the following properties of the space $\mathbf{X}_k(E)$. Also, the corresponding unisolvent degrees of freedom in $\mathbf{X}_k(E)$ can be divided into the following four types (see [5,6])

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

$$\int_E \mathbf{v}_h \cdot \mathbf{g}^{\perp}\, \mathrm{d}E, \qquad \forall \mathbf{g}^{\perp} \in \mathcal{G}_{k-2}^{\perp}(E),$$

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

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

We observe that the projectors $\boldsymbol{\Pi}_k^{\nabla,E}$, $\widehat{\boldsymbol{\Pi}}_k^{0,E}$ and $\boldsymbol{\Pi}_k^{0,E}$ can be computed using only the degrees of freedom $(\mathbf{D1_v})$–$(\mathbf{D4_v})$.

Finally, the global finite dimensional space $\mathbf{X}_h$, associated with the partition $\mathcal{T}_h$, is defined such that: (i) the restriction of every VE function $\mathbf{v}$ to the mesh element E belongs to $\mathbf{X}_k(E)$; (ii) the restriction of every VE function $\mathbf{v}$ to boundary is zero. On the other hand, the discrete pressure space is simply given by piecewise polynomials of degree up to $k-1$:

$$Y_h := \left\{ q_h \in Y : \quad q_h|_E \in \mathbb{P}_{k-1}(E), \quad \forall E \in \mathcal{T}_h \right\},$$

and we also remark that

$$\operatorname{div} \mathbf{X}_h \subseteq Y_h. \tag{2.2}$$

and the global projection operators $\boldsymbol{\Pi}_k^{\nabla}$, $\widehat{\boldsymbol{\Pi}}_k^{0}$ and $\boldsymbol{\Pi}_k^{0}$ are defined similarly as in the scalar case.

Approximation properties associated with the space $\mathbf{X}_k(E)$. The following estimates can be obtained using Assumption 2.1 (see, e.g., [6]):

- For any $\mathbf{z} \in [H^s(E)]^2$ with $s \in [1, k+1]$ there exists $\mathbf{z}_\pi \in [\mathbb{P}_k(E)]^2$ such that

$$\|\mathbf{z} - \mathbf{z}_\pi\|_{0,E} + h_E\, |\mathbf{z} - \mathbf{z}_\pi|_{1,E} \leq C h_E^s |\mathbf{z}|_{s,E}. \tag{2.3}$$

- For any $\mathbf{z} \in [H^s(E)]^2$ with $s \in [1, k+1]$ there exists $\mathbf{z}_I \in \mathbf{X}_k(E)$ such that

$$\|\mathbf{z} - \mathbf{z}_I\|_{0,E} + h_E\, |\mathbf{z} - \mathbf{z}_I|_{1,E} \leq C h_E^s |\mathbf{z}|_{s,E}. \tag{2.4}$$

2.4 The discrete forms and their properties

As usual in the VE literature [2, 3] we define computable discrete forms that approximate the continuous bilinear and trilinear forms in (1.3) using projections. Similarly to the FE 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 $\mathcal{M}^E_{1,h}(\cdot,\cdot): Z_k(E)\times Z_k(E)\to\mathbb{R}$ and $\mathcal{A}^E_{j,h}(\cdot,\cdot): Z_k(E)\times Z_k(E)\to\mathbb{R}$ for $j=1,2,3$ as

$$\mathcal{M}^E_{1,h}(\omega_h,z_h) := \mathcal{M}^E_1\left(\Pi^{0,E}_k\omega_h,\Pi^{0,E}_k z_h\right) + S^E_{\mathtt{m}}\left((\mathrm{I}-\Pi^{0,E}_k)\omega_h,(\mathrm{I}-\Pi^{0,E}_k)z_h\right), \tag{2.5}$$

and

$$\mathcal{A}^E_{j,h}(\omega_h,z_h) := \mathcal{A}^E_j\left(\Pi^{\nabla,E}_k\omega_h,\Pi^{\nabla,E}_k z_h\right) + |\lambda_j|S^E_{\mathtt{a}}\left((\mathrm{I}-\Pi^{\nabla,E}_k)\omega_h,(\mathrm{I}-\Pi^{\nabla,E}_k)z_h\right),\quad \lambda_j\in\{\kappa_1,\kappa_2,\epsilon\},$$

respectively, where the stabilizations $S^E_{\mathtt{m}}(\cdot,\cdot): Z_k(E)\times Z_k(E)\to\mathbb{R}$ and $S^E_{\mathtt{a}}(\cdot,\cdot): Z_k(E)\times Z_k(E)\to\mathbb{R}$ are symmetric, positive definite, bilinear forms such that

$$c_{0,\mathtt{m}}\|z_h\|^2_{0,E} \le S^E_{\mathtt{m}}(z_h,z_h) \le c_{1,\mathtt{m}}\|z_h\|^2_{0,E} \qquad \text{with } \Pi^{0,E}_k(z_h)=0, \tag{2.6a}$$
$$c_{0,\mathtt{a}}|z_h|^2_{1,E} \le S^E_{\mathtt{a}}(z_h,z_h) \le c_{1,\mathtt{a}}|z_h|^2_{1,E} \qquad \text{with } \Pi^{\nabla,E}_k(z_h)=0, \tag{2.6b}$$

for positive constants $c_{0,\mathtt{m}}$, $c_{1,\mathtt{m}}$, $c_{0,\mathtt{a}}$, $c_{1,\mathtt{a}}$ that are independent of h.

Moreover, trilinear form $\mathcal{C}^E_i(\cdot;\cdot,\cdot)$ for $i=1,2$ is replaced by

$$\mathcal{C}^E_{i,h}(\cdot;\cdot,\cdot): Z_k(E)\times \mathring{Z}_k(E)\times Z_k(E)\to\mathbb{R} \qquad \mathcal{C}^E_{i,h}(\omega_h;\psi_h,z_h) := \left(\kappa_i\Pi^{0,E}_k\omega_h\mathbf{\Pi}^{0,E}_{k-1}\nabla\psi_h,\ \mathbf{\Pi}^{0,E}_{k-1}\nabla z_h\right)_{0,E}.$$

Also, the discrete local forms $\mathcal{M}^E_{2,h}(\cdot,\cdot): \mathbf{X}_k(E)\times\mathbf{X}_k(E)\to\mathbb{R}$ and $\mathcal{K}^E_h(\cdot,\cdot): \mathbf{X}_k(E)\times\mathbf{X}_k(E)\to\mathbb{R}$ are defined as

$$\mathcal{M}^E_{2,h}(\mathbf{w}_h,\mathbf{v}_h) := \mathcal{M}^E_2\left(\mathbf{\Pi}^{0,E}_k\mathbf{w}_h,\mathbf{\Pi}^{0,E}_k\mathbf{v}_h\right) + \tilde{\mathcal{S}}^E_{\mathtt{m}}\left((\mathbf{I}-\mathbf{\Pi}^{0,E}_k)\mathbf{w}_h,(\mathbf{I}-\mathbf{\Pi}^{0,E}_k)\mathbf{v}_h\right),$$
$$\mathcal{K}^E_h(\mathbf{w}_h,\mathbf{v}_h) := \mathcal{K}^E\left(\mathbf{\Pi}^{\nabla,E}_k\mathbf{w}_h,\mathbf{\Pi}^{\nabla,E}_k\mathbf{v}_h\right) + \tilde{\mathcal{S}}^E_{\mathtt{a}}\left((\mathbf{I}-\mathbf{\Pi}^{\nabla,E}_k)\mathbf{w}_h,(\mathbf{I}-\mathbf{\Pi}^{\nabla,E}_k)\mathbf{v}_h\right),$$

respectively, where the stabilizers $\tilde{\mathcal{S}}^E_{\mathtt{m}}(\cdot,\cdot): \mathbf{X}_k(E)\times\mathbf{X}_k(E)\to\mathbb{R}$ and $\tilde{\mathcal{S}}^E_{\mathtt{a}}(\cdot,\cdot): \mathbf{X}_k(E)\times\mathbf{X}_k(E)\to\mathbb{R}$ are symmetric, positive definite bilinear forms satisfying

$$\tilde{c}_{0,\mathtt{m}}\|\mathbf{v}_h\|^2_{0,E} \le \tilde{\mathcal{S}}^E_{\mathtt{m}}(\mathbf{v}_h,\mathbf{v}_h) \le \tilde{c}_{1,\mathtt{m}}\|\mathbf{v}_h\|^2_{0,E}, \quad \text{with } \mathbf{\Pi}^{0,E}_k(\mathbf{v}_h)=\mathbf{0}, \tag{2.7a}$$
$$\tilde{c}_{0,\mathtt{a}}|\mathbf{v}_h|^2_{1,E} \le \tilde{\mathcal{S}}^E_{\mathtt{a}}(\mathbf{v}_h,\mathbf{v}_h) \le \tilde{c}_{1,\mathtt{a}}|\mathbf{v}_h|^2_{1,E}, \quad \text{with } \mathbf{\Pi}^{\nabla,E}_k(\mathbf{v}_h)=\mathbf{0}, \tag{2.7b}$$

for positive constants $\tilde{c}_{0,\mathtt{m}},\tilde{c}_{1,\mathtt{m}},\tilde{c}_{0,\mathtt{a}},\tilde{c}_{1,\mathtt{a}}$ that are independent of h. Finally, the skew-symmetric trilinear forms $\mathcal{E}^E(\mathbf{u};\mathbf{w},\mathbf{v})$ and $\mathcal{D}^E(\mathbf{u};\omega,z)$, as well as the trilinear form $(\omega_h\nabla\psi_h,\mathbf{v}_h)_{0,E}$ are replaced, respectively, by

$$\mathcal{E}^E_h(\mathbf{u}_h;\mathbf{w}_h,\mathbf{v}_h) := \frac{1}{2}\big[(\mathbf{\Pi}^{0,E}_k\mathbf{u}_h\cdot\widehat{\mathbf{\Pi}}^{0,E}_{k-1}\boldsymbol{\nabla}\mathbf{w}_h,\mathbf{\Pi}^{0,E}_k\mathbf{v}_h)_{0,E} - (\mathbf{\Pi}^{0,E}_k\mathbf{u}_h\cdot\widehat{\mathbf{\Pi}}^{0,E}_{k-1}\boldsymbol{\nabla}\mathbf{v}_h,\mathbf{\Pi}^{0,E}_k\mathbf{w}_h)_{0,E}\big], \tag{2.8a}$$
$$\mathcal{D}^E_h(\mathbf{u}_h;\omega_h,z_h) := \frac{1}{2}\big[(\mathbf{\Pi}^{0,E}_k\mathbf{u}_h\Pi^{0,E}_k\omega_h,\mathbf{\Pi}^{0,E}_{k-1}\nabla z_h)_{0,E} - (\mathbf{\Pi}^{0,E}_k\mathbf{u}_h\cdot\mathbf{\Pi}^{0,E}_{k-1}\nabla\omega_h,\Pi^{0,E}_k z_h)_{0,E}\big], \tag{2.8b}$$

and

$$(\omega_h\nabla\psi_h,\mathbf{v}_h)_h|_E := \left(\Pi^{0,E}_k\omega_h\mathbf{\Pi}^{0,E}_{k-1}\nabla\psi_h,\mathbf{\Pi}^{0,E}_k\mathbf{v}_h\right)_{0,E}.$$

These forms are continuous thanks to Cauchy–Schwarz inequality, the continuity of the projections with respect to the L^2-norm, and the stability properties (2.6a)–(2.7b):

$$\mathcal{M}_{1,h}(\omega_h,z_h) \le \alpha_1\|\omega_h\|_1\|z_h\|_1, \qquad \mathcal{A}_{j,h}(\omega_h,z_h) \le \alpha_{j+1}\|\omega_h\|_1\|z_h\|_1, \tag{2.9a}$$
$$\mathcal{M}_{2,h}(\mathbf{w}_h,\mathbf{v}_h) \le \tilde{\alpha}_1\|\mathbf{w}_h\|_1\|\mathbf{v}_h\|_1, \qquad \mathcal{K}_h(\mathbf{w}_h,\mathbf{v}_h) \le \tilde{\alpha}_2\|\mathbf{w}_h\|_1\|\mathbf{v}_h\|_1, \tag{2.9b}$$

for all $\omega_h, z_h\in Z_h$, $\mathbf{w}_h,\mathbf{v}_h\in\mathbf{X}_h$ and $j=1,2,3$.

The bilinear forms $\mathcal{M}_{1,h},\mathcal{M}_{2,h}$ and $\mathcal{A}_{j,h}$, $j=1,2,3$, turn out to be coercive owing to the stability properties of stabilizers (cf. (2.6a)-(2.7b)) together with Young and triangle inequalities

$$\mathcal{M}_{1,h}(z_h,z_h) \ge \beta_1\|z_h\|^2_0, \qquad \mathcal{A}_{j,h}(z_h,z_h) \ge \beta_{j+1}\|z_h\|^2_1, \tag{2.10a}$$
$$\mathcal{M}_{2,h}(\mathbf{v}_h,\mathbf{v}_h) \ge \tilde{\beta}_1\|\mathbf{v}_h\|^2_0, \tag{2.10b}$$

for all $z_h\in Z_h, \mathbf{v}_h\in\mathbf{X}_h$.

On the other hand, $\mathcal{K}_h$ is coercive on the discrete kernel $\widetilde{\mathbf{X}}_h$ of the bilinear form $\mathcal{B}(\cdot,\cdot)$

$$\mathcal{K}_h(\mathbf{v}_h,\mathbf{v}_h) \ge \tilde{\beta}_2\|\mathbf{v}_h\|^2_1, \qquad \forall\mathbf{v}_h\in\widetilde{\mathbf{X}}_h,$$

where

$$\widetilde{\mathbf{X}}_h = \{\mathbf{v}_h\in\mathbf{X}_h: \quad \mathcal{B}(q_h,\mathbf{v}_h)=0, \quad \forall q_h\in Y_h\}. \tag{2.11}$$

The continuity of $\mathcal{D}_h(\cdot;\cdot,\cdot)$ and $\mathcal{E}_h(\cdot;\cdot,\cdot)$ on Z_h and $\mathbf{X}_h$, respectively, is stated in the following result.

Lemma 2.1 *The trilinear forms $\mathcal{D}_h(\cdot;\cdot,\cdot)$ and $\mathcal{E}_h(\cdot;\cdot,\cdot)$ are continuous, with respective continuity constants*

$$\gamma_1 := \sup_{\mathbf{u}_h\in\mathbf{X}_h,\omega_h,z_h\in Z_h} \frac{|\mathcal{D}_h(\mathbf{u}_h;\omega_h,z_h)|}{\|\mathbf{u}_h\|_1\|\omega_h\|_1\|z_h\|_1}, \qquad \gamma_2 := \sup_{\mathbf{u}_h,\mathbf{w}_h,\mathbf{v}_h\in\mathbf{X}_h} \frac{|\mathcal{E}_h(\mathbf{u}_h;\mathbf{w}_h,\mathbf{v}_h)|}{\|\mathbf{u}_h\|_1\|\mathbf{w}_h\|_1\|\mathbf{v}_h\|_1}.$$

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

$$\begin{aligned}\mathcal{D}_h(\mathbf{u}_h;\omega_h,z_h) &= \frac{1}{2}\big[(\boldsymbol{\Pi}_k^0\mathbf{u}_h\ \Pi_k^0\omega_h, \boldsymbol{\Pi}_{k-1}^0\nabla z_h)_0 - (\boldsymbol{\Pi}_k^0\mathbf{u}_h\cdot\boldsymbol{\Pi}_{k-1}^0\nabla\omega_h, \Pi_k^0 z_h)_0\big]\\ &\le \|\boldsymbol{\Pi}_k^0\mathbf{u}_h\|_{0,4}\|\Pi_k^0\omega_h\|_{0,4}\|\boldsymbol{\Pi}_{k-1}^0\nabla z_h\|_0 + \|\boldsymbol{\Pi}_k^0\mathbf{u}_h\|_{0,4}\|\boldsymbol{\Pi}_{k-1}^0\nabla\omega_h\|_0\|\Pi_k^0 z_h\|_{0,4}. \end{aligned}\tag{2.12}$$

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

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

and similarly

$$\|\Pi_k^0\omega_h\|_{0,4} \le C_2\|\omega_h\|_{0,4}, \quad \|\Pi_k^0 z_h\|_{0,4} \le C_3\|z_h\|_{0,4}.$$

Combining the above estimates with Eq. (2.12), leads to

$$\mathcal{D}_h(\mathbf{u}_h;\omega_h,z_h) \le \frac{1}{2}\left(C_1C_2 + C_1C_3\right)\|\mathbf{u}_h\|_1\|\omega_h\|_1\|z_h\|_1,$$

which confirms the continuity of $\mathcal{D}_h(\cdot;\cdot,\cdot)$. The proof of continuity of $\mathcal{E}_h(\cdot;\cdot,\cdot)$ can be found in [6]. □

Lemma 2.2 *There exist constants γ_3 and γ_4 (independent of E and h) verifying*

$$\begin{aligned} \mathcal{C}_{i,h}(\omega_h;\psi_h,z_h) &\le \gamma_3\|\omega_h\|_\infty\|\psi_h\|_1\|z_h\|_1, && \forall\omega_h,z_h\in Z_h,\ \psi_h\in\mathring{Z}_h,\\ (\omega_h\nabla\psi_h,\mathbf{v}_h)_h &\le \gamma_4\|\omega_h\|_1\|\psi_h\|_1\|\mathbf{v}_h\|_1, && \forall\omega_h\in Z_h,\ \psi_h\in\mathring{Z}_h,\ \mathbf{v}_h\in\mathbf{X}_h. \end{aligned}$$

Proof. The proof is a direct consequence of the Hölder inequality, the continuity of Π_k^0 with respect to the L^∞-norm. □

Lemma 2.3 (Discrete inf-sup condition) *[6] Given the VE spaces $\mathbf{X}_h$ and Y_h defined in Section 2.3, there exists a positive constant $\widehat{\beta}$, independent of h, such that:*

$$\sup_{\mathbf{v}_h\in\mathbf{X}_h\mathbf{v}_h\neq\mathbf{0}} \frac{\mathcal{B}\left(\mathbf{v}_h,q_h\right)}{\|\mathbf{v}_h\|_1} \ge \widehat{\beta}\,\|q_h\|_0 \qquad \textit{for all } q_h\in Y_h.$$

Such a discrete inf-sup property together with (2.2), indicate that

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

The following result compares $\mathcal{M}_1^E, \mathcal{M}_2^E$, $\mathcal{A}_j^E$ and $\mathcal{K}^E$ against their computable counterparts.

Lemma 2.4 ([19]) *Let $\alpha_i,\tilde{\alpha}_r$, $i=1,\cdots,4$, $r=1,2$ be the constants from (2.9a) and (2.9b). Then for each $\omega,\mathrm{z}\in Z$ and $\mathbf{w},\mathbf{v}\in\mathbf{X}$, there hold*

$$\begin{aligned} |\mathcal{M}_1(\omega,\mathrm{z}) - \mathcal{M}_{1,h}(\omega,\mathrm{z})| &\le \alpha_1\|\omega - \Pi_k^0(\omega)\|_0\|\mathrm{z}\|_0,\\ |\mathcal{M}_2(\mathbf{w},\mathbf{v}) - \mathcal{M}_{2,h}(\mathbf{w},\mathbf{v})| &\le \tilde{\alpha}_1\|\mathbf{w} - \boldsymbol{\Pi}_k^0(\mathbf{w})\|_0\|\mathbf{v}\|_0,\\ |\mathcal{A}_i(\omega,\mathrm{z}) - \mathcal{A}_{i,h}(\omega,\mathrm{z})| &\le \alpha_{i+1}\|\omega - \Pi_k^\nabla(\omega)\|_1\|\mathrm{z}\|_1,\\ |\mathcal{K}(\mathbf{w},\mathbf{v}) - \mathcal{K}_h(\mathbf{w},\mathbf{v})| &\le \tilde{\alpha}_2\|\mathbf{w} - \boldsymbol{\Pi}_k^\nabla(\mathbf{w})\|_1\|\mathbf{v}\|_1. \end{aligned}$$

Lemma 2.5 *Assume that $\mathbf{w}\in\mathbf{X}\cap\mathbf{H}^{k+1}(\Omega)$. Then, it holds*

$$|\widehat{\mathcal{E}}(\mathbf{w};\mathbf{w},\mathbf{v}) - \mathcal{E}_h(\mathbf{w};\mathbf{w},\mathbf{v})| \le Ch^{k+1}|\mathbf{w}|_{k+1}\|\mathbf{w}\|_2\|\mathbf{v}\|_1, \qquad \forall\mathbf{v}\in\mathbf{X},$$

where

$$\widehat{\mathcal{E}}(\mathbf{w};\mathbf{w},\mathbf{v}) := \frac{1}{2}\big[(\boldsymbol{\Pi}_k^0(\mathbf{w}\cdot\boldsymbol{\nabla}\mathbf{w}),\mathbf{v})_0 - (\widehat{\boldsymbol{\Pi}}_{k-1}^0(\mathbf{w}\otimes\mathbf{w}),\boldsymbol{\nabla}\mathbf{v})_0\big].$$

Proof. First, by the definitions of the trilinear continuous and discrete forms $\widehat{\mathcal{E}}(\cdot;\cdot,\cdot)$ and $\mathcal{E}_h(\cdot;\cdot,\cdot)$, for any $E \in \mathcal{T}_h$ we have

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

The above terms will now be analyzed. Straightforward manipulations applied on $\boldsymbol{\eta}_1$, the definition of $\mathbf{L}^2$-projection $\boldsymbol{\Pi}_k^{0,E}$ and adding $\pm(\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\cdot\boldsymbol{\nabla}\mathbf{w},\boldsymbol{\Pi}_k^{0,E}\mathbf{v})_{0,E}$, give

$$\begin{aligned}\boldsymbol{\eta}_1 &= \int_E \left(\boldsymbol{\Pi}_k^{0,E}(\mathbf{w}\cdot\boldsymbol{\nabla}\mathbf{w})\cdot\mathbf{v} - (\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\cdot\widehat{\boldsymbol{\Pi}}_{k-1}^{0,E}\boldsymbol{\nabla}\mathbf{w})\cdot\boldsymbol{\Pi}_k^{0,E}\mathbf{v}\right)\mathrm{d}E\\ &= \int_E \left((\mathbf{w}\cdot\boldsymbol{\nabla}\mathbf{w})\cdot\boldsymbol{\Pi}_k^{0,E}\mathbf{v} - (\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\cdot\widehat{\boldsymbol{\Pi}}_{k-1}^{0,E}\boldsymbol{\nabla}\mathbf{w})\cdot\boldsymbol{\Pi}_k^{0,E}\mathbf{v}\right)\mathrm{d}E\\ &= \int_E \left(((\mathbf{I}-\boldsymbol{\Pi}_k^{0,E})\mathbf{w}\cdot\boldsymbol{\nabla}\mathbf{w})\cdot\boldsymbol{\Pi}_k^{0,E}\mathbf{v} + (\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\cdot(\mathbb{I}-\widehat{\boldsymbol{\Pi}}_{k-1}^{0,E})\boldsymbol{\nabla}\mathbf{w})\cdot\boldsymbol{\Pi}_k^{0,E}\mathbf{v}\right)\mathrm{d}E\\ &=: \boldsymbol{\eta}_1^1 + \boldsymbol{\eta}_1^2.\end{aligned} \tag{2.14}$$

Now, using the Hölder inequality, the approximation property given in (2.3) and the continuity of $\boldsymbol{\Pi}_k^{0,E}$ with respect to the $\mathbf{L}^4$-norm, allow us to conclude that

$$\begin{aligned}|\boldsymbol{\eta}_1^1| &= \left|\int_E \left(((\mathbf{I}-\boldsymbol{\Pi}_k^{0,E})\mathbf{w}\cdot\boldsymbol{\nabla}\mathbf{w})\cdot\boldsymbol{\Pi}_k^{0,E}\mathbf{v}\right)\mathrm{d}E\right| \le \|\boldsymbol{\nabla}\mathbf{w}\|_{0,4,E}\left\|(\mathbf{I}-\boldsymbol{\Pi}_k^{0,E})\mathbf{w}\right\|_{0,E}\left\|\boldsymbol{\Pi}_k^{0,E}\mathbf{v}\right\|_{0,4,E}\\ &\le \|\boldsymbol{\nabla}\mathbf{w}\|_{0,4,E}\, h_E^{k+1}|\mathbf{w}|_{k+1,E}\,\|\mathbf{v}\|_{0,4,E}\\ &\le Ch_E^{k+1}|\mathbf{w}|_{k+1,E}\|\mathbf{w}\|_{2,E}\|\mathbf{v}\|_{1,E},\end{aligned} \tag{2.15}$$

where in the last inequality we have used the Sobolev embeddings $\mathbf{H}^1 \subset \mathbf{L}^4$ and $\mathbf{H}^2 \subset \mathbf{W}^{1,4}$.

For the term $\boldsymbol{\eta}_1^2$ in (2.14), we realize that using the Hölder inequality, the continuity of $\boldsymbol{\Pi}_k^{0,E}$ and Gagliardo–Nirenberg inequality (cf. Lemma 1.1 with letting $j=0,\ m=1,\ q=4,\ r=p=2,\ a=0.5$), the inverse inequality (cf. (2.1) with $q=4,\ p=2$) and the Sobolev embeddings $\mathbf{H}^1 \subset \mathbf{L}^4$ and $\mathbf{H}^2 \subset \mathbf{W}^{1,4}$, it holds that

$$\begin{aligned}|\boldsymbol{\eta}_1^2| &= \left|\int_E \left((\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\cdot(\mathbb{I}-\widehat{\boldsymbol{\Pi}}_{k-1}^{0,E})\boldsymbol{\nabla}\mathbf{w})\cdot\boldsymbol{\Pi}_k^{0,E}\mathbf{v}\right)\mathrm{d}E\right| \le \left\|(\mathbb{I}-\widehat{\boldsymbol{\Pi}}_{k-1}^{0,E})\boldsymbol{\nabla}\mathbf{w}\right\|_{0,E}\left\|\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\right\|_{0,4,E}\left\|\boldsymbol{\Pi}_k^{0,E}\mathbf{v}\right\|_{0,4,E}\\ &\le h_E^k|\mathbf{w}|_{k+1,E}(\|\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\|_{0,E}^{\frac{1}{2}}\|\boldsymbol{\nabla}\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\|_{0,E}^{\frac{1}{2}})(\|\boldsymbol{\Pi}_k^{0,E}\mathbf{v}\|_{0,E}^{\frac{1}{2}}\|\boldsymbol{\nabla}\boldsymbol{\Pi}_k^{0,E}\mathbf{v}\|_{0,E}^{\frac{1}{2}})\\ &\le h_E^k|\mathbf{w}|_{k+1,E}(h_E^{\frac{1}{2}}\|\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\|_{0,4,E}^{\frac{1}{2}}\|\boldsymbol{\nabla}\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\|_{0,4,E}^{\frac{1}{2}})(h_E^{\frac{1}{4}}\|\boldsymbol{\Pi}_k^{0,E}\mathbf{v}\|_{0,4,E}^{\frac{1}{2}}\|\boldsymbol{\nabla}\boldsymbol{\Pi}_k^{0,E}\mathbf{v}\|_{0,E}^{\frac{1}{2}})\\ &\le h_E^{k+\frac{3}{4}}|\mathbf{w}|_{k+1,E}(\|\boldsymbol{\nabla}\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\|_{0,E}^{\frac{1}{2}}\|\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\|_{2,E}^{\frac{1}{2}})\|\boldsymbol{\Pi}_k^{0,E}\mathbf{v}\|_{1,E}\\ &\le h_E^{k+\frac{3}{4}}|\mathbf{w}|_{k+1,E}(h_E^{\frac{1}{4}}\|\boldsymbol{\nabla}\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\|_{0,4,E}^{\frac{1}{2}}\|\mathbf{w}\|_{2,E}^{\frac{1}{2}})\|\mathbf{v}\|_{1,E}\\ &\le h_E^{k+1}|\mathbf{w}|_{k+1,E}\|\mathbf{w}\|_{2,E}\|\mathbf{v}\|_{1,E}.\end{aligned} \tag{2.16}$$

Combining Eqs. (2.15) and (2.16) in (2.14) gives

$$\sum_{E\in\mathcal{T}_h} |\boldsymbol{\eta}_1| \le Ch^{k+1}|\mathbf{w}|_{k+1}\|\mathbf{w}\|_2\|\mathbf{v}\|_1. \tag{2.17}$$

On the other hand, the second term on the right-hand of (2.13) can be rewritten by applying analogous arguments used in (2.14):

$$\begin{aligned}\boldsymbol{\eta}_2 &= \int_E \left(\widehat{\boldsymbol{\Pi}}_{k-1}^{0,E}(\mathbf{w}\otimes\mathbf{w}) : \boldsymbol{\nabla}\mathbf{v} - (\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\otimes\boldsymbol{\Pi}_k^{0,E}\mathbf{w}) : \widehat{\boldsymbol{\Pi}}_{k-1}^{0,E}\boldsymbol{\nabla}\mathbf{v}\right)\mathrm{d}E\\ &= \int_E \left((\mathbf{w}\otimes\mathbf{w}) : \widehat{\boldsymbol{\Pi}}_{k-1}^{0,E}\boldsymbol{\nabla}\mathbf{v} - (\boldsymbol{\Pi}_k^{0,E}\mathbf{w}\otimes\boldsymbol{\Pi}_k^{0,E}\mathbf{w}) : \widehat{\boldsymbol{\Pi}}_{k-1}^{0,E}\boldsymbol{\nabla}\mathbf{v}\right)\mathrm{d}E\\ &= \int_E \left((\mathbf{w}\otimes(\mathbf{I}-\boldsymbol{\Pi}_k^{0,E})\mathbf{w}) : \widehat{\boldsymbol{\Pi}}_{k-1}^{0,E}\boldsymbol{\nabla}\mathbf{v} + ((\mathbf{I}-\boldsymbol{\Pi}_k^{0,E})\mathbf{w}\otimes\boldsymbol{\Pi}_k^{0,E}\mathbf{w}) : \widehat{\boldsymbol{\Pi}}_{k-1}^{0,E}\boldsymbol{\nabla}\mathbf{v}\right)\mathrm{d}E\\ &=: \boldsymbol{\eta}_2^1 + \boldsymbol{\eta}_2^2.\end{aligned} \tag{2.18}$$

Now, in order to bound the first term in (2.18), we employ the Hölder inequality, the continuity of $\widehat{\mathbf{\Pi}}_k^{0,E}$ and Gagliardo–Nirenberg inequality (cf. Lemma 1.1 with letting $j=0,\ m=1,\ q=\infty,\ r=p=4,\ a=0.5$), to find that

$$\begin{aligned}|\boldsymbol{\eta}_2^1| &= \left|\int_E \Big((\mathbf{w}\otimes(\mathbf{I}-\mathbf{\Pi}_k^{0,E})\mathbf{w}) : \widehat{\mathbf{\Pi}}_{k-1}^{0,E}\boldsymbol{\nabla}\mathbf{v}\Big)\ \mathrm{d}E\right| \leq \|\mathbf{w}\|_{\infty,E}\left\|(\mathbf{I}-\mathbf{\Pi}_k^{0,E})\mathbf{w}\right\|_{0,E}\left\|\widehat{\mathbf{\Pi}}_{k-1}^{0,E}\boldsymbol{\nabla}\mathbf{v}\right\|_{0,E}\\ &\leq (\|\mathbf{w}\|_{0,4,E}^{\frac12}\|\nabla\mathbf{w}\|_{0,4,E}^{\frac12})h_E^{k+1}|\mathbf{w}|_{k+1,E}\|\mathbf{v}\|_1\\ &\leq h_E^{k+1}|\mathbf{w}|_{k+1,E}\|\mathbf{w}\|_{2,E}\|\mathbf{v}\|_{1,E},\end{aligned} \tag{2.19}$$

where in the last step we have invoked the Sobolev embeddings. And using analogous arguments as those for $\boldsymbol{\eta}_2^1$ we can derive the bound

$$|\boldsymbol{\eta}_2^2| \leq Ch_E^{k+1}|\mathbf{w}|_{k+1,E}\|\mathbf{w}\|_{2,E}\|\mathbf{v}\|_{1,E},$$

which together with (2.19) and (2.18) implies

$$\sum_{E\in\mathcal{T}_h}|\boldsymbol{\eta}_2| \leq h^{k+1}|\mathbf{w}|_{k+1}\|\mathbf{w}\|_2\|\mathbf{v}\|_1. \tag{2.20}$$

The proof can be inferred by combining (2.17) and (2.20) in (2.13). □

Lemma 2.6 *Assume that* $\mathbf{w}\in \boldsymbol{X}\cap\mathbf{H}^{k+1}(\Omega)$, $\omega\in Z\cap\mathrm{H}^{k+1}(\Omega)$. *Then*

$$|\widehat{\mathcal{D}}(\mathbf{w};\omega,z)-\mathcal{D}_h(\mathbf{w};\omega,z)| \leq Ch^{k+1}\left(|\boldsymbol{w}|_{k+1}\|\rho\|_2+|\rho|_{k+1}\|\boldsymbol{w}\|_2\right)\|z\|_1 \qquad \forall z\in Z,$$

where

$$\widehat{\mathcal{D}}(\mathbf{w};\omega,z) := \frac12\big[(\mathbf{\Pi}_{k-1}^0(\mathbf{w}\ \omega),\nabla z)_0-(\mathbf{\Pi}_k^0(\mathbf{w}\cdot\nabla\omega),z)_0\big].$$

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

$$\begin{aligned}\widehat{\mathcal{D}}(\mathbf{w};\omega,z)-\mathcal{D}_h(\mathbf{w};\omega,z) &= \frac12\big[(\mathbf{\Pi}_{k-1}^0(\mathbf{w}\ \omega),\nabla z)_0-(\mathbf{\Pi}_k^0\mathbf{w}\cdot\Pi_k^0\omega,\mathbf{\Pi}_{k-1}^0\nabla z)_0\big]\\ &\quad-\frac12\big[(\mathbf{\Pi}_k^0(\mathbf{w}\cdot\nabla\omega),z)_0-(\mathbf{\Pi}_k^0\mathbf{w}\cdot\mathbf{\Pi}_{k-1}^0\nabla\omega,\Pi_k^0 z)_0\big]\\ &=: \frac12(\eta_1-\eta_2).\end{aligned} \tag{2.21}$$

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

$$\begin{aligned}\eta_1|_E &= \int_E\Big(\mathbf{\Pi}_{k-1}^{0,E}(\mathbf{w}\ \omega)\cdot\nabla z-(\mathbf{\Pi}_k^{0,E}\mathbf{w}\ \Pi_k^{0,E}\omega)\cdot\mathbf{\Pi}_{k-1}^{0,E}\nabla z\Big)\,\mathrm{d}E\\ &= \int_E\Big((\mathbf{I}-\mathbf{\Pi}_k^{0,E})\mathbf{w}\ \omega\ \mathbf{\Pi}_{k-1}^{0,E}\nabla z+\mathbf{\Pi}_k^{0,E}\mathbf{w}\ (\mathrm{I}-\Pi_k^{0,E})\omega\ \mathbf{\Pi}_{k-1}^{0,E}\nabla z\Big)\,\mathrm{d}E.\end{aligned} \tag{2.22}$$

Then, using the Hölder inequality, the continuity of $\mathbf{\Pi}_k^{0,E}$ (with respect to the $\mathbf{L}^4$-norm), Sobolev embeddings, as well as the Gagliardo–Nirenberg and inverse inequalities, we can control the terms on the right-hand side of (2.21) as follows

$$|\eta_1| \leq Ch^{k+1}\left(|\mathbf{w}|_{k+1}\|\omega\|_2+|\omega|_{k+1}\|\mathbf{w}\|_2\right)\|z\|_1, \tag{2.23a}$$
$$|\eta_2| \leq Ch^{k+1}\left(|\mathbf{w}|_{k+1}\|\omega\|_2+|\omega|_{k+1}\|\mathbf{w}\|_2\right)\|z\|_1. \tag{2.23b}$$

Consequently, the proof follows after putting together (2.23a) and (2.23b) into (2.22). □

Lemma 2.7 *Assume that* $\omega,\psi\in Z\cap\mathrm{H}^{k+1}(\Omega)$. *Then, it holds*

$$\left|\widehat{\mathcal{C}}_i(\omega;\psi,z)-\mathcal{C}_{i,h}(\omega;\psi,z)\right| \leq Ch^k\left(\|\omega\|_2|\psi|_{k+1}+\|\psi\|_2|\omega|_{k+1}\right)\|z\|_1 \qquad \forall z\in Z, \tag{2.24}$$

where

$$\widehat{\mathcal{C}}_i(\omega;\psi,z) := \left(\kappa_i\mathbf{\Pi}_{k-1}^0(\omega\nabla\psi),\nabla z\right)_0.$$

Proof. We first write, on each element $E\in\mathcal{T}_h$, the following relation (which follows using the orthogonality property of $\mathbf{\Pi}_k^{0,E}$ and adding $\pm(\kappa_i\omega\mathbf{\Pi}_{k-1}^0\nabla\psi,\mathbf{\Pi}_{k-1}^0\nabla z)_{0,E}$):

$$\begin{aligned}\widehat{\mathcal{C}}_i^E(\omega;\psi,z)-\mathcal{C}_{i,h}^E(\omega;\psi,z) &= \int_E\kappa_i\mathbf{\Pi}_{k-1}^{0,E}(\omega\nabla\psi)\cdot\nabla z\ \ \mathrm{d}E-\int_E\kappa_i\Pi_k^{0,E}\omega\ \mathbf{\Pi}_{k-1}^{0,E}\nabla\psi\cdot\mathbf{\Pi}_{k-1}^{0,E}\nabla z\ \ \mathrm{d}E\\ &= \int_E\kappa_i\omega\nabla\psi\cdot\mathbf{\Pi}_{k-1}^{0,E}\nabla z\ \ \mathrm{d}E-\int_E\kappa_i\Pi_k^{0,E}\omega\ \mathbf{\Pi}_{k-1}^{0,E}\nabla\psi\cdot\mathbf{\Pi}_{k-1}^{0,E}\nabla z\ \ \mathrm{d}E\end{aligned}$$

$$
\begin{aligned}
&= \int_E \kappa_i \boldsymbol{\Pi}_{k-1}^{0,E} \nabla z \cdot \left((\mathbf{I} - \boldsymbol{\Pi}_{k-1}^{0,E}) \nabla \psi \right) \omega \ \mathrm{d}E + \int_E \kappa_i \boldsymbol{\Pi}_{k-1}^{0,E} \nabla z \cdot \boldsymbol{\Pi}_{k-1}^{0,E} \nabla \psi \left((\mathrm{I} - \Pi_k^{0,E}) \omega \right) \mathrm{d}E \\
&=: \theta_1 + \theta_2.
\end{aligned} \tag{2.25}
$$

Applying the continuity and approximation properties of $\boldsymbol{\Pi}_{k-1}^{0,E}$, and, as before, Hölder, Gagliardo–Nirenberg and Sobolev inequalities, we have

$$
\begin{aligned}
|\theta_1| &= \left| \int_E \boldsymbol{\Pi}_{k-1}^{0,E} \nabla z \left((\mathbf{I} - \boldsymbol{\Pi}_{k-1}^{0,E}) \nabla \psi \right) \omega \ \mathrm{d}E \right| \\
&\leq \|\boldsymbol{\Pi}_{k-1}^{0,E} \nabla z\|_{0,E} \|(\mathbf{I} - \boldsymbol{\Pi}_{k-1}^{0,E}) \nabla \psi\|_{0,E} \|\omega\|_{\infty,E} \\
&\leq C \|\nabla z\|_{0,E} h_E^k |\nabla \psi|_{k,E} \|\omega\|_{0,4,E}^{1/2} \|\nabla \omega\|_{0,4,E}^{1/2} \\
&\leq C h_E^k \|\omega\|_{2,E} |\psi|_{k+1,E} \|z\|_{1,E},
\end{aligned}
$$

and the term θ_2 can be estimated using similar arguments as follows

$$
|\theta_2| \leq C h_E^k |\omega|_{k+1,E} \|\psi\|_{2,E} \|z\|_{1,E},
$$

which, substituted back in (2.25) and summing over $E \in \mathcal{T}_h$, yields (2.24). □

2.5 Semi-discrete and fully-discrete schemes

With the aid of the discrete forms (2.5)-(2.8a) we can state the semi-discrete VE scheme as:
Find $\{(c_{1,h}(\cdot,t), c_{2,h}(\cdot,t)), \phi_h(\cdot,t)\} \in \mathbf{Z}_h \times \mathring{Z}_h$ and $\{\mathbf{u}_h(\cdot,t), p_h(\cdot,t)\} \in \mathbf{X}_h \times Y_h$ such that for almost all $t \in (0, t_F]$

$$
\begin{aligned}
\mathcal{M}_{1,h}(\partial_t c_{i,h}, z_{i,h}) + \mathcal{A}_{i,h}(c_{i,h}, z_{i,h}) + e_i \mathcal{C}_{i,h}(c_{i,h}; \phi_h, z_{i,h}) - \mathcal{D}_h(\mathbf{u}_h; c_{i,h}, z_{i,h}) &= 0 && \forall z_{i,h} \in Z_h, \\
\mathcal{A}_{3,h}(\phi_h, \psi_h) - \mathcal{M}_{1,h}(c_{1,h}, \psi_h) + \mathcal{M}_{1,h}(c_{2,h}, \psi_h) &= 0 && \forall \psi_h \in \mathring{Z}_h, \\
\mathcal{M}_{2,h}(\partial_t \mathbf{u}_h, \mathbf{v}_h) + \mathcal{K}_h(\mathbf{u}_h, \mathbf{v}_h) + \mathcal{E}_h(\mathbf{u}_h; \mathbf{u}_h, \mathbf{v}_h) - \mathcal{B}(p_h, \mathbf{v}_h) + ((c_{1,h} - c_{2,h}) \nabla \phi_h, \mathbf{v}_h)_h &= 0 && \forall \mathbf{v}_h \in \mathbf{X}_h, \\
\mathcal{B}(q_h, \mathbf{u}_h) &= 0 && \forall q_h \in Y_h,
\end{aligned}
$$

with initial conditions $c_{i,h}(\cdot,0) := \Pi_k^0 c_{i,0}$ and $\mathbf{u}_h(\cdot,0) := \boldsymbol{\Pi}_k^0 \mathbf{u}_0$.

Next, we discretize in time using the backward Euler method with constant step-size $\tau = \frac{t_F}{N}$ and for a generic function ϱ, denote $\varrho^n = \varrho(\cdot, t_n)$, $\delta_t \varrho^n = \frac{\varrho^n - \varrho^{n-1}}{\tau}$. The fully discrete system reads: for $n = 1, \cdots, N$ find $\{(c_{1,h}^n, c_{2,h}^n), \phi_h^n\} \in \mathbf{Z}_h \times \mathring{Z}_h$, $\{\mathbf{u}_h^n, p_h^n\} \in \mathbf{X}_h \times Y_h$ such that

$$
\mathcal{M}_{1,h}(\delta_t c_{i,h}^n, z_{i,h}) + \mathcal{A}_{i,h}(c_{i,h}^n, z_{i,h}) + e_i \mathcal{C}_{i,h}(c_{i,h}^n; \phi_h^n, z_{i,h}) - \mathcal{D}_h(\mathbf{u}_h^n; c_{i,h}^n, z_{i,h}) = 0, \tag{2.26a}
$$
$$
\mathcal{A}_{3,h}(\phi_h^n, \psi_h) - \mathcal{M}_{1,h}(c_{1,h}^n, \psi_h) + \mathcal{M}_{1,h}(c_{2,h}^n, \psi_h) = 0, \tag{2.26b}
$$
$$
\mathcal{M}_{2,h}(\delta_t \mathbf{u}_h^n, \mathbf{v}_h) + \mathcal{K}_h(\mathbf{u}_h^n, \mathbf{v}_h) + \mathcal{E}_h(\mathbf{u}_h^n; \mathbf{u}_h^n, \mathbf{v}_h) - \mathcal{B}(p_h^n, \mathbf{v}_h) + \left((c_{1,h}^n - c_{2,h}^n) \nabla \phi_h^n, \mathbf{v}_h\right)_h = 0, \tag{2.26c}
$$
$$
\mathcal{B}(q_h, \mathbf{u}_h^n) = 0, \tag{2.26d}
$$

for all $\{(z_{1,h}, z_{2,h}), \psi_h\} \in \mathbf{Z}_h \times \mathring{Z}_h$ and $\{\mathbf{v}_h, q_h\} \in \mathbf{X}_h \times Y_h$, where $c_{i,h}^0 = c_{i,h}(\cdot,0)$, $\mathbf{u}_h^0 = \mathbf{u}_h(\cdot,0)$.

Remark 2.1 Equation (2.26d) along with the property (2.2), implies that the discrete velocity $\mathbf{u}_h^n \in \mathbf{X}_k^h$ is exactly divergence-free. More generally, introducing the continuous kernel:

$$
\widetilde{\mathbf{X}} = \{ \mathbf{v} \in \mathbf{X} : \quad \mathcal{B}(q, \mathbf{v}) = 0, \quad \forall q \in Y \},
$$

and discrete kernel $\widetilde{\mathbf{X}}_h$ given in (2.11), we can readily check that $\widetilde{\mathbf{X}}_h \subseteq \widetilde{\mathbf{X}}$. Therefore we consider the following reduced problem (equivalent to (2.26)): Find $\{(c_{1,h}^n, c_{2,h}^n), \phi_h^n\} \in \mathbf{Z}_h \times \mathring{Z}_h$, $\mathbf{u}_h^n \in \widetilde{\mathbf{X}}_h$ and $n = 1, \cdots, N$ such that

$$
\mathcal{M}_{1,h}(\delta_t c_{i,h}^n, z_{i,h}) + \mathcal{A}_{i,h}(c_{i,h}^n, z_{i,h}) + e_i \mathcal{C}_{i,h}(c_{i,h}^n; \phi_h^n, z_{i,h}) - \mathcal{D}_h(\mathbf{u}_h^n; c_{i,h}^n, z_{i,h}) = 0, \tag{2.27a}
$$
$$
\mathcal{A}_{3,h}(\phi_h^n, \psi_h) - \mathcal{M}_{1,h}(c_{1,h}^n, \psi_h) + \mathcal{M}_{1,h}(c_{2,h}^n, \psi_h) = 0, \tag{2.27b}
$$
$$
\mathcal{M}_{2,h}(\delta_t \mathbf{u}_h^n, \mathbf{v}_h) + \mathcal{K}_h(\mathbf{u}_h^n, \mathbf{v}_h) + \mathcal{E}_h(\mathbf{u}_h^n; \mathbf{u}_h^n, \mathbf{v}_h) + \left((c_{1,h}^n - c_{2,h}^n) \nabla \phi_h^n, \mathbf{v}_h\right)_h = 0, \tag{2.27c}
$$

for all $\{(z_{1,h}, z_{2,h}), \psi_h\} \in \mathbf{Z}_h \times \mathring{Z}_h$ and $\mathbf{v}_h \in \widetilde{\mathbf{X}}_h$.

3 Well-posedness analysis

We begin by introducing a fixed-point operator

$$\mathbf{T}:\mathbf{Z}_h\times\mathbf{X}_h\to\mathbf{Z}_h\times\mathbf{X}_h,\quad(\boldsymbol{\xi}_h^n,\mathbf{w}_h^n)\mapsto\mathbf{T}(\boldsymbol{\xi}_h^n,\mathbf{w}_h^n):=(\widehat{\mathbf{c}}_h^n,\widehat{\mathbf{u}}_h^n),$$

with $\boldsymbol{\xi}_h^n:=(\xi_{1,h}^n,\xi_{2,h}^n)\in\mathbf{Z}_h$, $\widehat{\mathbf{c}}_h^n:=(\widehat{c}_{1,h}^n,\widehat{c}_{2,h}^n)$, and where $(\widehat{\mathbf{c}}_h^n,\widehat{\mathbf{u}}_h^n)$ are the first and third components of the solution of the linearized version of problem (2.27): Given $\widehat{\mathbf{c}}_h^0=(\Pi_k^0c_{1,0},\Pi_k^0c_{2,0})$, $\widehat{\mathbf{u}}_h^0=\mathbf{\Pi}_k^0\mathbf{u}_0$, find $\{(\widehat{\mathbf{c}}_h^n,\widehat{\phi}_h^n),\widehat{\mathbf{u}}_h^n\}$ for $i=1,2$, $n=1,\cdots,N$ such that

$$\begin{aligned}\mathcal{M}_{1,h}(\delta_t\widehat{c}_{i,h}^n,z_{i,h})+\mathcal{A}_{i,h}(\widehat{c}_{i,h}^n,z_{i,h})+e_i\mathcal{C}_{i,h}(\xi_{i,h}^n;\widehat{\phi}_h^n,z_{i,h})-\mathcal{D}_h(\mathbf{w}_h^n;\widehat{c}_{i,h}^n,z_{i,h})&=0,\\ \mathcal{A}_{3,h}(\widehat{\phi}_h^n,\psi_h)&=\mathcal{M}_{1,h}(\widehat{c}_{1,h}^n,\psi_h)-\mathcal{M}_{1,h}(\widehat{c}_{2,h}^n,\psi_h),\\ \mathcal{M}_{2,h}(\delta_t\widehat{\mathbf{u}}_h^n,\mathbf{v}_h)+\mathcal{K}_h(\widehat{\mathbf{u}}_h^n,\mathbf{v}_h)+\mathcal{E}_h(\mathbf{w}_h^n;\widehat{\mathbf{u}}_h^n,\mathbf{v}_h)&=-\Big((\xi_{1,h}^n-\xi_{2,h}^n)\nabla\widehat{\phi}_h^n,\mathbf{v}_h\Big)_h.\end{aligned}\tag{3.1}$$

System (3.1) can be reformulated as follows:

$$\widehat{\mathbf{A}}_{\boldsymbol{\xi}_h^n,\mathbf{w}_h^n}\Big((\widehat{\mathbf{c}}_h^n,\widehat{\phi}_h^n,\widehat{\mathbf{u}}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\Big)=\mathcal{M}_{1,h}(\widehat{c}_{1,h}^{n-1},z_{1,h})+\mathcal{M}_{1,h}(\widehat{c}_{2,h}^{n-1},z_{2,h})+\mathcal{M}_{2,h}(\widehat{\mathbf{u}}_h^{n-1},\mathbf{v}_h),\tag{3.2}$$

where

$$\widehat{\mathbf{A}}_{\boldsymbol{\xi}_h^n,\mathbf{w}_h^n}\left((\boldsymbol{\rho}_h^n,\zeta_h^n,\mathbf{z}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right):=\mathbf{A}\left((\boldsymbol{\rho}_h^n,\zeta_h^n,\mathbf{z}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right)+\tau\mathbf{B}_{\boldsymbol{\xi}_h^n,\mathbf{w}_h^n}\left((\boldsymbol{\rho}_h^n,\zeta_h^n,\mathbf{z}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right),\tag{3.3}$$

with

$$\begin{aligned}&\mathbf{A}\left((\boldsymbol{\rho}_h^n,\zeta_h^n,\mathbf{z}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right):=\mathcal{M}_{1,h}(\rho_{1,h}^n,z_{1,h})+\tau\mathcal{A}_{1,h}(\rho_{1,h}^n,z_{1,h})+\mathcal{M}_{1,h}(\rho_{2,h}^n,z_{2,h})+\tau\mathcal{A}_{2,h}(\rho_{2,h}^n,z_{2,h})\\ &\quad+\tau\mathcal{A}_{3,h}(\zeta_h^n,\psi_h)-\tau\mathcal{M}_{1,h}(\rho_{1,h}^n,\psi_h)+\tau\mathcal{M}_{1,h}(\rho_{2,h}^n,\psi_h)+\mathcal{M}_{2,h}(\mathbf{z}_h^n,\mathbf{v}_h)+\tau\mathcal{K}_h(\mathbf{z}_h^n,\mathbf{v}_h),\\ &\mathbf{B}_{\boldsymbol{\xi}_h^n,\mathbf{w}_h^n}\left((\boldsymbol{\rho}_h^n,\zeta_h^n,\mathbf{z}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right):=\mathcal{C}_{i,h}(\xi_{1,h}^n;\zeta_h^n,z_{1,h})-\mathcal{C}_{i,h}(\xi_{2,h}^n;\zeta_h^n,z_{2,h})-\mathcal{D}_h(\mathbf{w}_h^n;\rho_{1,h}^n,z_{1,h})\\ &\quad-\mathcal{D}_h(\mathbf{w}_h^n;\rho_{2,h}^n,z_{2,h})+\mathcal{E}_h(\mathbf{w}_h^n;\mathbf{z}_h^n,\mathbf{v}_h)+\left((\xi_{1,h}^n-\xi_{2,h}^n)\nabla\zeta_h^n,\mathbf{v}_h\right)_h,\end{aligned}$$

for all $(\mathbf{z}_h,\psi_h)\in\mathbf{Z}_h\times\mathring{Z}_h$ and $\mathbf{v}_h\in\mathbf{X}_h$.

Lemma 3.1 (Discrete global inf-sup condition) *For each $\boldsymbol{\xi}_h^n\in\boldsymbol{Z}_h$ and $\boldsymbol{w}_h^n\in\boldsymbol{X}_h$ such that $\|\boldsymbol{w}_h^n\|_1\le\frac{\widehat{\alpha}}{6(\gamma_1+\gamma_2)}$, $\|\boldsymbol{\xi}_h^n\|_\infty\le\frac{\widehat{\alpha}}{6\gamma_3}$ and $\|\boldsymbol{\xi}_h^n\|_{\boldsymbol{Z}}\le\frac{\widehat{\alpha}}{6\gamma_4}$, there exists a positive constant $\widehat{\alpha}$ satisfying*

$$\sup_{\substack{(\boldsymbol{z}_h,\psi_h,\boldsymbol{v}_h)\in\boldsymbol{Z}_h\times\mathring{Z}_h\times\boldsymbol{X}_h\\(\boldsymbol{z}_h,\psi_h,\boldsymbol{v}_h)\neq\mathbf{0}}}\frac{\widehat{\mathbf{A}}_{\boldsymbol{\xi}_h^n,\boldsymbol{w}_h^n}\left((\boldsymbol{\rho}_h^n,\zeta_h^n,\boldsymbol{z}_h^n),(\boldsymbol{z}_h,\psi_h,\boldsymbol{v}_h)\right)}{\|(\boldsymbol{z}_h,\psi_h,\boldsymbol{v}_h)\|_{\boldsymbol{Z}\times Z\times\boldsymbol{X}}}\ge\beta_1\|\boldsymbol{\rho}_h^n\|_0+\tilde{\beta}_1\|\boldsymbol{z}_h^n\|_0+\tau\frac{\widehat{\alpha}}{2}\|(\boldsymbol{\rho}_h^n,\zeta_h^n,\boldsymbol{z}_h^n)\|_{\boldsymbol{Z}\times Z\times\boldsymbol{X}}.\tag{3.4}$$

Proof. First, note that the ellipticity of $\mathcal{M}_{1,h},\mathcal{A}_{i,h}$ and $\mathcal{M}_{2,h},\mathcal{K}_h$, will imply an inf-sup condition for $\mathbf{A}$. That is, there exists $\widehat{\alpha}>0$, such that

$$\sup_{\substack{(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\in\mathbf{Z}_h\times\mathring{Z}_h\times\mathbf{X}_h\\(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\neq\mathbf{0}}}\frac{\mathbf{A}\left((\boldsymbol{\rho}_h^n,\zeta_h^n,\mathbf{z}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right)}{\|(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\|_{\mathbf{Z}\times Z\times\mathbf{X}}}\ge\beta_1\|\boldsymbol{\rho}_h^n\|_0+\tilde{\beta}_1\|\mathbf{z}_h^n\|_0+\tau\widehat{\alpha}\,\|(\boldsymbol{\rho}_h^n,\zeta_h^n,\mathbf{z}_h^n)\|_{\mathbf{Z}\times Z\times\mathbf{X}},\tag{3.5}$$

for all $(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\in\mathbf{Z}_h\times\mathring{Z}_h\times\mathbf{X}_h$. Employing (3.5) and the boundedness for $\mathcal{C}_{i,h},\mathcal{D}_h,\mathcal{E}_h,(\cdot,\cdot)_h$ stated in Lemmas 2.1 and 2.2, we readily obtain

$$\begin{aligned}&\sup_{\substack{(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\in\mathbf{Z}_h\times\mathring{Z}_h\times\mathbf{X}_h\\(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\neq\mathbf{0}}}\frac{\widehat{\mathbf{A}}_{\boldsymbol{\xi}_h^n,\mathbf{w}_h^n}\left((\boldsymbol{\rho}_h^n,\zeta_h^n,\mathbf{z}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right)}{\|(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\|_{\mathbf{Z}\times Z\times\mathbf{X}}}\\ &\qquad\ge\beta_1\|\boldsymbol{\rho}_h^n\|_0+\tilde{\beta}_1\|\mathbf{z}_h^n\|_0+\tau(\widehat{\alpha}-(\gamma_1+\gamma_2)\|\mathbf{w}_h^n\|_1-\gamma_3\|\boldsymbol{\xi}_h^n\|_\infty-\gamma_4\|\boldsymbol{\xi}_h^n\|_{\mathbf{Z}})\,\|(\boldsymbol{\rho}_h^n,\zeta_h^n,\mathbf{z}_h^n)\|_{\mathbf{Z}\times Z\times\mathbf{X}},\end{aligned}$$

and (3.4) follows as a consequence of the assumptions $\|\mathbf{w}_h^n\|_1\le\frac{\widehat{\alpha}}{6(\gamma_1+\gamma_2)}$, $\|\boldsymbol{\xi}_h^n\|_\infty\le\frac{\widehat{\alpha}}{6\gamma_3}$ and $\|\boldsymbol{\xi}_h^n\|_1\le\frac{\widehat{\alpha}}{6\gamma_4}$. □ Now we are ready to show that $\mathbf{T}$ is well-defined, or equivalently, that problem (3.2) is uniquely solvable.

Lemma 3.2 (Well-definedness of T) *Let the assumptions of Lemma 3.1 be satisfied. Then, there exists a unique $\{(\widehat{\boldsymbol{c}}_h^n,\widehat{\phi}_h^n),\widehat{\boldsymbol{u}}_h^n\}$ solution to (3.1). In addition, for any $1\le n\le N$, there holds*

$$\begin{aligned}\|\boldsymbol{T}(\boldsymbol{\xi}_h^n,\boldsymbol{w}_h^n)\|_0+\tau\sum_{j=0}^n\|\boldsymbol{T}(\boldsymbol{\xi}_h^j,\boldsymbol{w}_h^j)\|_{\boldsymbol{Z}\times\boldsymbol{X}}&=\|\widehat{\boldsymbol{c}}_h^n\|_0+\|\widehat{\boldsymbol{u}}_h^n\|_0+\tau\sum_{j=0}^n(\|\widehat{\boldsymbol{c}}_h^j\|_{\boldsymbol{Z}}+\|\widehat{\boldsymbol{u}}_h^j\|_1)\\ &\le\max\{c_1,c_2\}\max\{c_1,c_2,\frac{\widehat{\alpha}}{2}\}\left(\|\boldsymbol{c}_0\|_0+\|\boldsymbol{u}_0\|_0\right).\end{aligned}\tag{3.6}$$

Proof. A straightforward application of the classical Babuška–Brezzi theory and Lemma 3.1 implies that problem (3.1) is well-posed. The continuous dependence on data then gives

$$\beta_1\|\widehat{\mathbf{c}}_h^n\|_0+\tilde\beta_1\|\widehat{\mathbf{u}}_h^n\|_0+\tau\frac{\widehat\alpha}{2}\left\|(\widehat{\mathbf{c}}_h^n,\widehat\phi_h^n,\widehat{\mathbf{u}}_h^n)\right\|_{\mathbf{Z}\times Z\times\mathbf{X}}\le\alpha_1\|\widehat{\mathbf{c}}_h^{n-1}\|_0+\tilde\alpha_1\|\widehat{\mathbf{u}}_h^{n-1}\|_0,$$

which, after a simple manipulation of the terms, leads to

$$\underbrace{\min\{\beta_1,\alpha_1\}}_{c_1}\left[\|\widehat{\mathbf{c}}_h^n\|_0-\|\widehat{\mathbf{c}}_h^{n-1}\|_0\right]+\underbrace{\min\{\tilde\beta_1,\tilde\alpha_1\}}_{c_2}\left[\|\widehat{\mathbf{u}}_h^n\|_0-\|\widehat{\mathbf{u}}_h^{n-1}\|_0\right]+\tau\frac{\widehat\alpha}{2}\left\|(\widehat{\mathbf{c}}_h^n,\widehat\phi_h^n,\widehat{\mathbf{u}}_h^n)\right\|_{\mathbf{Z}\times Y\times\mathbf{X}}\le 0.$$

Summing up the above inequality for n, produces

$$\|\widehat{\mathbf{c}}_h^n\|_0+\|\widehat{\mathbf{u}}_h^n\|_0+\tau\sum_{j=0}^{n}\left\|(\widehat{\mathbf{c}}_h^j,\widehat\phi_h^j,\widehat{\mathbf{u}}_h^j)\right\|_{\mathbf{Z}\times Y\times\mathbf{X}}\le\max\{c_1,c_2\}\max\{c_1,c_2,\frac{\widehat\alpha}{2}\}\left(\|\mathbf{c}_0\|_0+\|\mathbf{u}_0\|_0\right),$$

which yields (3.6). □

The next step is to show that $\mathbf{T}$ maps a closed ball in $\mathbf{Z}_h\times\mathbf{X}_h$ into itself. Let us define the set

$$V_h:=\left\{(\boldsymbol{\xi}_h^n,\mathbf{w}_h^n)\in\mathbf{Z}_h\times\mathbf{X}_h:\quad\|\mathbf{w}_h^n\|_1\le\frac{\widehat\alpha}{6(\gamma_1+\gamma_2)},\quad\|\boldsymbol{\xi}_h^n\|_\infty\le\frac{\widehat\alpha}{6\gamma_3},\quad\|\boldsymbol{\xi}_h^n\|_{\mathbf{Z}}\le\frac{\widehat\alpha}{6\gamma_4}\right\}.$$

Lemma 3.3 *Let*

$$C_{\mathtt{stab}}:=\max\{c_1,c_2\}\max\{c_1,c_2,\frac{\widehat\alpha}{2}\},\quad\textit{and}\quad\tilde C_{\mathtt{stab}}:=t_F^{-1}\min\{\frac{\widehat\alpha}{6\alpha_4},\frac{\widehat\alpha}{6(\gamma_1+\gamma_2)}\}.$$

Suppose that the data satisfy

$$C_{\mathtt{stab}}\tilde C_{\mathtt{stab}}\left(\|c_{1,0}\|_0+\|c_{2,0}\|_0+\|\boldsymbol{u}_0\|_0\right)\le 1.$$

Then, $\boldsymbol{T}(V_h)\subset V_h$.

Proof. It is deduced straightforwardly from Lemma 3.2 and the a priori estimate stated in (3.6). □

Lemma 3.4 (Lipschitz-continuity of T) *For any $1\le n\le N$, there holds*

$$\|\boldsymbol{T}(\boldsymbol{\xi}_h^n,\boldsymbol{w}_h^n)-\boldsymbol{T}(\boldsymbol{\rho}_h^n,\boldsymbol{z}_h^n)\|_{\boldsymbol{Z}\times\boldsymbol{X}}\le\hat C_{\mathtt{stab}}\left(\|\boldsymbol{\xi}_h^n-\boldsymbol{\rho}_h^n\|_{\boldsymbol{Z}}+\|\boldsymbol{w}_h^n-\boldsymbol{z}_h^n\|_1\right),$$

in which

$$\hat C_{\mathtt{stab}}:=2c_{\mathrm{p}}^2\max\{\frac{\alpha_1}{3\beta_4},\frac{\gamma_1}{6\gamma_4}+\frac{\gamma_2}{6(\gamma_1+\gamma_2)}\}.$$

Proof. Given $(\boldsymbol{\xi}_h^n,\mathbf{w}_h^n)\in V_h$ and $(\boldsymbol{\rho}_h^n,\mathbf{z}_h^n)\in V_h$, we let $\mathbf{T}(\boldsymbol{\xi}_h^n,\mathbf{w}_h^n)=(\widehat{\mathbf{c}}_h^n,\widehat{\mathbf{u}}_h^n)\in V_h$ and $\mathbf{T}(\boldsymbol{\rho}_h^n,\mathbf{z}_h^n)=(\tilde{\mathbf{c}}_h^n,\tilde{\mathbf{u}}_h^n)\in V_h$, where $\{(\widehat{\mathbf{c}}_h^n,\widehat\phi_h^n),\widehat{\mathbf{u}}_h^n)\}$ and $\{(\tilde{\mathbf{c}}_h^n,\tilde\phi_h^n),\tilde{\mathbf{u}}_h^n\}$ are the unique solutions of (3.1) (equivalently (3.2)) with $(\boldsymbol{\xi}_h^n,\mathbf{w}_h^n)=(\boldsymbol{\rho}_h^n,\mathbf{z}_h^n)$. It follows from (3.2) that

$$\widehat{\mathbf{A}}_{\boldsymbol{\xi}_h^n,\mathbf{w}_h^n}\left((\widehat{\mathbf{c}}_h^n,\widehat\phi_h^n,\widehat{\mathbf{u}}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right)=\widehat{\mathbf{A}}_{\boldsymbol{\rho}_h^n,\mathbf{z}_h^n}\left((\tilde{\mathbf{c}}_h^n,\tilde\phi_h^n,\tilde{\mathbf{u}}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right),$$

for all $(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\in\mathbf{Z}_h\times\mathring{Z}_h\times\mathbf{X}_h$, which, according to the definition of $\widehat{\mathbf{A}}_{\boldsymbol{\xi}_h^n,\mathbf{w}_h^n}$ (cf. (3.3)), becomes

$$\mathbf{A}\left((\widehat{\mathbf{c}}_h^n,\widehat\phi_h^n,\widehat{\mathbf{u}}_h^n)-(\tilde{\mathbf{c}}_h^n,\tilde\phi_h^n,\tilde{\mathbf{u}}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right)=\tau\left[\mathbf{B}_{\boldsymbol{\rho}_h^n,\mathbf{z}_h^n}((\tilde{\mathbf{c}}_h^n,\tilde\phi_h^n,\tilde{\mathbf{u}}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h))-\mathbf{B}_{\boldsymbol{\xi}_h^n,\mathbf{w}_h^n}((\widehat{\mathbf{c}}_h^n,\widehat\phi_h^n,\widehat{\mathbf{u}}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h))\right].$$

This result, combined with (3.3) by setting $(\boldsymbol{\rho}_h^n,\zeta_h^n,\mathbf{z}_h^n)=(\widehat{\mathbf{c}}_h^n-\tilde{\mathbf{c}}_h^n,\widehat\phi_h^n-\tilde\phi_h^n,\widehat{\mathbf{u}}_h^n-\tilde{\mathbf{u}}_h^n)$ yields

$$\begin{aligned}\widehat{\mathbf{A}}_{\boldsymbol{\xi}_h^n,\mathbf{w}_h^n}\left((\widehat{\mathbf{c}}_h^n,\widehat\phi_h^n,\widehat{\mathbf{u}}_h^n)-(\tilde{\mathbf{c}}_h^n,\tilde\phi_h^n,\tilde{\mathbf{u}}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right)&=\mathbf{A}\left((\widehat{\mathbf{c}}_h^n,\widehat\phi_h^n,\widehat{\mathbf{u}}_h^n)-(\tilde{\mathbf{c}}_h^n,\tilde\phi_h^n,\tilde{\mathbf{u}}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right)\\&\quad+\tau\mathbf{B}_{\boldsymbol{\xi}_h^n,\mathbf{w}_h^n}\left((\widehat{\mathbf{c}}_h^n,\widehat\phi_h^n,\widehat{\mathbf{u}}_h^n)-(\tilde{\mathbf{c}}_h^n,\tilde\phi_h^n,\tilde{\mathbf{u}}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right)\\&=\tau\mathbf{B}_{\boldsymbol{\rho}_h^n-\boldsymbol{\xi}_h^n,\mathbf{z}_h^n-\mathbf{w}_h^n}\left((\tilde{\mathbf{c}}_h^n,\tilde\phi_h^n,\tilde{\mathbf{u}}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right).\end{aligned}$$

Hence, we apply the inf-sup condition stated in Lemma 3.1 in the left-hand side of the above equation and utilize the estimates given in Lemmas 2.1 and 2.2 for $\mathcal{C}_{i,h},\mathcal{D}_h,\mathcal{E}_h,(\cdot,\cdot)_h$, to get

$$\tau\frac{\widehat\alpha}{2}\left\|(\widehat{\mathbf{c}}_h^n,\widehat\phi_h^n,\widehat{\mathbf{u}}_h^n)-(\tilde{\mathbf{c}}_h^n,\tilde\phi_h^n,\tilde{\mathbf{u}}_h^n)\right\|_{\mathbf{Z}\times Z\times\mathbf{X}}\le\sup_{(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\neq\mathbf{0}}\frac{\tau\mathbf{B}_{\boldsymbol{\rho}_h^n-\boldsymbol{\xi}_h^n,\mathbf{z}_h^n-\mathbf{w}_h^n}\left((\tilde{\mathbf{c}}_h^n,\tilde\phi_h^n,\tilde{\mathbf{u}}_h^n),(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\right)}{\|(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\|_{\mathbf{Z}\times Z\times\mathbf{X}}}$$

$$= \tau \sup_{(\mathbf{z}_h,\psi_h,\mathbf{v}_h)\neq\mathbf{0}} \frac{\mathcal{C}_{i,h}(\boldsymbol{\rho}_h^n - \boldsymbol{\xi}_h^n; \tilde{\phi}_h^n, \mathbf{z}_h) - \mathcal{D}_h(\mathbf{z}_h^n - \mathbf{w}_h^n; \tilde{\mathbf{c}}_h^n, \mathbf{z}_h) + \mathcal{E}_h(\mathbf{z}_h^n - \mathbf{w}_h^n; \tilde{\mathbf{u}}_h^n, \mathbf{v}_h) + ((\boldsymbol{\rho}_h^n - \boldsymbol{\xi}_h^n)\nabla\tilde{\phi}_h^n, \mathbf{v}_h)_h}{\|(\mathbf{z}_h, \psi_h, \mathbf{v}_h)\|_{\mathbf{Z}\times Z\times\mathbf{X}}}$$

$$\leq \tau\Big\{\gamma_3\|\boldsymbol{\rho}_h^n - \boldsymbol{\xi}_h^n\|_0\|\tilde{\phi}_h^n\|_{1,\infty} + \gamma_1\|\mathbf{z}_h^n - \mathbf{w}_h^n\|_1\|\tilde{\mathbf{c}}_h^n\|_{\mathbf{Z}} + \gamma_2\|\mathbf{z}_h^n - \mathbf{w}_h^n\|_1\|\tilde{\mathbf{u}}_h^n\|_1 + \gamma_4\|\boldsymbol{\rho}_h^n - \boldsymbol{\xi}_h^n\|_{\mathbf{Z}}\|\tilde{\phi}_h^n\|_1\Big\}$$

$$\leq \tau(\gamma_3 c_{\mathtt{P}}\|\tilde{\phi}_h^n\|_{1,\infty} + \gamma_4\|\tilde{\phi}_h^n\|_1)\|\boldsymbol{\rho}_h^n - \boldsymbol{\xi}_h^n\|_{\mathbf{Z}} + \tau(\gamma_1\frac{\widehat{\alpha}}{6\gamma_4} + \gamma_2\frac{\widehat{\alpha}}{6(\gamma_1+\gamma_2)})\|\mathbf{z}_h^n - \mathbf{w}_h^n\|_1, \tag{3.7}$$

where in the last inequality we have used the Poincaré inequality and the fact that $(\tilde{\mathbf{c}}_h^n, \tilde{\mathbf{u}}_h^n) \in V_h$. In addition, a bound for the terms $\|\tilde{\phi}_h^n\|_1$ and $\|\tilde{\phi}_h^n\|_{1,\infty}$ can be derived using that $\{(\tilde{\mathbf{c}}_h^n, \tilde{\phi}_h^n), \tilde{\mathbf{u}}_h^n\}$ is actually a solution to (3.1), that is

$$\mathcal{A}_{3,h}(\tilde{\phi}_h^n, \psi_h) = \mathcal{M}_{1,h}(\tilde{c}_{1,h}^n, \psi_h) - \mathcal{M}_{1,h}(\tilde{c}_{2,h}^n, \psi_h).$$

Letting $\psi_h = \tilde{\phi}_h^n$ in the above equation and invoking Eqs. (2.9a) and (2.10a), we readily get

$$\beta_4\|\tilde{\phi}_h^n\|_1^2 \leq \alpha_1\left(\|\tilde{c}_{1,h}^n\|_0 + \|\tilde{c}_{2,h}^n\|_0\right)\|\tilde{\phi}_h^n\|_0.$$

Appealing to Poincaré and inverse inequalities, implies that

$$\|\tilde{\phi}_h^n\|_1 \leq \frac{\alpha_1}{\beta_4}c_{\mathtt{P}}^2\|\tilde{\mathbf{c}}_h^n\|_{\mathbf{Z}}, \qquad \text{and} \qquad \|\tilde{\phi}_h^n\|_{1,\infty} \leq \frac{\alpha_1}{\beta_4}c_{\mathtt{P}}\|\tilde{\mathbf{c}}_h^n\|_\infty,$$

which together with the fact that $(\tilde{\mathbf{c}}_h^n, \tilde{\mathbf{u}}_h^n) \in V_h$, leads us to

$$\|\tilde{\phi}_h^n\|_1 \leq \frac{\alpha_1\widehat{\alpha}}{6\gamma_4\beta_4}c_{\mathtt{P}}^2, \qquad \text{and} \qquad \|\tilde{\phi}_h^n\|_{1,\infty} \leq \frac{\widehat{\alpha}\alpha_1}{6\gamma_3\beta_4}c_{\mathtt{P}}. \tag{3.8}$$

Finally, combining (3.8), (3.7) and observing that

$$\|\mathbf{T}(\boldsymbol{\xi}_h^n, \mathbf{w}_h^n) - \mathbf{T}(\boldsymbol{\rho}_h^n, \mathbf{z}_h^n)\|_{\mathbf{Z}\times\mathbf{X}} \leq \|(\widehat{\mathbf{c}}_h^n, \widehat{\phi}_h^n, \widehat{\mathbf{u}}_h^n) - (\tilde{\mathbf{c}}_h^n, \tilde{\phi}_h^n, \tilde{\mathbf{u}}_h^n)\|_{\mathbf{Z}\times Z\times\mathbf{X}},$$

the desired continuity follows. □

The main result of this section is summarized in the following theorem.

Theorem 3.1 *Assume that the data satisfy*

$$C_{\mathtt{stab}}\tilde{C}_{\mathtt{stab}}\left(\|c_{1,0}\|_0 + \|c_{2,0}\|_0 + \|\boldsymbol{u}_0\|_0\right) \leq 1.$$

Then, there exists a unique solution $\{(\boldsymbol{c}_h^n, \phi_h^n), \boldsymbol{u}_h^n\} \in \boldsymbol{Z}_h \times \mathring{Z}_h \times \boldsymbol{X}_h$ *with* $(\boldsymbol{c}_h^n, \boldsymbol{u}_h^n) \in V_h$ *for the fully discrete problem* (2.27)*, and for any* $1 \leq n \leq N$*, there holds*

$$\|\boldsymbol{c}_h^n\|_0 + \|\boldsymbol{u}_h^n\|_0 + \tau\sum_{j=0}^n \left\|(\boldsymbol{c}_h^j, \phi_h^j, \boldsymbol{u}_h^j)\right\|_{\boldsymbol{Z}\times Z\times\boldsymbol{X}} \leq C_{\mathtt{stab}}\left(\|c_{1,0}\|_0 + \|c_{2,0}\|_0 + \|\boldsymbol{u}_0\|_0\right). \tag{3.9}$$

Proof. Firstly we realize that solving (2.27) (or equivalently (3.2)) is equivalent to finding $\mathbf{c}_h^n, \mathbf{u}_h^n$ such that

$$\begin{cases} \mathbf{T}(\mathbf{c}_h^n, \mathbf{u}_h^n) = (\mathbf{c}_h^n, \mathbf{u}_h^n), & n = 1, \cdots, N, \\ \mathbf{c}_h^0 = (\Pi_k^0 c_{1,0}, \Pi_k^0 c_{2,0}),\ \mathbf{u}_h^0 = \boldsymbol{\Pi}_k^0\mathbf{u}_0. \end{cases}$$

Finally, the compactness of $\mathbf{T}$ (on the ball V_h) and its Lipschitz-continuity are guaranteed by Lemmas 3.3 and 3.4. Hence, it suffices to apply Banach's fixed-point theorem to the fully discrete VE scheme (2.27) to conclude the existence and uniqueness of solution. Furthermore, the stability result (3.9) is derived directly from (3.6), provided in Lemma 3.2. □

4 Discrete mass conservation and discrete thermal energy decay

This section is devoted to investigate discrete mass conservative and discrete energy decaying properties of (2.27). To that end, first we recall the $k-$consistency of $\mathcal{M}_{1,h}$ and $\mathcal{A}_{i,h}$.

Lemma 4.1 ([13]) *For every polynomial* $q_k \in \mathbb{P}_k(E)$ *and every VE function* $z_h \in Z_k(E)$ *it holds that*

$$\mathcal{M}_{1,h}^E(q_k, z_h) = \mathcal{M}_1^E(q_k, z_h), \quad \text{and} \quad \mathcal{A}_{i,h}^E(q_k, z_h) = \mathcal{A}_i^E(q_k, z_h), \qquad \text{for } i = 1, 2.$$

Lemma 4.2 *Suppose* $\{(c_{1,h}^n, c_{2,h}^n), \phi_h^n\} \in \boldsymbol{Z}_h \times \mathring{Z}_h$ *is the solution of* (2.27a)-(2.27b)*. Then there holds*

$$\|\phi_h^n\|_{1,\infty} \leq C\|c_{1,h}^n - c_{2,h}^n\|_{0,4}.$$

Proof. It is easy to see that the discrete weak formulation (2.27b) for ϕ_h^n can be interpreted as the VEM solution to the following Poisson equation

$$-\Delta\phi = c_{1,h}^n - c_{2,h}^n \qquad \text{in } \Omega,$$

with homogeneous Neumann boundary condition. From $W^{1,\infty}$-estimate of the VEMs [57] and using the Gagliardo–Nirenberg inequality and the regularity estimate, we obtain

$$\|\phi_h^n\|_{1,\infty} \leq C_{\mathtt{inf}}\|\phi\|_{1,\infty} \leq C_{\mathtt{inf}}C_{\mathtt{GN}}\|\phi\|_{2,4} \leq C_{\mathtt{GN}}C_{\mathtt{inf}}\|c_{1,h}^n - c_{2,h}^n\|_{0,4}.$$

This completes the proof. □

Theorem 4.1 (Discrete mass conservation) *Let $\{(c_{1,h}^n, c_{2,h}^n, \phi_h^n), \mathbf{u}_h^n\}_{n=1}^N$ be a solution of the VE scheme (2.27). Then the approximate concentrations satisfy*

$$\sum_{E\in\mathcal{T}_h}\int_E c_{i,h}^n \;\mathrm{d}E = \sum_{E\in\mathcal{T}_h}\int_E c_{i,h}^0 \;\mathrm{d}E, \qquad i=1,2. \tag{4.1}$$

Proof. It follows from (2.27a) by letting $z_{i,h}=1$, $i=1,2$, applying Lemma 4.1 and the definitions of $\mathcal{C}_{i,h}$ and $\mathcal{A}_i$ that

$$\mathcal{M}_1(\delta_t c_{i,h}^n, 1) = \mathcal{D}_h(\mathbf{u}_h^n; c_{i,h}^n, 1). \tag{4.2}$$

By the definition of $\mathcal{D}_h$ given in (2.8b), and using orthogonality property of $\mathbf{\Pi}_k^{0,E}$ and the exactly divergence-free property of the discrete velocity (cf. Remark 2.1) and the fact that $\mathbf{\Pi}_{k-1}^{0,E}\nabla z_h = \nabla\Pi_k^{\nabla,E}z_h$ for any $z_h\in Z_h$, we can get

$$\mathcal{D}_h^E(\mathbf{u}_h^n; c_{i,h}^n, 1) = -\frac{1}{2}\int_E \mathbf{\Pi}_k^{0,E}\mathbf{u}_h^n\mathbf{\Pi}_{k-1}^{0,E}\nabla c_{i,h}^n\,\mathrm{d}E = -\frac{1}{2}\int_E \mathbf{u}_h^n\mathbf{\Pi}_{k-1}^{0,E}\nabla c_{i,h}^n\,\mathrm{d}E = \frac{1}{2}\int_E \mathrm{div}(\mathbf{u}_h^n)\Pi_k^{\nabla,E}c_{i,h}^n\,\mathrm{d}E = 0, \tag{4.3}$$

which by combining (4.2) and (4.3), and summing on n completes the proof. □

Remark 4.1 Equation (4.1) along with the property (1.2), implies that the difference $c_{1,h}^n - c_{2,h}^n$ belongs to the space $\mathring{Z}_h$. More precisely, we have

$$\sum_{E\in\mathcal{T}_h}\int_E \left(c_{1,h}^n - c_{2,h}^n\right)\,\mathrm{d}E = \sum_{E\in\mathcal{T}_h}\int_E \left(c_{1,h}^0 - c_{2,h}^0\right)\,\mathrm{d}E = \sum_{E\in\mathcal{T}_h}\int_E (c_{1,0}-c_{2,0})\,\mathrm{d}E = 0. \tag{4.4}$$

We now establish a discrete energy decay, independently of the discretization parameters h, τ. We define the total free energy as follows (see [47]):

$$E_h(\phi_h^n, \mathbf{u}_h^n) := \frac{1}{2}\left[\|\phi_h^n\|_1^2 + \|\mathbf{u}_h^n\|_0^2\right].$$

Theorem 4.2 (Discrete energy decay) *Let $\{(c_{1,h}^n, c_{2,h}^n, \phi_h^n), \mathbf{u}_h^n\}_{n=1}^N$ be a solution of (2.27). Then*

$$E_h(\phi_h^n, \mathbf{u}_h^n) + \tau\sum_{j=0}^n\left[\beta_1\|c_{1,h}^j - c_{2,h}^j\|_0^2 + \tilde{\beta}_1\|\mathbf{u}_h^j\|_0^2\right] + \frac{\tau^2}{2}\left[\beta_4\|\delta_t\phi_h^n\|_1^2 + \tilde{\beta}_1\|\delta_t\mathbf{u}_h^n\|_0^2\right] \leq E_h(\phi_h^0, \mathbf{u}_h^0). \tag{4.5}$$

Proof. Using as test functions $(z_{i,h}, \psi_h) = (\tau\phi_h^n, \tau(c_{1,h}^n - c_{2,h}^n))$ and $\mathbf{v}_h = \tau\mathbf{u}_h^n$ in (2.27), gives

$$\mathcal{M}_{1,h}(\delta_t c_{i,h}^n, \tau\phi_h^n) + \mathcal{A}_{i,h}(c_{i,h}^n, \tau\phi_h^n) + e_i\mathcal{C}_{i,h}(c_{i,h}^n; \phi_h^n, \tau\phi_h^n) - \mathcal{D}_h(\mathbf{u}_h^n; c_{i,h}^n, \tau\phi_h^n) = 0, \tag{4.6a}$$

$$\mathcal{A}_{3,h}(\tau\phi_h^n, c_{1,h}^n - c_{2,h}^n) - \tau\mathcal{M}_{1,h}(c_{1,h}^n - c_{2,h}^n, c_{1,h}^n - c_{2,h}^n) = 0, \tag{4.6b}$$

$$\mathcal{M}_{2,h}(\delta_t\mathbf{u}_h^n, \tau\mathbf{u}_h^n) + \mathcal{K}_h(\mathbf{u}_h^n, \tau\mathbf{u}_h^n) + \mathcal{E}_h(\mathbf{u}_h^n; \mathbf{u}_h^n, \tau\mathbf{u}_h^n) + \left((c_{1,h}^n - c_{2,h}^n)\nabla\phi_h^n, \tau\mathbf{u}_h^n\right)_h = 0. \tag{4.6c}$$

Next we proceed to differentiate (2.27c) with respect to t, leading to

$$\mathcal{A}_{3,h}(\partial_t\phi_h^n, \psi_h) = \mathcal{M}_{1,h}(\partial_t c_{1,h}^n, \psi_h) - \mathcal{M}_{1,h}(\partial_t c_{2,h}^n, \psi_h) \qquad \forall\psi_h\in\mathring{Z}_h.$$

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

$$\mathcal{A}_{3,h}(\delta_t\phi_h^n, \psi_h) = \mathcal{M}_{1,h}(\delta_t c_{1,h}^n, \psi_h) - \mathcal{M}_{1,h}(\delta_t c_{2,h}^n, \psi_h) \qquad \forall\psi_h\in\mathring{Z}_h,$$

and then taking $\psi_h = \tau\phi_h^n$ implies that

$$\mathcal{A}_{3,h}(\delta_t\phi_h^n, \tau\phi_h^n) = \mathcal{M}_{1,h}(\delta_t c_{1,h}^n, \tau\phi_h^n) - \mathcal{M}_{1,h}(\delta_t c_{2,h}^n, \tau\phi_h^n). \tag{4.7}$$

Combining (4.6a)-(4.6b) and (4.7), and using the chain of identities

$$\mathcal{A}_{3,h}(\delta_t\phi_h^n, \tau\phi_h^n) = \mathcal{A}_{3,h}(\phi_h^n - \phi_h^{n-1}, \phi_h^n) = \frac{1}{2}\mathcal{A}_{3,h}(\phi_h^n - \phi_h^{n-1}, (\phi_h^n - \phi_h^{n-1}) + (\phi_h^n + \phi_h^{n-1}))$$

$$= \frac{\tau^2}{2}\mathcal{A}_{3,h}(\delta_t\phi_h^n,\delta_t\phi_h^n) + \frac{\tau}{2}\delta_t\mathcal{A}_{3,h}(\phi_h^n,\phi_h^n), \tag{4.8}$$

we can readily conclude that

$$\frac{\tau^2}{2}\mathcal{A}_{3,h}(\delta_t\phi_h^n,\delta_t\phi_h^n) + \frac{\tau}{2}\delta_t\mathcal{A}_{3,h}(\phi_h^n,\phi_h^n) = -\tau\mathcal{M}_{1,h}(c_{1,h}^n - c_{2,h}^n, c_{1,h}^n - c_{2,h}^n) - \mathcal{C}_{i,h}(c_{1,h}^n - c_{2,h}^n;\phi_h^n,\tau\phi_h^n) + \mathcal{D}_h(\mathbf{u}_h^n; c_{1,h}^n - c_{2,h}^n, \tau\phi_h^n).$$

Also, after applying the fact that $\mathcal{E}_h(\mathbf{u}_h^n;\mathbf{u}_h^n,\tau\mathbf{u}_h^n) = 0$ and its analogous identity (4.8) in (4.6c), we obtain

$$\frac{\tau^2}{2}\mathcal{M}_{2,h}(\delta_t\mathbf{u}_h^n,\delta_t\mathbf{u}_h^n) + \frac{\tau}{2}\delta_t\mathcal{M}_{2,h}(\mathbf{u}_h^n,\mathbf{u}_h^n) + \tau\mathcal{K}_h(\mathbf{u}_h^n,\mathbf{u}_h^n) = -\tau\left((c_{1,h}^n - c_{2,h}^n)\nabla\phi_h^n,\mathbf{u}_h^n\right)_h.$$

Summing the last two inequalities and employing the coercivity of $\mathcal{A}_{3,h}$, $\mathcal{M}_{1,h}$, $\mathcal{M}_{2,h}$ stated in Eqs. (2.10a) and (2.10b), respectively, allows us to assert that

$$\begin{aligned}\frac{\tau^2}{2}\big[\beta_4\|\delta_t\phi_h^n\|_1^2 + \tilde{\beta}_1\|\delta_t\mathbf{u}_h^n\|_0^2\big] + \frac{\tau}{2}\big[\beta_4\delta_t\|\phi_h^n\|_1^2 + \tilde{\beta}_1\delta_t\|\mathbf{u}_h^n\|_0^2\big] + \tau\big[\beta_1\|c_{1,h}^n - c_{2,h}^n\|_0^2 + \tilde{\beta}_1\|\mathbf{u}_h^n\|_0^2\big]\\ \le \big|\mathcal{D}_h(\mathbf{u}_h^n; c_{1,h}^n - c_{2,h}^n,\tau\phi_h^n) - \tau\left((c_{1,h}^n - c_{2,h}^n)\nabla\phi_h^n,\mathbf{u}_h^n\right)_h - \mathcal{C}_{i,h}(c_{1,h}^n - c_{2,h}^n;\phi_h^n,\tau\phi_h^n)\big|.\end{aligned} \tag{4.9}$$

The second term on the right-hand side of the above inequality can be rewritten by using that $\mathbf{u}_h$ is exactly divergence-free, as follows:

$$\begin{aligned}\left((c_{1,h}^n - c_{2,h}^n)\nabla\phi_h^n,\mathbf{u}_h^n\right)_h &= \left(\Pi_k^0(c_{1,h}^n - c_{2,h}^n)\boldsymbol{\Pi}_k^0\mathbf{u}_h^n, \nabla\Pi_k^\nabla\phi_h^n\right)_0 = -\left(\operatorname{div}(\Pi_k^0(c_{1,h}^n - c_{2,h}^n)\boldsymbol{\Pi}_k^0\mathbf{u}_h^n), \Pi_k^\nabla\phi_h^n\right)_0\\ &= -\left(\operatorname{div}(\boldsymbol{\Pi}_k^0\mathbf{u}_h^n)\Pi_k^0(c_{1,h}^n - c_{2,h}^n), \Pi_k^\nabla\phi_h^n\right)_0 - \left(\boldsymbol{\Pi}_k^0\mathbf{u}_h^n\cdot\nabla\Pi_k^0(c_{1,h}^n - c_{2,h}^n), \Pi_k^\nabla\phi_h^n\right)_0\\ &= -\frac{1}{2}\Big[\left(\boldsymbol{\Pi}_k^0\mathbf{u}_h^n\nabla\Pi_k^0(c_{1,h}^n - c_{2,h}^n), \Pi_k^\nabla\phi_h^n\right)_h - \left(\boldsymbol{\Pi}_k^0\mathbf{u}_h^n\Pi_k^0(c_{1,h}^n - c_{2,h}^n), \nabla\Pi_k^\nabla\phi_h^n\right)_0\Big]\\ &\quad - \frac{1}{2}\left(\operatorname{div}(\boldsymbol{\Pi}_k^0\mathbf{u}_h^n)\Pi_k^0(c_{1,h}^n - c_{2,h}^n), \Pi_k^\nabla\phi_h^n\right)_0.\end{aligned} \tag{4.10}$$

Now, we show that the last term of the above equation is zero. Using the definition of $\boldsymbol{\Pi}_k^0$ and Π_k^0 and Remark 2.1, for any $q_{k-1}\in Y_h$ we have

$$\int_E \operatorname{div}(\boldsymbol{\Pi}_k^0\mathbf{u}_h^n)q_{k-1}\,\mathrm{d}E = -\int_E \boldsymbol{\Pi}_k^0\mathbf{u}_h^n\cdot\nabla q_{k-1}\,\mathrm{d}E = -\int_E \mathbf{u}_h^n\cdot\nabla q_{k-1}\,\mathrm{d}E = \int_E \operatorname{div}(\mathbf{u}_h^n)q_{k-1}\,\mathrm{d}E = 0.$$

Combining the above equation with (4.10) and the definition of $\mathcal{D}_h$ stated in (2.8b) yields

$$\left((c_{1,h}^n - c_{2,h}^n)\nabla\phi_h^n,\mathbf{u}_h^n\right)_h = \mathcal{D}_h(\mathbf{u}_h^n;(c_{1,h}^n - c_{2,h}^n),\phi_h^n). \tag{4.11}$$

On the other hand, for term $\mathcal{C}_{i,h}(c_{1,h}^n - c_{2,h}^n;\phi_h^n,\tau\phi_h^n)$ using Hölder inequality and Lemma 4.2, we have

$$\begin{aligned}0 \le \big|\mathcal{C}_{i,h}(c_{1,h}^n - c_{2,h}^n;\phi_h^n,\tau\phi_h^n)\big| &\le \tau\|c_{1,h}^n - c_{2,h}^n\|_{0,1}\|\phi_h^n\|_{1,\infty}^2\\ &\le \tau\|c_{1,h}^n - c_{2,h}^n\|_{0,1}\left(\|c_{1,h}^n\|_1 + \|c_{2,h}^n\|_1\right)^2,\end{aligned}$$

which together with (4.4) and a priori estimate (3.9) leads to

$$\big|\mathcal{C}_{i,h}(c_{1,h}^n - c_{2,h}^n;\phi_h^n,\tau\phi_h^n)\big| = 0.$$

Then, combining this result with (4.9) and (4.11) yields

$$\begin{aligned}\frac{\tau^2}{2}\big[\beta_4\|\delta_t\phi_h^n\|_1^2 + \tilde{\beta}_1\|\delta_t\mathbf{u}_h^n\|_0^2\big] + \frac{1}{2}\big[\beta_4\|\phi_h^n\|_1^2 + \tilde{\beta}_1\|\mathbf{u}_h^n\|_0^2\big] + \tau\beta_1\|c_{1,h}^n - c_{2,h}^n\|_0^2 + \tau\tilde{\beta}_1\|\mathbf{u}_h^n\|_0^2\\ \le \frac{1}{2}\big[\beta_4\|\phi_h^{n-1}\|_1^2 + \tilde{\beta}_1\|\mathbf{u}_h^{n-1}\|_0^2\big].\end{aligned}$$

Finally, summing up the above inequality on n $(1\le n\le N)$, leads to (4.5). □

5 Convergence analysis

We split the error analysis in two steps. Firstly, we estimate the velocity and pressure discretization errors, $\|\mathbf{u}^n - \mathbf{u}_h^n\|_0$, $\|\mathbf{u}^n - \mathbf{u}_h^n\|_1$, and $\|p^n - p_h^n\|_0$, respectively; and the second stage corresponds to establishing bounds for the concentration error $\|c_i^n - c_{i,h}^n\|_0$ and electrostatic potential error $\|\phi^n - \phi_h^n\|_0$.

5.1 Error bounds: velocity and pressure

We apply the classical Stokes projection to derive optimal error estimates. For a prescribed $\mathbf{F} \in \mathbf{L}^2(\Omega)$, we consider $(\mathbf{w}, s) \in \mathbf{X} \times Y$ as the solution of the following steady Stokes problem

$$-\boldsymbol{\Delta}\mathbf{w} + \nabla s = \mathbf{F}, \qquad \operatorname{div}(\mathbf{w}) = 0, \quad \text{in } \Omega, \qquad \mathbf{w}|_{\partial\Omega} = \mathbf{0}. \tag{5.1}$$

We also consider, for the moment, the approximation of the steady state Stokes problem (5.1) by VEM, as: find $(\mathbf{w}_h, s_h) \in \mathbf{X}_h \times Y_h$ such that

$$\begin{cases} \mathcal{K}_h(\mathbf{w}_h, \mathbf{v}_h) - \mathcal{B}(\mathbf{v}_h, s_h) = (\mathbf{F}_h, \mathbf{v}_h) & \forall \mathbf{v}_h \in \mathbf{X}_h, \\ \mathcal{B}(\mathbf{w}_h, q_h) = 0 & \forall q_h \in Y_h, \end{cases} \tag{5.2}$$

where $\mathbf{F}_h := \boldsymbol{\Pi}_k^0(\mathbf{f})$. We have the following result.

Lemma 5.1 *Let $\mathbf{F}$, $\mathbf{F}_h$, $\mathbf{w}, s$ and $\mathbf{w}_h, s_h$ be as above and suppose that $(\mathbf{F} - \mathbf{F}_h, \mathbf{v}_\pi)_0 = 0$ for $\mathbf{v}_\pi \in \mathbf{P}_k(\mathcal{T}_h)$. Then*

$$\|\mathbf{w} - \mathbf{w}_h\|_0 + h|\mathbf{w} - \mathbf{w}_h|_1 \leq Ch^{k+1} + Ch \sup\left\{ \frac{(\mathbf{F} - \mathbf{F}_h, \mathbf{v}_h)_0}{\|\boldsymbol{\nabla}\mathbf{v}_h\|_0}, \quad \mathbf{v}_h \in \mathbf{X}_h, \ \mathbf{v}_h \neq \mathbf{0} \right\}. \tag{5.3}$$

Proof. First, we split $\mathbf{w} - \mathbf{w}_h = \mathbf{w} - \mathbf{w}_I + \mathbf{w}_I - \mathbf{w}_h$. Then, by setting $\boldsymbol{\vartheta}_{\mathbf{w}} := \mathbf{w}_h - \mathbf{w}_I$, it holds that $\boldsymbol{\vartheta}_{\mathbf{w}} \in \widetilde{\mathbf{X}}_h$. Hence, employing the discrete coercivity of $\mathcal{K}_h(\cdot, \cdot)$, we can assert that

$$\begin{aligned} \tilde{\beta}_2 |\boldsymbol{\vartheta}_{\mathbf{w}}|_1^2 \leq \mathcal{K}_h(\boldsymbol{\vartheta}_{\mathbf{w}}, \boldsymbol{\vartheta}_{\mathbf{w}}) &= \mathcal{K}_h(\mathbf{w}_h, \boldsymbol{\vartheta}_{\mathbf{w}}) - \mathcal{K}_h(\mathbf{w}_I, \boldsymbol{\vartheta}_{\mathbf{w}}) \\ &= (\mathbf{F}_h, \boldsymbol{\vartheta}_{\mathbf{w}}) - \mathcal{K}_h(\mathbf{w}_I, \boldsymbol{\vartheta}_{\mathbf{w}}) + \left[\mathcal{K}(\mathbf{w}, \boldsymbol{\vartheta}_{\mathbf{w}}) - (\mathbf{F}, \boldsymbol{\vartheta}_{\mathbf{w}})_0\right] \\ &= \mathcal{K}_h(\mathbf{w} - \mathbf{w}_I, \boldsymbol{\vartheta}_{\mathbf{w}}) + \left[\mathcal{K}(\mathbf{w}, \boldsymbol{\vartheta}_{\mathbf{w}}) - \mathcal{K}_h(\mathbf{w}, \boldsymbol{\vartheta}_{\mathbf{w}})\right] + \left[(\mathbf{F}_h, \boldsymbol{\vartheta}_{\mathbf{w}})_0 - (\mathbf{F}, \boldsymbol{\vartheta}_{\mathbf{w}})_0\right], \end{aligned}$$

which together with discrete continuity of $\mathcal{K}_h(\cdot, \cdot)$, the estimate (2.4) and Lemma 2.4, allow us to deduce the following bound

$$|\mathbf{w} - \mathbf{w}_h|_1 \leq Ch^k + \sup\left\{ \frac{(\mathbf{F} - \mathbf{F}_h, \mathbf{v}_h)_0}{\|\boldsymbol{\nabla}\mathbf{v}_h\|_0}, \quad \mathbf{v}_h \in \mathbf{X}_h, \ \mathbf{v}_h \neq \mathbf{0} \right\}. \tag{5.4}$$

To derive an error estimate in the L^2-norm, we use a duality argument. Let $\boldsymbol{\Phi} \in \widetilde{\mathbf{X}}$, $r \in Y$, be the (unique) solution of the auxiliary Stokes problem

$$-\boldsymbol{\Delta}\boldsymbol{\Phi} + \nabla r = \mathbf{w} - \mathbf{w}_h, \quad \text{in } \Omega. \tag{5.5}$$

Moreover, we have the following regularity result

$$\|\boldsymbol{\Phi}\|_2 + \|r\|_1 \leq c_{\mathtt{reg}} \|\mathbf{w} - \mathbf{w}_h\|_0. \tag{5.6}$$

Then, the testing of the Eq. (5.5) against $\mathbf{w} - \mathbf{w}_h$ yields

$$\|\mathbf{w} - \mathbf{w}_h\|_0^2 = \mathcal{K}(\boldsymbol{\Phi}, \mathbf{w} - \mathbf{w}_h) = \mathcal{K}(\boldsymbol{\Phi} - \boldsymbol{\Phi}_I, \mathbf{w} - \mathbf{w}_h) + \mathcal{K}(\boldsymbol{\Phi}_I, \mathbf{w} - \mathbf{w}_h). \tag{5.7}$$

The first and second terms in (5.7) can be estimated as

$$\mathcal{K}(\boldsymbol{\Phi} - \boldsymbol{\Phi}_I, \mathbf{w} - \mathbf{w}_h) \leq \tilde{\beta}_1 Ch \|\boldsymbol{\Phi}\|_2 |\mathbf{w} - \mathbf{w}_h|_1, \tag{5.8}$$

and

$$\mathcal{K}(\boldsymbol{\Phi}_I, \mathbf{w} - \mathbf{w}_h) = \underbrace{\mathcal{K}_h(\boldsymbol{\Phi}_I, \mathbf{w}_h) - \mathcal{K}(\boldsymbol{\Phi}_I, \mathbf{w}_h)}_{T_1} + \underbrace{\mathcal{K}(\boldsymbol{\Phi}_I, \mathbf{w}) - \mathcal{K}_h(\boldsymbol{\Phi}_I, \mathbf{w}_h)}_{T_2}, \tag{5.9}$$

respectively. Applying the polynomial consistency property of $\mathcal{K}_h(\cdot, \cdot)$ and Cauchy–Schwarz inequality, implies

$$\begin{aligned} T_1 &= \mathcal{K}_h(\mathbf{w}_h - \mathbf{w}_\pi, \boldsymbol{\Phi}_I - \boldsymbol{\Phi}_\pi) - \mathcal{K}(\mathbf{w}_h - \mathbf{w}_\pi, \boldsymbol{\Phi}_I - \boldsymbol{\Phi}_\pi) \\ &\leq C\left(|\mathbf{w}_h - \mathbf{w}|_1 + |\mathbf{w} - \mathbf{w}_\pi|_1\right)\left(|\boldsymbol{\Phi}_I - \boldsymbol{\Phi}|_1 + |\boldsymbol{\Phi} - \boldsymbol{\Phi}_\pi|_1\right) \\ &\leq Ch\|\boldsymbol{\Phi}\|_2 \left(|\mathbf{w}_h - \mathbf{w}|_1 + h^k |\mathbf{w}|_{k+1}\right). \end{aligned}$$

Also, an application of (5.1) and (5.2) by taking $\mathbf{v} = \boldsymbol{\Phi}_I$ and $\mathbf{v}_h = \boldsymbol{\Phi}_I$, respectively and invoking the assumption that $(\mathbf{F} - \mathbf{F}_h, \mathbf{v}_\pi)_0 = 0$ for $\mathbf{v}_\pi \in \mathbf{P}_k(\mathcal{T}_h)$, yields

$$T_2 = (\mathbf{F} - \mathbf{F}_h, \boldsymbol{\Phi}_I)_0 = (\mathbf{F} - \mathbf{F}_h, \boldsymbol{\Phi}_I - \boldsymbol{\Phi}_\pi)_0 \leq Ch\|\boldsymbol{\Phi}\|_2 \sup\left\{ \frac{(\mathbf{F} - \mathbf{F}_h, \mathbf{v}_h)_0}{\|\boldsymbol{\nabla}\mathbf{v}_h\|_0}, \quad \mathbf{v}_h \in \mathbf{X}_h, \ \mathbf{v}_h \neq \mathbf{0} \right\}.$$

Finally, substituting the bounds (5.8) and (5.9) into (5.7) and using regularity (5.6) gives,

$$\|\mathbf{w} - \mathbf{w}_h\|_0 \leq Ch\left(|\mathbf{w}_h - \mathbf{w}|_1 + \sup\left\{ \frac{(\mathbf{F} - \mathbf{F}_h, \mathbf{v}_h)_0}{\|\boldsymbol{\nabla}\mathbf{v}_h\|_0}, \quad \mathbf{v}_h \in \mathbf{X}_h, \ \mathbf{v}_h \neq \mathbf{0} \right\} \right) + h^{k+1}|\mathbf{w}|_{k+1},$$

which, together with estimate (5.4), completes the proof of this theorem. □

Next we define approximations $(\mathbf{R}_h\mathbf{u}, Q_h p)$ for the solution $(\mathbf{u}, p)$ of the Navier–Stokes problem (1.3c)-(1.3d), by requiring

$$\begin{cases} \mathcal{K}_h(\mathbf{R}_h\mathbf{u}, \mathbf{v}_h) - \mathcal{B}(\mathbf{v}_h, Q_h p) = \mathcal{K}(\mathbf{\Pi}_k^0\mathbf{u}, \mathbf{v}_h) - \mathcal{B}(\mathbf{v}_h, \Pi_{k-1}^0 p) & \forall \mathbf{v}_h \in \mathbf{X}_h, \\ \mathcal{B}(\mathbf{R}_h\mathbf{u} - \mathbf{u}, q_h) = 0 & \forall q_h \in Y_h. \end{cases} \tag{5.10}$$

Lemma 5.2 *For all $t \in (0, t_F]$, the solution of the Navier–Stokes equations (1.3c)-(1.3d) satisfies*

$$\|\mathbf{u} - \mathbf{R}_h\mathbf{u}\|_0 + h|\mathbf{u} - \mathbf{R}_h\mathbf{u}|_1 \le Ch^{k+1}. \tag{5.11}$$

Proof. To apply Lemma 5.1, we make the identification $\mathbf{w} = \mathbf{u}$ and $\mathbf{w}_h = \mathbf{R}_h\mathbf{u}$. Then, referring to (5.1) and (5.2), we set $\mathbf{F} = -\partial_t\mathbf{u} - (\mathbf{u}\cdot\boldsymbol{\nabla})\mathbf{u} - (c_1 - c_2)\nabla\phi \in \mathbf{L}^2(\Omega)$, and define the corresponding functional $\mathbf{F}_h$ by

$$(\mathbf{F}_h, \mathbf{v}_h)_0 := \mathcal{K}(\mathbf{\Pi}_k^0\mathbf{u}, \mathbf{v}_h) - \mathcal{B}(\mathbf{v}_h, \Pi_{k-1}^0 p), \qquad \forall \mathbf{v}_h \in \mathbf{X}_h. \tag{5.12}$$

Our aim is now to show that $(\mathbf{F} - \mathbf{F}_h, \mathbf{v}_\pi)_0 = 0$ for $\mathbf{v}_\pi \in \mathbf{P}_k(\mathcal{T}_h)$. For Eq. (1.3c), we choose the test function $\mathbf{v} = \mathbf{\Pi}_k^0\mathbf{v}_h$, to get

$$\begin{aligned} 0 &= \mathcal{M}_2(\partial_t\mathbf{u}, \mathbf{\Pi}_k^0\mathbf{v}_h) + \mathcal{K}(\mathbf{u}, \mathbf{\Pi}_k^0\mathbf{v}_h) + \mathcal{E}(\mathbf{u};\mathbf{u}, \mathbf{\Pi}_k^0\mathbf{v}_h) - \mathcal{B}(p, \mathbf{\Pi}_k^0\mathbf{v}_h) + \big((c_1 - c_2)\nabla\phi, \mathbf{\Pi}_k^0\mathbf{v}_h\big) \\ &= \mathcal{M}_2(\mathbf{\Pi}_k^0\partial_t\mathbf{u}, \mathbf{v}_h) + \mathcal{K}(\mathbf{\Pi}_k^0\mathbf{u}, \mathbf{v}_h) + \frac{1}{2}\big[(\mathbf{\Pi}_k^0(\mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{u}), \mathbf{v}_h)_0 - (\widehat{\mathbf{\Pi}}_{k-1}^0(\mathbf{u}\otimes\mathbf{u}), \boldsymbol{\nabla}\mathbf{v}_h)\big] - \mathcal{B}(\Pi_{k-1}^0 p, \mathbf{v}_h) \\ &\quad + (\mathbf{\Pi}_k^0\left((c_1 - c_2)\nabla\phi\right), \mathbf{v}_h)_0, \end{aligned} \tag{5.13}$$

where the orthogonality property of $\mathbf{\Pi}_k^0$ was used in the last step. Combining Eqs. (5.12) and (5.13), we find

$$(\mathbf{F}_h, \mathbf{v}_h)_0 = -\mathcal{M}_2(\mathbf{\Pi}_k^0\partial_t\mathbf{u}, \mathbf{v}_h) - \frac{1}{2}\big[(\mathbf{\Pi}_k^0(\mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{u}), \mathbf{v}_h)_0 - (\widehat{\mathbf{\Pi}}_{k-1}^0(\mathbf{u}\otimes\mathbf{u}), \boldsymbol{\nabla}\mathbf{v}_h)\big] - (\mathbf{\Pi}_k^0\left((c_1 - c_2)\nabla\phi\right), \mathbf{v}_h)_0.$$

Then, clearly, $(\mathbf{F} - \mathbf{F}_h, \mathbf{v}_\pi)_0 = 0$ for $\mathbf{v}_\pi \in \mathbf{P}_k(\mathcal{T}_h)$. Moreover, as a consequence of Lemmas 2.4 and 2.5 we have

$$\begin{aligned} (\mathbf{F} - \mathbf{F}_h, \mathbf{v}_h)_{0,E} &= -\int_E (\mathbf{I} - \mathbf{\Pi}_k^{0,E})(\partial_t\mathbf{u})\cdot\mathbf{v}_h\,\mathrm{d}E - \frac{1}{2}\int_E (\mathbf{I} - \mathbf{\Pi}_{k-2}^{0,E})(\mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{u})\cdot(\mathbf{I} - \mathbf{\Pi}_k^{0,E})\mathbf{v}_h\,\mathrm{d}E \\ &\quad + \frac{1}{2}\int_E (\mathbb{I} - \widehat{\mathbf{\Pi}}_{k-1}^{0,E})(\mathbf{u}\otimes\mathbf{u}) : (\mathbb{I} - \widehat{\mathbf{\Pi}}_{k-1}^{0,E})\boldsymbol{\nabla}\mathbf{v}_h\,\mathrm{d}E - \int_E (\mathbf{I} - \mathbf{\Pi}_{k-2}^{0,E})((c_1 - c_2)\nabla\phi)\cdot(\mathbf{I} - \mathbf{\Pi}_k^{0,E})\mathbf{v}_h\,\mathrm{d}E, \end{aligned}$$

and therefore, each of the terms above are estimated as follows:

$$\begin{aligned} \left|\int_E (\mathbf{I} - \mathbf{\Pi}_k^{0,E})(\partial_t\mathbf{u})\cdot\mathbf{v}_h\,\mathrm{d}E\right| &\le Ch^k|\partial_t\mathbf{u}|_{k+1,E}\|\mathbf{v}_h\|_{1,E}, \\ \left|\int_E (\mathbf{I} - \mathbf{\Pi}_{k-2}^{0,E})(\mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{u})\cdot(\mathbf{I} - \mathbf{\Pi}_k^{0,E})\mathbf{v}_h\,\mathrm{d}E\right| &\le Ch^k|\mathbf{u}|_{k,E}|\mathbf{u}|_{k+1,E}\|\mathbf{v}_h\|_{1,E}, \\ \left|\int_E (\mathbb{I} - \widehat{\mathbf{\Pi}}_{k-1}^{0,E})(\mathbf{u}\otimes\mathbf{u}) : (\mathbb{I} - \widehat{\mathbf{\Pi}}_{k-1}^{0,E})\boldsymbol{\nabla}\mathbf{v}_h\,\mathrm{d}E\right| &\le Ch^k|\mathbf{u}|_{k+1,E}^2\|\mathbf{v}_h\|_{1,E}, \\ \left|\int_E (\mathbf{I} - \mathbf{\Pi}_{k-2}^{0,E})((c_1 - c_2)\nabla\phi)\cdot(\mathbf{I} - \mathbf{\Pi}_k^{0,E})\mathbf{v}_h\,\mathrm{d}E\right| &\le Ch^k|(c_1 - c_2)|_{k,E}|\phi|_{k+1,E}\|\mathbf{v}_h\|_{1,E}, \end{aligned}$$

which leads to

$$\sup\left\{\frac{(\mathbf{F} - \mathbf{F}_h, \mathbf{v}_h)_0}{\|\boldsymbol{\nabla}\mathbf{v}_h\|_0}, \quad \mathbf{v}_h \in \mathbf{X}_h,\ \mathbf{v}_h \neq \mathbf{0}\right\} \le Ch^k\left(|\partial_t\mathbf{u}|_{k+1} + |\mathbf{u}|_k|\mathbf{u}|_{k+1} + |\mathbf{u}|_{k+1}^2 + |(c_1 - c_2)|_k|\phi|_{k+1}\right).$$

Consequently, the estimate (5.3) implies (5.11). □

Now, we consider the following problem:

$$\mathcal{M}_{2,h}(\delta_t\mathbf{u}_h^n, \mathbf{v}_h) + \mathcal{K}_h(\mathbf{u}_h^n, \mathbf{v}_h) + \mathcal{E}_h(\mathbf{u}_h^n;\mathbf{u}_h^n, \mathbf{v}_h) = -\left((c_{1,h}^n - c_{2,h}^n)\nabla\phi_h^n, \mathbf{v}_h\right)_h, \quad \forall \mathbf{v}_h \in \widetilde{\mathbf{X}}_h, \tag{5.14}$$

where $\{c_{1,h}^n, c_{2,h}^n, \phi_h^n\}$ is an approximate solution of the PNP system (2.26) 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 $\|c_i^n - c_{i,h}^n\|_0$ and $\|\phi^n - \phi_h^n\|_0$. For this purpose, we split the error $\mathbf{e}^n = \mathbf{u}^n - \mathbf{u}_h^n$ into two parts, $\mathbf{e}^n := \boldsymbol{\xi}^n + \boldsymbol{\eta}^n$, where, $\boldsymbol{\xi}^n = \mathbf{u}^n - \mathbf{w}_h^n$ represents the error inherent in the VEM approximation of a linearized (Stokes) problem, and $\boldsymbol{\eta}^n = \mathbf{w}_h^n - \mathbf{u}_h^n$ represents the error caused by the presence of the nonlinearity in problem (1.3c)-(1.3d). The linearized equation to be satisfied by the auxiliary function $\mathbf{w}_h^n$ is

$$\mathcal{M}_{2,h}(\delta_t\mathbf{w}_h^n, \mathbf{v}_h) + \mathcal{K}_h(\mathbf{w}_h^n, \mathbf{v}_h) = -\widehat{\mathcal{E}}(\mathbf{u}^n;\mathbf{u}^n, \mathbf{v}_h) - \left(\mathbf{\Pi}_k^0((c_1^n - c_2^n)\nabla\phi^n), \mathbf{v}_h\right), \quad \forall \mathbf{v}_h \in \widetilde{\mathbf{X}}_h, \tag{5.15}$$

where the trilinear form $\widehat{\mathcal{E}}(\cdot;\cdot,\cdot)$ is stated in Lemma 2.5.

Lemma 5.3 *Let $\mathbf{w}_h^n \in \widetilde{\boldsymbol{X}}_h$ be the solution of (5.15) corresponding to the initial value $\mathbf{w}_h^0 = \boldsymbol{\Pi}_k^0 \mathbf{u}_0$. Then, the error $\boldsymbol{\xi}^n$ satisfies*

$$\max_{1\le n\le N} \sum_{j=1}^{n} \|\boldsymbol{\xi}^j\|_0^2 + \max_{1\le n\le N} \tau \sum_{j=1}^{n} \left(h^2 \|\boldsymbol{\xi}^j\|_1^2 + h^2 \|\delta_t \boldsymbol{\xi}^j\|_0^2\right) \le C(h^{2(k+1)} + \tau^2). \tag{5.16}$$

Proof. We start writing the error equation in terms of $\boldsymbol{\xi}^n$ and combine (1.3c) with (5.15). Using Eq. (5.13) gives

$$\begin{aligned}\mathcal{M}_{2,h}(\frac{\boldsymbol{\xi}^n - \boldsymbol{\xi}^{n-1}}{\tau}, \mathbf{v}_h) + \mathcal{K}_h(\boldsymbol{\xi}^n, \mathbf{v}_h) &= \left[\mathcal{M}_{2,h}(\delta_t \mathbf{u}^n, \mathbf{v}_h) + \mathcal{K}_h(\mathbf{u}^n, \mathbf{v}_h)\right] - \left[\mathcal{M}_{2,h}(\delta_t \mathbf{w}_h^n, \mathbf{v}_h) + \mathcal{K}_h(\mathbf{w}_h^n, \mathbf{v}_h)\right] \\ &= \left[\mathcal{M}_{2,h}(\delta_t \mathbf{u}^n, \mathbf{v}_h) - \mathcal{M}_2(\boldsymbol{\Pi}_k^0 \partial_t \mathbf{u}^n, \mathbf{v}_h)\right] + \left[\mathcal{K}_h(\mathbf{u}^n, \mathbf{v}_h) - \mathcal{K}(\boldsymbol{\Pi}_k^0 \mathbf{u}^n, \mathbf{v}_h)\right].\end{aligned} \tag{5.17}$$

We divide the rest proof into two steps.

Step 1: error in $\mathbf{H}^1$-norm. First, we take $\mathbf{v}_h = \boldsymbol{\xi}^n$ to obtain

$$\begin{aligned}\mathcal{M}_{2,h}(\frac{\boldsymbol{\xi}^n - \boldsymbol{\xi}^{n-1}}{\tau}, \boldsymbol{\xi}^n) + \mathcal{K}_h(\boldsymbol{\xi}^n, \boldsymbol{\xi}^n) &= \left[\mathcal{M}_{2,h}(\delta_t \mathbf{u}^n, \boldsymbol{\xi}^n) - \mathcal{M}_2(\boldsymbol{\Pi}_k^0 \partial_t \mathbf{u}^n, \boldsymbol{\xi}^n)\right] + \left[\mathcal{K}_h(\mathbf{u}^n, \boldsymbol{\xi}^n) - \mathcal{K}(\boldsymbol{\Pi}_k^0 \mathbf{u}^n, \boldsymbol{\xi}^n)\right] \\ &=: S_1 + S_2.\end{aligned} \tag{5.18}$$

The terms on the right-hand side will be handled separately: For S_1 we first notice that, by adding and subtracting $\mathcal{M}_{2,h}(\partial_t \mathbf{u}^n, \boldsymbol{\xi}^n)$, we can write

$$S_1 = \mathcal{M}_{2,h}(\partial_t \mathbf{u}^n, \boldsymbol{\xi}^n) - \mathcal{M}_2(\boldsymbol{\Pi}_k^0 \partial_t \mathbf{u}^n, \boldsymbol{\xi}^n) + \mathcal{M}_{2,h}(\delta_t \mathbf{u}^n - \partial_t \mathbf{u}^n, \boldsymbol{\xi}^n). \tag{5.19}$$

To determine upper bounds for the terms in the right-hand side of (5.19), we use Cauchy–Schwarz inequality, Lemma 2.4, and the continuity of the L^2-projector $\boldsymbol{\Pi}_k^0$. This gives

$$\left|\mathcal{M}_2(\partial_t \mathbf{u}^n, \boldsymbol{\Pi}_k^0 \boldsymbol{\xi}^n) - \mathcal{M}_{2,h}(\partial_t \mathbf{u}^n, \boldsymbol{\xi}^n)\right| \le \tilde{\alpha}_1 \|\partial_t \mathbf{u}^n - \boldsymbol{\Pi}_k^0 \partial_t \mathbf{u}^n\|_0 \|\boldsymbol{\xi}^n\|_0 \le C h^{k+1} |\partial_t \mathbf{u}^n|_{k+1} \|\boldsymbol{\xi}^n\|_0, \tag{5.20}$$

and

$$\left|\mathcal{M}_{2,h}(\partial_t \mathbf{u}^n - \delta_t \mathbf{u}^n, \boldsymbol{\xi}^n)\right| \le \tilde{\alpha}_1 \tau^{1/2} \|\partial_{tt} \mathbf{u}\|_{\mathrm{L}^2(\mathrm{L}^2)} \|\boldsymbol{\xi}^n\|_0.$$

After combining this estimate with (5.20) and (5.19), we can conclude that

$$|S_1| \le \left\{C h^{k+1} |\partial_t \mathbf{u}^n|_{k+1} + \tau^{1/2} \|\partial_{tt} \mathbf{u}\|_{\mathrm{L}^2(\mathrm{L}^2)}\right\} \|\boldsymbol{\xi}^n\|_0 ,$$

and similarly

$$|S_2| = \left|\mathcal{K}(\mathbf{u}^n, \boldsymbol{\Pi}_k^0 \boldsymbol{\xi}^n) - \mathcal{K}_h(\mathbf{u}^n, \boldsymbol{\xi}^n)\right| \le \tilde{\alpha}_2 |\mathbf{u}^n - \boldsymbol{\Pi}_k^\nabla \mathbf{u}^n|_1 |\boldsymbol{\xi}^n|_1 \le C h^k |\mathbf{u}^n|_{k+1} |\boldsymbol{\xi}^n|_1.$$

Finally, inserting the bounds on S_1 and S_2 into (5.18), yields

$$\mathcal{M}_{2,h}(\frac{\boldsymbol{\xi}^n - \boldsymbol{\xi}^{n-1}}{\tau}, \boldsymbol{\xi}^n) + \mathcal{K}_h(\boldsymbol{\xi}^n, \boldsymbol{\xi}^n) \le \widehat{\varpi}_1^n \|\boldsymbol{\xi}^n\|_0 + \widehat{\varpi}_2^n \|\boldsymbol{\xi}^n\|_1 ,$$

with positive scalars

$$\widehat{\varpi}_1^n \le \overline{C}_1 h^{k+1} + \tau^{1/2} O_1^n, \quad \widehat{\varpi}_2^n \le \overline{C}_2 h^k, \tag{5.21}$$

where

$$\overline{C}_1 \le |\partial_t \mathbf{u}^n|_{k+1}, \quad O_1 \le \|\partial_{tt} \mathbf{u}\|_{\mathrm{L}^2(\mathrm{L}^2)} , \qquad \overline{C}_2 \le |\mathbf{u}^n|_{k+1}.$$

Also, it is not difficult to verify that

$$\mathcal{M}_{2,h}(\frac{\boldsymbol{\xi}^n - \boldsymbol{\xi}^{n-1}}{\tau}, \boldsymbol{\xi}^n) \ge \frac{1}{2\tau}\left(\tilde{\beta}_1 \|\boldsymbol{\xi}^n\|_0^2 - \tilde{\alpha}_1 \|\boldsymbol{\xi}^{n-1}\|_0^2\right), \qquad \mathcal{K}_h(\boldsymbol{\xi}^n, \boldsymbol{\xi}^n) \ge \tilde{\beta}_2 \|\boldsymbol{\xi}^n\|_1^2. \tag{5.22}$$

And employing the inequalities above, gives

$$\frac{1}{2\tau}\left(\|\boldsymbol{\xi}^n\|_0^2 - \|\boldsymbol{\xi}^{n-1}\|_0^2\right) + \tilde{\beta}_2 \|\boldsymbol{\xi}^n\|_1^2 \le \frac{1}{2}(\widehat{\varpi}_1^n)^2 + \frac{1}{2}\|\boldsymbol{\xi}^n\|_0^2 + \frac{(\widehat{\varpi}_2^n)^2}{2\tilde{\beta}_2} + \frac{\tilde{\beta}_2}{2}\|\boldsymbol{\xi}^n\|_1^2 .$$

Then we proceed to sum up the above inequality over n, $1 \le n \le N$, which gives

$$\|\boldsymbol{\xi}^n\|_0^2 + \tau \tilde{\beta}_2 \sum_{j=1}^{n} \|\boldsymbol{\xi}^j\|_1^2 \le \|\boldsymbol{\xi}^0\|_0^2 + \tau \sum_{j=1}^{n} \left[(\widehat{\varpi}_1^j)^2 + (\widehat{\varpi}_2^j)^2\right] + \tau \sum_{j=1}^{n} \|\boldsymbol{\xi}^j\|_0^2. \tag{5.23}$$

Using the fact that $\sum_{j=1}^{n}\tau \le t_F$ along with the definition of $\widehat{\varpi}_1^n$ in (5.21), we obtain

$$\begin{aligned}\tau\sum_{j=1}^{n}\left[(\widehat{\varpi}_1^j)^2+(\widehat{\varpi}_2^j)^2\right]+\tau\sum_{j=1}^{n}\|\boldsymbol{\xi}^j\|_0^2 &\le \sum_{j=1}^{n}\tau\left(\overline{C}_1^2h^{2(k+1)}+\tau(O_1^n)^2+\overline{C}_2^2h^{2k}\right)+\tau\sum_{j=1}^{n}\|\boldsymbol{\xi}^j\|_0^2\\ &\le \left[h^{2(k+1)}\overline{C}_1^2+h^{2k}\overline{C}_2^2\right]\sum_{j=1}^{n}\tau+\tau^2\sum_{j=1}^{n}(O_1^n)^2+\|\boldsymbol{\xi}\|^2_{\mathrm{L}^\infty(\mathrm{L}^2)}\sum_{j=1}^{n}\tau\\ &\le C(h^{2k}+\tau^2)+\|\boldsymbol{\xi}\|^2_{\mathrm{L}^\infty(\mathrm{L}^2)},\end{aligned}$$

which, together with (5.23), yield

$$\max_{1\le n\le N}\tau\sum_{j=1}^{n}\|\boldsymbol{\xi}^j\|_1^2 \le C(h^{2k}+\tau^2). \tag{5.24}$$

Moreover, taking $\mathbf{v}_h=\delta_t\boldsymbol{\xi}^n$ in (5.18) and using similar arguments as before, one can have

$$\max_{1\le n\le N}\tau\sum_{j=1}^{n}\|\delta_t\boldsymbol{\xi}^j\|_0^2 \le C(h^{2k}+\tau^2). \tag{5.25}$$

Step 2: error in $\mathbf{L}^2$-norm. To estimate the L^2-error, we use a parabolic duality argument. For $n=1,\cdots,N$, let $\boldsymbol{\Phi}^j\in\widetilde{\mathbf{X}}$, $r^j\in Y$, be the solution of the *backward* Stokes problem

$$\delta_t\boldsymbol{\Phi}^j+\boldsymbol{\Delta}\boldsymbol{\Phi}^j-\nabla r^j=\boldsymbol{\xi}^j,\qquad \text{for } 0\le j\le n,\qquad \boldsymbol{\Phi}^n=\mathbf{0}.$$

We note that the above problem has a unique solution $(\boldsymbol{\Phi}^j,r^j)\in\widetilde{\mathbf{X}}\times Y$ and satisfies (see [58] for more details)

$$\tau\sum_{j=0}^{n}\left(\|\boldsymbol{\Delta}\boldsymbol{\Phi}^j\|_0^2+\|\delta_t\boldsymbol{\Phi}^j\|_0^2+\|\nabla r^j\|_0\right)\le\tau\sum_{j=0}^{n}\|\boldsymbol{\xi}^j\|_0^2. \tag{5.26}$$

On the other hand, for any $j=0,\cdots,n$, we have

$$\begin{aligned}\|\boldsymbol{\xi}^j\|_0^2 &= \mathcal{M}_2(\delta_t\boldsymbol{\Phi}^j,\boldsymbol{\xi}^j)-\mathcal{K}(\boldsymbol{\Phi}^{j-1},\boldsymbol{\xi}^j)\\ &= \left[\mathcal{M}_2(\delta_t\boldsymbol{\Phi}^j,\boldsymbol{\xi}^j)+\mathcal{M}_2(\boldsymbol{\Phi}^{j-1},\delta_t\boldsymbol{\xi}^j)\right]-\mathcal{M}_2(\boldsymbol{\Phi}^{j-1},\delta_t\boldsymbol{\xi}^j)-\mathcal{K}(\boldsymbol{\Phi}^{j-1},\boldsymbol{\xi}^j)\\ &= \left[\mathcal{M}_2(\boldsymbol{\Phi}^j,\boldsymbol{\xi}^j)-\mathcal{M}_2(\boldsymbol{\Phi}^{j-1},\boldsymbol{\xi}^{j-1})\right]-\mathcal{M}_2(\boldsymbol{\Phi}^{j-1},\delta_t\boldsymbol{\xi}^j)-\mathcal{K}(\boldsymbol{\Phi}^{j-1},\boldsymbol{\xi}^j)\\ &= \left[\mathcal{M}_2(\delta_t\boldsymbol{\Phi}^j,\boldsymbol{\xi}^j)+\mathcal{M}_2(\boldsymbol{\Phi}^{j-1},\delta_t\boldsymbol{\xi}^j)\right]-\left[\mathcal{M}_2(\boldsymbol{\Phi}^{j-1}-\boldsymbol{\Phi}_I^{j-1},\delta_t\boldsymbol{\xi}^j)+\mathcal{K}(\boldsymbol{\Phi}^{j-1}-\boldsymbol{\Phi}_I^{j-1},\boldsymbol{\xi}^j)\right]\\ &\quad -\left[\mathcal{M}_2(\boldsymbol{\Phi}_I^{j-1},\delta_t\boldsymbol{\xi}^j)+\mathcal{K}(\boldsymbol{\Phi}_I^{j-1},\boldsymbol{\xi}^j)\right]\\ &=: L_1^j+L_2^j+L_3^j.\end{aligned} \tag{5.27}$$

In the following, first we focus on the estimation of the last term. Recalling $\boldsymbol{\xi}^j=\mathbf{u}^j-\mathbf{w}_h^j$ and using (5.15) with $\mathbf{v}_h=\boldsymbol{\Phi}_I^j$, one obtains

$$\begin{aligned}L_3^j &= \left[\mathcal{M}_2(\boldsymbol{\Phi}_I^{j-1},\delta_t\mathbf{w}_h^j)+\mathcal{K}(\boldsymbol{\Phi}_I^{j-1},\mathbf{w}_h^j)\right]-\left[\mathcal{M}_2(\boldsymbol{\Phi}_I^{j-1},\delta_t\mathbf{u}^j)+\mathcal{K}(\boldsymbol{\Phi}_I^{j-1},\mathbf{u}^j)\right]\\ &= \left[\mathcal{M}_2(\boldsymbol{\Phi}_I^{j-1},\delta_t\mathbf{w}_h^j)-\mathcal{M}_{2,h}(\boldsymbol{\Phi}_I^{j-1},\delta_t\mathbf{w}_h^j)\right]+\left[\mathcal{K}(\boldsymbol{\Phi}_I^{j-1},\mathbf{w}_h^j)-\mathcal{K}_h(\boldsymbol{\Phi}_I^{j-1},\mathbf{w}_h^j)\right]\\ &= \left[\mathcal{M}_2(\boldsymbol{\Phi}_I^{j-1}-\boldsymbol{\Pi}_{k-1}^0\boldsymbol{\Phi}^{j-1},\delta_t\mathbf{w}_h^j-\delta_t\mathbf{u}_\pi^j)-\mathcal{M}_{2,h}(\boldsymbol{\Phi}_I^{j-1}-\boldsymbol{\Pi}_{k-1}^0\boldsymbol{\Phi}^{j-1},\delta_t\mathbf{w}_h^j-\delta_t\mathbf{u}_\pi^j)\right]\\ &\quad+\left[\mathcal{K}(\boldsymbol{\Phi}_I^{j-1}-\boldsymbol{\Pi}_k^0\boldsymbol{\Phi}^{j-1},\mathbf{w}_h^j-\mathbf{u}_\pi^j)-\mathcal{K}_h(\boldsymbol{\Phi}_I^{j-1}-\boldsymbol{\Pi}_k^0\boldsymbol{\Phi}^{j-1},\mathbf{w}_h^j-\mathbf{u}_\pi^j)\right].\end{aligned}$$

Hence, the terms L_2^j and L_3^j are bounded as

$$\begin{aligned}|L_2^j| &\le Ch|\boldsymbol{\Phi}^{j-1}|_1\|\delta_t\boldsymbol{\xi}^j\|_0+Ch|\boldsymbol{\Phi}^{j-1}|_2|\boldsymbol{\xi}^j|_1,\\ |L_3^j| &\le \left(h^k|\mathbf{u}^j|_{k+1}+\|\delta_t\boldsymbol{\xi}^j\|_0+|\boldsymbol{\xi}^j|_1\right)h|\boldsymbol{\Phi}^{j-1}|_2.\end{aligned}$$

Finally, employing the above bounds in (5.27), and summing over j then using $\boldsymbol{\xi}^0=\mathbf{0}$, $\boldsymbol{\Phi}^n=\mathbf{0}$ together with the Cauchy–Schwarz and Young inequalities give

$$\begin{aligned}\tau\sum_{j=0}^{n}\|\boldsymbol{\xi}^j\|_0^2 &= \sum_{j=0}^{n}\left(\mathcal{M}_2(\boldsymbol{\Phi}^j,\boldsymbol{\xi}^j)-\mathcal{M}_2(\boldsymbol{\Phi}^{j-1},\boldsymbol{\xi}^{j-1})\right)+\tau\sum_{j=1}^{n}\left[L_2^j+L_3^j\right]\\ &\le \frac{1}{3}\tau\sum_{j=0}^{n}\left(|\boldsymbol{\Phi}^j|_1^2+|\boldsymbol{\Phi}^j|_2^2\right)+\frac{3}{2}h^2\tau\sum_{j=0}^{n}\left(\|\delta_t\boldsymbol{\xi}^j\|_0^2+\|\boldsymbol{\xi}^j\|_1^2+h^{2k}|\mathbf{u}^j|_{k+1}^2\right),\end{aligned}$$

which, according to the regularity estimates given by (5.26), along with (5.24) and (5.16), yields (5.25) and finishes the proof. ◻

Lemma 5.4 *For any $n = 1, \cdots, N$, the error $\boldsymbol{\xi}^n = \mathbf{u}^n - \mathbf{w}_h^n$ defined in Lemma 5.3 satisfies*

$$\|\boldsymbol{\xi}^n\|_0 + h|\boldsymbol{\xi}^n|_1 \le C(h^{k+1} + \tau). \tag{5.28}$$

Proof. Using the equations (5.15) and (5.10), satisfied by $\mathbf{w}_h^n$ and $\mathbf{R}_h\mathbf{u}^n$, respectively, we find by an elementary calculation:

$$\begin{aligned}\mathcal{M}_{2,h}(\delta_t(\mathbf{R}_h\mathbf{u}^n - \mathbf{w}_h^n), \mathbf{v}_h) + \mathcal{K}_h(\mathbf{R}_h\mathbf{u}^n - \mathbf{w}_h^n, \mathbf{v}_h) &= \mathcal{M}_{2,h}(\delta_t\mathbf{R}_h\mathbf{u}^n, \mathbf{v}_h) - \mathcal{M}(\boldsymbol{\Pi}_k^0(\partial_t\mathbf{u}^n), \mathbf{v}_h)\\ &= \mathcal{M}_{2,h}(\delta_t\mathbf{R}_h\mathbf{u}^n - \boldsymbol{\Pi}_k^0(\partial_t\mathbf{u}^n), \mathbf{v}_h), \qquad \forall \mathbf{v}_h \in \widetilde{\mathbf{X}}_h.\end{aligned}$$

Thus, setting $\mathbf{v}_h = \mathbf{R}_h\mathbf{u}^n - \mathbf{w}_h^n$, we have

$$\begin{aligned}\frac{1}{2\tau}\left(\|\mathbf{R}_h\mathbf{u}^n - \mathbf{w}_h^n\|_0^2 - \|\mathbf{R}_h\mathbf{u}^{n-1} - \mathbf{w}_h^{n-1}\|_0^2\right) &\le \|\delta_t\mathbf{R}_h\mathbf{u}^n - \boldsymbol{\Pi}_k^0(\partial_t\mathbf{u}^n)\|_0\|\mathbf{R}_h\mathbf{u}^n - \mathbf{w}_h^n\|_0\\ &\le \left(\|\delta_t(\mathbf{R}_h\mathbf{u}^n - \mathbf{u}^n)\|_0 + \|\delta_t\mathbf{u}^n - \partial_t\mathbf{u}^n\|_0 + \|(\mathbf{I} - \boldsymbol{\Pi}_k^0)\partial_t\mathbf{u}^n\|_0\right)\\ &\quad\times\left(\|\mathbf{R}_h\mathbf{u}^n - \mathbf{u}^n\|_0 + \|\mathbf{u}^n - \mathbf{w}_h^n\|_0\right).\end{aligned}$$

Next we use the following bounds (which hold for the terms on the right-hand side of the above inequality)

$$\begin{aligned}\|\delta_t(\mathbf{R}_h\mathbf{u}^n - \mathbf{u}^n)\|_0 &\le \|\partial_t(\mathbf{R}_h\mathbf{u} - \mathbf{u})\|_{\mathrm{L}^\infty(\mathrm{L}^2)}\\ &\le Ch^{k+1}\|\partial_t\mathbf{u}\|_{\mathrm{L}^\infty(\mathrm{L}^2)},\\ \|\delta_t\mathbf{u}^n - \partial_t\mathbf{u}^n\|_0 &\le \tau^{1/2}\|\partial_{tt}\mathbf{u}\|_{\mathrm{L}^2(\mathrm{L}^2)},\\ \|(\mathbf{I} - \boldsymbol{\Pi}_k^0)\partial_t\mathbf{u}^n\|_0 &\le h^{k+1}|\partial_t\mathbf{u}^n|_{k+1},\\ \|\mathbf{R}_h\mathbf{u}^n - \mathbf{u}^n\|_0 &\le Ch^{k+1},\end{aligned}$$

and proceed to sum over n and to employ $\mathbf{R}\mathbf{u}^0 = \mathbf{w}_h^0$, $\sum_{j=0}^n \tau < t_F$ and Lemma 5.3. These steps lead to

$$\|\mathbf{R}_h\mathbf{u}^n - \mathbf{w}_h^n\|_0^2 \le C(h^{2(k+1)} + \tau^2).$$

Combining this bound with the inverse inequality (i.e., $\|\nabla v\|_0 \le h^{-1}\|v\|_0$ for all v), we get

$$\|\mathbf{R}_h\mathbf{u}^n - \mathbf{w}_h^n\|_0 + h\|\mathbf{R}_h\mathbf{u}^n - \mathbf{w}_h^n\|_1 \le C(h^{k+1} + \tau).$$

Finally, this last step together with (5.11), yields (5.28). □

Lemma 5.5 *The function $\mathbf{w}_h^n$ defined in Lemma 5.3 satisfies*

$$\|\mathbf{w}_h^n\|_\infty + \|\nabla\mathbf{w}_h^n\|_{0,4} \le C\|\mathbf{u}^n\|_1^{1/2}\|\mathbf{u}^n\|_2^{1/2} + Ch^{\frac{2k-1}{2}}. \tag{5.29}$$

Proof. By a standard argument including the inverse estimate and Gagliardo–Nirenberg inequality and using Lemma 5.4, we obtain (remembering that $\boldsymbol{\xi}^n = \mathbf{u}^n - \mathbf{w}_h^n$)

$$\begin{aligned}\|\mathbf{w}_h^n\|_\infty \le \|\mathbf{u}^n\|_\infty + Ch^{-1}\|\boldsymbol{\xi}^n\|_0 &\le C\|\mathbf{u}^n\|_{0,4}^{1/2}\|\nabla\mathbf{u}^n\|_{0,4}^{1/2} + Ch^k\\ &\le C\|\mathbf{u}^n\|_1^{1/2}\|\mathbf{u}^n\|_2^{1/2} + Ch^k,\end{aligned} \tag{5.30}$$

and analogously,

$$\|\nabla\mathbf{w}_h^n\|_{0,4} \le \|\nabla\mathbf{u}^n\|_{0,4} + h^{-\frac{1}{2}}\|\nabla\boldsymbol{\xi}^n\|_0 \le C\|\mathbf{u}^n\|_1^{1/2}\|\mathbf{u}^n\|_2^{1/2} + Ch^{k-\frac{1}{2}}.$$

Thus, we can put together this last bound with (5.30), which readily implies (5.29). □

Lemma 5.6 *Let $\mathbf{w}_h^n$ be as defined in Lemma 5.3 and $c_i^n \in \mathrm{H}^{k+1}(\Omega)$, $\phi^n \in \mathrm{H}^{k+1}(\Omega) \cap W^{1,\infty}(\Omega)$, $\mathbf{u}^n \in \mathbf{H}^{k+1}(\Omega)$. Then, for $n = 1, \cdots, N$, the error $\boldsymbol{\eta}^n = \mathbf{w}_h^n - \mathbf{u}_h^n$ satisfies*

$$\|\boldsymbol{\eta}^n\|_0 + h|\boldsymbol{\eta}^n|_1 \le C(h^{k+1} + \tau) + \left(\tau\sum_{j=1}^n\left[\|c_1^j - c_{1,h}^j\|_0^2 + \|c_2^j - c_{2,h}^j\|_0^2 + \|\mathcal{R}_{3,h}\phi^j - \phi_h^j\|_1^2\right]\right)^{1/2}, \tag{5.31}$$

where the projection $\mathcal{P}_{3,h}$ is defined in (5.43).

Proof. We combine the equations (5.15) and (2.27c), satisfied by $\mathbf{w}_h^n$ and $\mathbf{u}_h^n$, respectively, to obtain

$$\begin{aligned}\mathcal{M}_{2,h}(\delta_t\boldsymbol{\eta}^n,\boldsymbol{\eta}^n)+\mathcal{K}_h(\boldsymbol{\eta}^n,\boldsymbol{\eta}^n)&=\left[\mathcal{E}_h(\mathbf{u}_h^n;\mathbf{u}_h^n,\boldsymbol{\eta}^n)-\widehat{\mathcal{E}}(\mathbf{u}^n;\mathbf{u}^n,\boldsymbol{\eta}^n)\right]\\&\quad+\left[((c_{1,h}^n-c_{2,h}^n)\nabla\phi_h^n,\boldsymbol{\eta}^n)_h-(\boldsymbol{\Pi}_{k-2}^0((c_1^n-c_2^n)\nabla\phi^n),\boldsymbol{\eta}^n)_0\right]\\&=:\delta_1+\delta_2.\end{aligned}$$

The terms δ_1 and δ_2 can be rewritten by adding and subtracting some suitable terms

$$\delta_1=\left[\mathcal{E}_h(\mathbf{u}^n;\mathbf{u}^n,\boldsymbol{\eta}^n)-\widehat{\mathcal{E}}(\mathbf{u}^n;\mathbf{u}^n,\boldsymbol{\eta}^n)\right]+\left[\mathcal{E}_h(\mathbf{u}_h^n;\mathbf{u}_h^n,\boldsymbol{\eta}^n)-\mathcal{E}_h(\mathbf{u}^n;\mathbf{u}^n,\boldsymbol{\eta}^n)\right]=:\delta_1^1+\delta_1^2,\tag{5.32}$$

and

$$\begin{aligned}\delta_2&=\left[\,((c_1^n-c_2^n)\nabla\phi^n,\boldsymbol{\eta}^n)_h-\left(\boldsymbol{\Pi}_{k-2}^0((c_1^n-c_2^n)\nabla\phi^n),\boldsymbol{\eta}^n\right)_0\right]+\left[\,\left((c_{1,h}^n-c_{2,h})\nabla\phi_h^n,\boldsymbol{\eta}^n\right)_h-((c_1^n-c_2^n)\nabla\phi^n,\boldsymbol{\eta}^n)_h\,\right]\\&=:\delta_2^1+\delta_2^2.\end{aligned}\tag{5.33}$$

The first term of Eq. (5.32) is estimated using Lemma 2.5 in the following manner

$$|\delta_1^1|\le Ch^{k+1}|\mathbf{u}^n|_{k+1}(|\mathbf{u}^n|_2+|\mathbf{u}^n|_1)\|\boldsymbol{\eta}^n\|_1,\tag{5.34}$$

while for the second term we use the skew-symmetry of $\mathcal{E}_h$, and we recall that $\boldsymbol{\eta}^n=\mathbf{w}_h^n-\mathbf{u}_h^n$, which leads to

$$\begin{aligned}\delta_1^2&=\mathcal{E}_h(\mathbf{u}^n;\mathbf{u}^n-\mathbf{w}_h^n,\boldsymbol{\eta}^n)+\mathcal{E}_h(\mathbf{u}^n;\mathbf{w}_h^n,\boldsymbol{\eta}^n)-\mathcal{E}_h(\mathbf{u}_h^n;\mathbf{u}_h^n+\boldsymbol{\eta}^n,\boldsymbol{\eta}^n)\\&=\mathcal{E}_h(\mathbf{u}^n;\boldsymbol{\xi}^n,\boldsymbol{\eta}^n)+\mathcal{E}_h(\mathbf{u}^n-\mathbf{u}_h^n;\mathbf{w}_h^n,\boldsymbol{\eta}^n).\end{aligned}\tag{5.35}$$

Then, employing the Hölder inequality and Gagliardo-Nirenberg and inverse inequalities, we get

$$\mathcal{E}_h(\mathbf{u}^n;\boldsymbol{\xi}^n,\boldsymbol{\eta}^n)\le\|\mathbf{u}^n\|_{0,4}\left(\|\nabla\boldsymbol{\xi}^n\|_0\|\boldsymbol{\eta}^n\|_{0,4}+\|\boldsymbol{\xi}^n\|_{0,4}\|\nabla\boldsymbol{\eta}^n\|_0\right)\le Ch|\mathbf{u}^n|_1\|\nabla\boldsymbol{\xi}^n\|_0|\boldsymbol{\eta}^n|_1,$$

and

$$\begin{aligned}\mathcal{E}_h(\mathbf{u}^n-\mathbf{u}_h^n;\mathbf{w}_h^n,\boldsymbol{\eta}^n)&\le\|\mathbf{u}^n-\mathbf{u}_h^n\|_0\|\nabla\boldsymbol{\eta}^n\|_0\left(\|\mathbf{w}_h^n\|_\infty+\|\nabla\mathbf{w}_h^n\|_{0,4}\right)\\&\le C\|\mathbf{u}^n-\mathbf{u}_h^n\|_0|\boldsymbol{\eta}^n|_1\left(|\mathbf{u}^n|_1^{1/2}|\mathbf{u}^n|_2^{1/2}+h^{\frac{2k-1}{2}}\right),\end{aligned}$$

where in the last inequality we have invoked the estimate (5.29). Substituting these expressions back into (5.35) and Lemma 5.4, we arrive at

$$\left|\delta_1^2\right|\le C\left(\tilde{c}(\|\boldsymbol{\xi}^n\|_0+\|\boldsymbol{\eta}^n\|_0)+h|\mathbf{u}^n|_1\|\boldsymbol{\xi}^n\|_1\right)\|\boldsymbol{\eta}^n\|_1\le C(|\mathbf{u}^n|_1)\left(h^{k+1}+\tau+\tilde{c}\|\boldsymbol{\eta}^n\|_0\right)\|\boldsymbol{\eta}^n\|_1,\tag{5.36}$$

with $\tilde{c}=|\mathbf{u}^n|_1^{1/2}|\mathbf{u}^n|_2^{1/2}+h^{\frac{2k-1}{2}}$. By combining (5.34) and (5.36) in (5.32) we finally get

$$\left|\delta_1\right|\le C(|\mathbf{u}^n|_1)\left(|\mathbf{u}^n|_{k+1}h^{k+1}+\tau+\tilde{c}\|\boldsymbol{\eta}^n\|_0\right)\|\boldsymbol{\eta}^n\|_1.$$

On the other hand, by arguments similar to those used in the proof of Lemma 2.5, we obtain

$$\left|\delta_2^1\right|\le Ch^{k+1}\left(|c_1^n-c_2^n|_2|\phi^n|_{k+1}+|c_1^n-c_2^n|_{k+1}|\phi^n|_2\right)\|\boldsymbol{\eta}^n\|_1.\tag{5.37}$$

The second term in (5.33) can be estimated by the Hölder inequality, Sobolev embedding $\mathrm{H}^k\subset W^{k-1,4}$ and the continuity of $\boldsymbol{\Pi}_k^{0,E}$ with respect to the L^4-norm, as follows

$$\begin{aligned}\delta_2^2&=\left((c_1^n-c_2^n)\nabla\phi^n-(c_{1,h}^n-c_{2,h}^n)\nabla\phi_h^n,\boldsymbol{\eta}^n\right)_h\\&=((c_1^n-c_2^n)(\nabla\phi^n-\nabla\mathcal{R}_{3,h}\phi^n),\boldsymbol{\eta}^n)_h+\left(((c_1^n-c_2^n)-(c_{1,h}^n-c_{2,h}^n))\nabla\mathcal{R}_{3,h}\phi^n,\boldsymbol{\eta}^n\right)_h\\&\quad+\left((c_{1,h}^n-c_{2,h}^n)(\nabla\mathcal{R}_{3,h}\phi^n-\nabla\phi^n),\boldsymbol{\eta}^n\right)_h\\&\le\Bigg(h|c_1^n-c_2^n|_2\|\nabla\phi^n-\nabla\mathcal{R}_{3,h}\phi^n\|_0+\|\mathcal{R}_{3,h}\phi^n\|_{1,\infty}(\|c_1^n-c_{1,h}^n\|_0+\|c_2^n-c_{2,h}^n\|_0)\\&\quad+(|c_{1,h}^n|_1+|c_{2,h}^n|_1)\|\nabla\mathcal{R}_{3,h}\phi^n-\nabla\phi_h^n\|_0\Bigg)\|\boldsymbol{\eta}^n\|_1.\end{aligned}\tag{5.38}$$

Now, it suffices to substitute (5.37) and (5.38) back into (5.33) and use Theorem 3.1, to arrive at

$$\begin{aligned}\left|\delta_2\right|&\le Ch^{k+1}\left(|c_1^n-c_2^n|_2|\phi^n|_{k+1}+|c_1^n-c_2^n|_{k+1}|\phi^n|_2\right)\|\boldsymbol{\eta}^n\|_1\\&\quad+\Bigg((\|c_1^n-c_{1,h}^n\|_0+\|c_2^n-c_{2,h}^n\|_0)\|\phi^n\|_{1,\infty}+C_{\mathtt{stab}}\left(\|c_{1,0}\|_0+\|c_{2,0}\|_0+\|\mathbf{u}_0\|_0\right)\|\phi_h^n-\mathcal{R}_{3,h}\phi^n\|_1\Bigg)\|\boldsymbol{\eta}^n\|_1.\end{aligned}$$

Inserting the bounds on δ_1 and δ_2 into (5.17), yields

$$\mathcal{M}_{2,h}(\frac{\boldsymbol{\eta}^n-\boldsymbol{\eta}^{n-1}}{\tau},\boldsymbol{\eta}^n)+\mathcal{K}_h(\boldsymbol{\eta}^n,\boldsymbol{\eta}^n)\leq\big[\widehat{\varpi}_1^n+(\|c_1^n-c_{1,h}^n\|_0+\|c_2^n-c_{2,h}^n\|_0)\|\phi^n\|_{1,\infty}$$
$$+\widehat{\varpi}_2^n\|\phi_h^n-\mathcal{R}_{3,h}\phi^n\|_1+\tilde{c}\|\boldsymbol{\eta}^n\|_0\big]\,\|\boldsymbol{\eta}^n\|_1\,,$$

with positive scalars

$$\widehat{\varpi}_1^n\leq\overline{C}_1h^{k+1}+\tau\tilde{c},\quad\widehat{\varpi}_2^n\leq C_{\mathtt{stab}}\left(\|c_{1,0}\|_0+\|c_{2,0}\|_0+\|\mathbf{u}_0\|_0\right),\tag{5.39}$$

where

$$\overline{C}_1\leq\tilde{c}+|\mathbf{u}^n|_{k+1}(|\mathbf{u}^n|_2+|\mathbf{u}^n|_1)+|c_1^n-c_2^n|_2|\phi^n|_{k+1}+|c_1^n-c_2^n|_{k+1}|\phi^n|_2.$$

Furthermore, employing inequalities similarly as in (5.22), gives

$$\frac{1}{2\tau}\left(\|\boldsymbol{\eta}^n\|_0^2-\|\boldsymbol{\eta}^{n-1}\|_0^2\right)+\tilde{\beta}_2\|\boldsymbol{\eta}^n\|_1^2\leq\tilde{c}^2\|\boldsymbol{\eta}^n\|_0^2+\big[\widehat{\varpi}_1^n+(\|c_1^n-c_{1,h}^n\|_0+\|c_2^n-c_{2,h}^n\|_0)\|\phi^n\|_{1,\infty}\big]^2$$
$$+(\widehat{\varpi}_2^n)^2\|\phi_h^n-\mathcal{R}_{3,h}\phi^n\|_1^2+\frac{\tilde{\beta}_2}{4}\,\|\boldsymbol{\eta}^n\|_1^2\,.$$

Finally, removing the non-negative term $\|\boldsymbol{\eta}^n\|_1^2$ and then summing up the obtained inequality over n, $1\leq n\leq N$, we find

$$\|\boldsymbol{\eta}^n\|_0^2\leq\|\boldsymbol{\eta}^0\|_0^2+\tau\sum_{j=1}^n\tilde{c}^2\|\boldsymbol{\eta}^j\|_0^2+\tau\sum_{j=1}^n\big[\widehat{\varpi}_1^j+(\|c_1^j-c_{1,h}^j\|_0+\|c_2^j-c_{2,h}^j\|_0)\|\phi^j\|_{1,\infty}+\widehat{\varpi}_2^n\|\phi_h^j-\mathcal{R}_{3,h}\phi^j\|_1\big]^2.\tag{5.40}$$

Using the fact that $\sum_{j=1}^n\tau\leq t_F$ along with the definition of $\widehat{\varpi}_1^n$ in (5.39), we obtain

$$\begin{aligned}\tau\sum_{j=1}^n(\widehat{\varpi}_1^j)^2&\leq\sum_{j=1}^n\tau\left(\overline{C}_1h^{k+1}+\tilde{C}\tau\right)^2\\&\leq\big[h^{2(k+1)}\overline{C}_1^2+\tau^2\tilde{C}\big]\sum_{j=1}^n\tau\\&\leq C(h^{2(k+1)}+\tau^2),\end{aligned}$$

which, after an application of Eq. (5.40) and discrete Gronwall inequality, yield the required estimate in the L^2-norm. Hence, the inverse inequality implies the desired estimate (5.31), and this completes the proof. □

Theorem 5.1 *Given $\{\mathbf{c}_h^n,\phi_h^n\}\in\boldsymbol{Z}_h\times\mathring{Z}_h$, let $\mathbf{u}_h^n\in\widetilde{\mathbf{X}}_h$ be the solution to (5.14) and $\{\mathbf{c}^n,\phi^n\}$, $\{\mathbf{u}^n,p^n\}$ be the solution of (1.1) satisfying the following regularity conditions*

$$\|\partial_t\mathbf{u}\|_{\mathrm{L}^\infty(\mathrm{H}^{k+1})}+\|\mathbf{u}\|_{\mathrm{L}^\infty(\mathrm{H}^{k+1})}+\|\partial_{tt}\mathbf{u}\|_{\mathrm{L}^2(\mathrm{L}^2)}+\|\partial_t\mathbf{u}\|_{\mathrm{L}^2(\mathrm{H}^{k+1})}+(\|\mathbf{u}^n\|_k+\|\mathbf{u}^n\|_1+\|\mathbf{u}^n\|_{k+1}+1)\,\|\mathbf{u}^n\|_{k+1}\leq C,$$

$$(\|c_1^n\|_1+\|c_2^n\|_1)(\|\phi^n\|_2+\|\phi^n\|_{s+1})+(\|c_1^n\|_{k+1}+\|c_2^n\|_{k+1})\|\phi^n\|_1\leq C.$$

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

$$\|\mathbf{u}^n-\mathbf{u}_h^n\|_0+h\|\mathbf{u}^n-\mathbf{u}_h^n\|_1\leq C(h^{k+1}+\tau)+\left(\tau\sum_{j=1}^n\big[\|c_1^j-c_{1,h}^j\|_0^2+\|c_2^j-c_{2,h}^j\|_0^2+\|\mathcal{P}_{3,h}\phi^j-\phi_h^j\|_1^2\big]\right)^{1/2}.$$

Proof. It follows straightforwardly from Lemmas 5.4 and 5.6. □

5.2 Error bounds: concentrations and electrostatic potential

Let us now consider the following problem:

$$\mathcal{M}_{1,h}(\delta_t c_{i,h}^n, z_{i,h}) + \mathcal{A}_{i,h}(c_{i,h}^n, z_{i,h}) + e_i\mathcal{C}_{i,h}(c_{i,h}^n;\phi_h^n, z_{i,h}) - \mathcal{D}_h(\mathbf{u}_h^n; c_{i,h}^n, z_{i,h}) = 0, \tag{5.41a}$$

$$\mathcal{A}_{3,h}(\phi_h^n, \psi_h) - \mathcal{M}_{1,h}(c_{1,h}^n, \psi_h) + \mathcal{M}_{1,h}(c_{2,h}^n, \psi_h) = 0, \tag{5.41b}$$

where $\mathbf{u}_h^n \in \widetilde{\mathbf{X}}_h$ is the solution from (2.27) for $n = 1, \cdots, N$. The aim of this part is to attain an upper bound for $\|c_i^n - c_{i,h}^n\|_0$. Next we define discrete projection operators that will be instrumental in deriving error estimates for concentrations and electrostatic potential. For this purpose, for a fixed $\mathbf{u}(t) \in \mathbf{X}$ and $t \in J$, we define the discrete projection operators $\mathcal{P}_{i,h} : Z \to Z_h$ and $\mathcal{P}_{3,h} : \mathring{Z} \to \mathring{Z}_h$, as follows

$$\underbrace{\mathcal{A}_{i,h}(\mathcal{P}_{i,h}c_i, z_{i,h}) + e_i\mathcal{C}_{i,h}(\mathcal{P}_{i,h}c_i;\mathcal{P}_{3,h}\phi, z_{i,h})}_{:=\overline{\mathcal{B}}_{i,h}(\mathcal{P}_{i,h}c_i;\phi,z_{i,h})} = \underbrace{\mathcal{A}_i(\Pi_k^0 c_i, z_{i,h}) + e_i\widehat{\mathcal{C}}(c_i;\phi, z_{i,h})}_{:=\mathcal{L}_i(z_{i,h})}, \tag{5.42}$$

and

$$\mathcal{A}_{3,h}(\mathcal{P}_{3,h}\phi, \psi_h) = \mathcal{A}_3(\phi, \psi_h), \tag{5.43}$$

respectively, where

$$\widehat{\mathcal{C}}(c_i;\phi, z_i) := \left(\mathbf{\Pi}_{k-1}^0(c_i\nabla\phi), \nabla z_i\right)_0.$$

Lemma 5.7 *Assume that $\mathbf{u} \in \mathbf{L}^\infty(\Omega)$ and $\phi \in W^{1,\infty}(\Omega)$ for all $t \in (0, t_F]$. Then, the operator $\mathcal{P}_{i,h} : Z \to Z_h$ in (5.42) is well-defined.*

Proof. We proceed by the generalized 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 (5.42) satisfies the following two conditions:

(i) There exists $\hat{c}_1$ such that

$$\sup_{z_h\in Z_h} \frac{\overline{\mathcal{B}}_{i,h}(\omega_h;\phi, z_h)}{\|z_h\|_1} \geq \hat{c}_1\|\omega_h\|_1;$$

(ii)

$$\sup_{z_h\in Z_h} \left|\overline{\mathcal{B}}_h(\omega_h;\phi, z_h)\right| > 0.$$

The proof of cases (i) and (ii) can be found in Ref. [59]. The second step proves that the right-hand side functional is bounded over Z_h. Continuity of $\mathcal{L}_i$ is achieved by the continuity of the form $\mathcal{A}_i(\cdot,\cdot)$ and projection $\mathbf{\Pi}_{k-1}^0$, and Poincaré inequality with

$$\widehat{\mathcal{C}}(c_i;\phi, z_i) = (\mathbf{\Pi}_{k-1}^0(c_i\nabla\phi), \nabla z_i)_0 \leq \|\mathbf{\Pi}_{k-1}^0(c_i\nabla\phi)\|_0|z_i|_1 \leq \|\phi\|_{1,\infty}|c_i|_1|z_i|_1,$$

Then, combining this result with (2.10a) completes the proof. □

Now we derive the error estimates of $\phi - \mathcal{P}_{3,h}\phi$, $c_1 - \mathcal{P}_{1,h}c_1$ and $c_2 - \mathcal{P}_{2,h}c_2$ in the L^2-norm.

Lemma 5.8 ([50]) *Assume that $\phi \in \mathrm{H}^{k+1}(\Omega) \cap \mathrm{H}^1(\Omega)$. Then, there exists a unique $\mathcal{P}_{3,h}\phi \in Z_h$ solution of (5.43) satisfying*

$$\|\phi - \mathcal{P}_{3,h}\phi\|_0 + h|\phi - \mathcal{P}_{3,h}\phi|_1 \leq Ch^{k+1}|\phi|_{k+1},$$
$$|\phi - \mathcal{P}_{3,h}\phi|_{1,\infty} \leq Ch^k|\phi|_{k+1,\infty}.$$

Lemma 5.9 *Suppose that $\{c_1, c_2, \phi\}$ is the solution of (1.1) satisfying the following regularity assumptions*

$$|c_i|_1 + |c_i|_{k+1} + |\phi|_{1,\infty} + |\phi|_2 + |\phi|_{k+1} \leq C,$$

and $\mathcal{P}_{i,h}$ is defined as in (5.42). Then for $t \in (0, t_F]$, we have the following error estimates

$$\|c_i - \mathcal{P}_{i,h}c_i\|_0 + h|c_i - \mathcal{P}_{i,h}c_i|_1 \leq Ch^{k+1}.$$

Proof. We first bound the term $c_i - \mathcal{P}_{i,h}c_i$ in the H^1-norm for any $t \in (0, t_F]$. To this end, for $\{c_1, c_2\} \in \mathrm{H}^{k+1}(\Omega)\times\mathrm{H}^{k+1}(\Omega)$ we recall the estimate of its interpolant $\{c_{1,I}, c_{2,I}\}$ given in (2.4). Let $\theta_i := \mathcal{P}_{i,h}c_i - c_{i,I}$ be elements of Z_h. Employing the discrete coercivity of $\mathcal{L}_{i,h}$ (cf. proof of Lemma 5.7) and Eq. (5.42), yields

$$\begin{aligned}
|\theta_i|_1^2 &\leq \mathcal{A}_{i,h}(\theta_i, \theta_i) = \mathcal{A}_{i,h}(\mathcal{P}_{i,h}c_i - c_{i,I}, \theta_i)\\
&= \left[\mathcal{A}_i(\Pi_k^0 c_i, \theta_i) + e_i\widehat{\mathcal{C}}(c_i;\phi, \theta_i) - e_i\mathcal{C}_{i,h}(\mathcal{P}_{i,h}c_i;\mathcal{P}_{3,h}\phi, \theta_i^n)\right] - \mathcal{A}_{i,h}(c_{i,I}, \theta_i)\\
&= \mathcal{A}_{i,h}(c_i - c_{i,I}, \theta_i) + \left[\mathcal{A}_i(\Pi_k^0 c_i, \theta_i) - \mathcal{A}_{i,h}(c_i, \theta_i)\right]\\
&\quad + e_i\left[\widehat{\mathcal{C}}_i(c_i;\phi, \theta_i^n) - \mathcal{C}_{i,h}(\mathcal{P}_{i,h}c_i;\mathcal{P}_{3,h}\phi, \theta_i)\right]
\end{aligned}$$

$$=: L_1 + L_2. \tag{5.44}$$

First, we will bound the term L_1 in the above decomposition. This is achieved by Lemma 2.4 and (2.9a) as

$$\begin{aligned}\mathcal{A}_{i,h}(c_i - c_{i,I}, \theta_i) &\le Ch^k |c_i|_{k+1} |\theta_i|_1,\\ \left|\mathcal{A}_i(\Pi_k^0 c_i, \theta_i) - \mathcal{A}_{i,h}(c_i, \theta_i)\right| &\le \left|\mathcal{A}_i(\Pi_k^0 c_i^n - c_i^n, \theta_i^n)\right| + \left|\mathcal{A}_i(c_i^n, \theta_i^n) - \mathcal{A}_{i,h}(c_i, \theta_i)\right|\\ &\le Ch^k |c_i|_{k+1} |\theta_i|_1,\end{aligned}$$

which leads to

$$L_1 \le Ch^k |c_i|_{k+1} |\theta_i|_1.$$

Next, in order to estimate L_2, we add zero in the form $\pm\mathcal{C}_{i,h}(c_i;\phi,\theta_i)$, to find that

$$L_2 = \underbrace{\left[\widehat{\mathcal{C}}_i(c_i;\phi,\theta_i) - \mathcal{C}_{i,h}(c_i;\phi,\theta_i)\right]}_{L_2^{(1)}} + \underbrace{\mathcal{C}_{i,h}(c_i;\phi - \mathcal{P}_{3,h}\phi, \theta_i)}_{L_2^{(2)}} + \underbrace{\mathcal{C}_{i,h}(c_i - \mathcal{P}_{i,h}c_i; \mathcal{P}_{3,h}\phi, \theta_i)}_{L_2^{(3)}}. \tag{5.45}$$

Note that from Lemma 2.7, it holds

$$L_2^{(1)} \le Ch^k \left(|c_i|_1 |\phi|_{k+1} + |\phi|_1 |c_i|_{k+1}\right) |\theta_i|_1.$$

For the term $L_2^{(2)}$, from Hölder inequality and the approximation property of $\mathcal{P}_{3,h}$ and Theorem 3.1, we obtain

$$|L_2^{(2)}| \le \|c_i\|_0 \|\phi - \mathcal{P}_{3,h}\|_{1,\infty} |\theta_i|_1 \le h^k |c_i|_1 |\phi|_{k+1} |\theta_i|_1.$$

For the last term of (5.45), by similar arguments, we derive

$$|L_2^{(3)}| \le \gamma_3 \|\theta_i\|_0 \|\nabla \mathcal{P}_{3,h}\phi\|_\infty \|\theta_i\|_1,$$

and using the triangle inequality and Lemma 5.8, we obtain the following upper bound

$$\|\nabla \mathcal{P}_{3,h}\phi\|_\infty \le \|\nabla\phi\|_\infty + \|\nabla(\phi - \mathcal{P}_{3,h}\phi)\|_\infty \le \|\phi\|_{1,\infty}, \tag{5.46}$$

which implies

$$|L_2^{(3)}| \le \gamma_3 \|\theta_i\|_0 \|\phi\|_{1,\infty} |\theta_i|_1.$$

Thus, the H^1-seminorm estimate is derived by inserting the bounds for $L_1^{(1)}$, $L_1^{(2)}$ and $L_1^{(3)}$ into L_2 and then substituting the obtained estimates for L_1 and L_2 in (5.44) as

$$|\theta_i|_1 \le Ch^k + \|\theta_i\|_0. \tag{5.47}$$

In order to present the L^2 estimate for θ_i we shall use duality arguments. For $\phi \in W^{1,\infty}(\Omega)$, let $w_i \in \mathrm{H}^2(\Omega)$ be the solution of

$$-\Delta w_i + e_i \nabla\phi \cdot \nabla w_i = c_i - \mathcal{P}_i c_i, \qquad \text{in } \Omega, \qquad \nabla w_i \cdot \mathbf{n}|_{\partial\Omega} = 0. \tag{5.48}$$

By the regularity theory of second-order elliptic equations [22], we have that

$$\|w_i\|_2 \le C\|\hat{\theta}_i\|_0. \tag{5.49}$$

Setting $\hat{\theta}_i := c_i - \mathcal{P}_i c_i$ and taking the test function $\hat{\theta}_i$ in (5.48) and adding and subtracting an appropriate expression, we obtain

$$\begin{aligned}\|\hat{\theta}_i\|_0^2 &= \mathcal{A}_i(w_i, \hat{\theta}_i) + e_i \mathcal{C}_i(\hat{\theta}_i;\phi, w_i)\\ &= \left[\mathcal{A}_i(w_i,\hat{\theta}_i) - \mathcal{A}_i(w_{i,I}, \Pi_k^0\hat{\theta}_i)\right] + e_i\left[\mathcal{C}_i(\hat{\theta}_i;\phi,w_i) - \widehat{\mathcal{C}}_i(\hat{\theta}_i;\phi,w_{i,I})\right] + \mathcal{A}_i(w_{i,I},\Pi_k^0\hat{\theta}_i) + e_i\widehat{\mathcal{C}}_i(\hat{\theta}_i;\phi,w_{i,I})\\ &= \left[\mathcal{A}_i(w_i,\hat{\theta}_i) - \mathcal{A}_i(w_{i,I}, \Pi_k^0\hat{\theta}_i)\right] + e_i\left[\mathcal{C}_i(\hat{\theta}_i;\phi,w_i) - \widehat{\mathcal{C}}_i(\hat{\theta}_i;\phi,w_{i,I})\right]\\ &\quad + \mathcal{A}_i(w_{i,I}, \Pi_k^0(c_i - \mathcal{P}_i c_i)) + e_i\widehat{\mathcal{C}}_i(c_i - \mathcal{P}_{i,h}c_i;\phi,w_{i,I})\\ &\quad + \mathcal{A}_{i,h}(w_{i,I},\mathcal{P}_i c_i) + e_i\mathcal{C}_{i,h}(\mathcal{P}_{i,h}c_i;\phi,w_{i,I}) - \mathcal{A}_{i,h}(w_{i,I},\mathcal{P}_i c_i) - e_i\mathcal{C}_{i,h}(\mathcal{P}_i c_i;\phi,w_{i,I})\\ &= \left[\mathcal{A}_i(w_i,\hat{\theta}_i) - \mathcal{A}_i(w_{i,I}, \Pi_k^0\hat{\theta}_i)\right] + e_i\left[\mathcal{C}_i(\hat{\theta}_i;\phi,w_i) - \widehat{\mathcal{C}}_i(\hat{\theta}_i;\phi,w_{i,I})\right]\\ &\quad + \left[\mathcal{A}_{i,h}(w_{i,I},\mathcal{P}_i c_i) - \mathcal{A}_i(w_{i,I},\Pi_k^0(\mathcal{P}_i c_i))\right] + e_i\left[\mathcal{C}_{i,h}(\mathcal{P}_i c_i;\mathcal{P}_3\phi,w_{i,I}) - \widehat{\mathcal{C}}_i(\mathcal{P}_i c_i;\phi,w_{i,I})\right],\end{aligned} \tag{5.50}$$

where the definition of the projector $\mathcal{R}_{i,h}$ (cf. (5.42)) was applied in the last step. The first three terms on the right-hand side of the above equation can be estimated using similar arguments as in the proof of Lemma 5.3 as

$$\left|\mathcal{A}_i(w_i,\hat{\theta}_i) - \mathcal{A}_i(w_{i,I},\Pi_k^0\hat{\theta}_i)\right| \le \left|\mathcal{A}_i(w_i - w_{i,I},\hat{\theta}_i)\right| + \left|\mathcal{A}_i(w_{i,I} - \Pi_k^0 w_i, (I - \Pi_k^0)\hat{\theta}_i)\right|$$

$$
\begin{aligned}
&\le Ch|w_i|_2|\hat{\theta}_i|_1, && (5.51a)\\
\left|\mathcal{C}_i(\hat{\theta}_i;\phi,w_i)-\widehat{\mathcal{C}}_i(\hat{\theta}_i;\phi,w_{i,I})\right| &\le \left|\mathcal{C}_i(\hat{\theta}_i;\phi,w_i-w_{i,I})\right| + \left|\Big((\mathbf{I}-\mathbf{\Pi}^0_{k-2})(\hat{\theta}_i\nabla\phi),\nabla(w_{i,I}-\Pi^\nabla_k w_i)\Big)_0\right| \\
&\le Ch\|\phi\|_2|w_i|_2|\hat{\theta}_i|_1, && (5.51b)\\
\left|\mathcal{A}_{i,h}(w_{i,I},\mathcal{P}_ic_i)-\mathcal{A}_i(w_{i,I},\Pi^0_k(\mathcal{P}_ic_i))\right| &\le \left|\mathcal{A}_{i,h}(w_{i,I}-\Pi^0_k w_i,\mathcal{P}_ic_i-c_{i,\pi})\right| \\
&\quad + \left|\mathcal{A}_i(w_{i,I}-\Pi^0_k w_i,\Pi^0_k(\mathcal{P}_ic_i-c_{i,\pi}))\right| \\
&\le \left(h^k|c_i|_{k+1}+|\hat{\theta}_i|_1\right)h|w_i|_2. && (5.51c)
\end{aligned}
$$

It remains to estimate the last term on the right-hand side of Eq. (5.50). Adding and subtracting suitable terms, there holds

$$
\begin{aligned}
\mathcal{C}_{i,h}(\mathcal{P}_ic_i;\mathcal{P}_3\phi,w_{i,I})-\widehat{\mathcal{C}}_i(\mathcal{P}_ic_i;\phi,w_{i,I}) &= \mathcal{C}_{i,h}(\mathcal{P}_ic_i;\mathcal{P}_3\phi,w_{i,I}-w_i)-\widehat{\mathcal{C}}_i(\mathcal{P}_ic_i;\phi,w_{i,I}-w_i)\\
&\quad+\mathcal{C}_{i,h}(\mathcal{P}_ic_i;\mathcal{P}_3\phi,w_i)-\widehat{\mathcal{C}}_i(\mathcal{P}_ic_i;\phi,w_i)\\
&=\left[\mathcal{C}_{i,h}(\mathcal{P}_ic_i-c_i;\mathcal{P}_3\phi,w_{i,I}-w_i)-\widehat{\mathcal{C}}_i(\mathcal{P}_ic_i-c_i;\phi,w_{i,I}-w_i)\right]\\
&\quad+\left[\mathcal{C}_{i,h}(c_i;\mathcal{P}_3\phi,w_{i,I}-w_i)-\widehat{\mathcal{C}}_i(c_i;\phi,w_{i,I}-w_i)\right]\\
&\quad+\left[\mathcal{C}_{i,h}(\mathcal{P}_ic_i-c_i;\mathcal{P}_3\phi,w_i)-\widehat{\mathcal{C}}_i(\mathcal{P}_ic_i-c_i;\phi,w_i)\right]+\mathcal{C}_{i,h}(c_i;\mathcal{P}_3\phi-\phi,w_i)\\
&\quad+\left[\mathcal{C}_{i,h}(c_i;\phi,w_i)-\widehat{\mathcal{C}}_i(c_i;\phi,w_i)\right]\\
&=:\sum_{i=1}^5 S_i. && (5.52)
\end{aligned}
$$

By Cauchy–Schwarz inequality, the approximation property of the interpolate $w_{i,I}$, the boundedness of forms $\mathcal{C}_i$ and $\mathcal{C}_{i,h}$ and Lemma 2.7, we get

$$
\begin{aligned}
|S_1| &\le \left|\mathcal{C}_{i,h}(\hat{\theta}_i;\mathcal{P}_3\phi,w_{i,I}-w_i)\right|+\left|\widehat{\mathcal{C}}_i(\hat{\theta}_i;\phi,w_{i,I}-w_i)\right|\\
&\le \left(\|\mathcal{P}_3\phi\|_2+\|\phi\|_2\right)|\hat{\theta}_i|_1 h|w_i|_2, && (5.53a)\\
|S_2| &\le \left|\mathcal{C}_{i,h}(c_i;\mathcal{P}_3\phi-\phi,w_{i,I}-w_i)\right|+\left|\mathcal{C}_{i,h}(c_i;\phi,w_{i,I}-w_i)-\widehat{\mathcal{C}}_i(c_i;\phi,w_{i,I}-w_i)\right|\\
&\le h^k\left(2|c_i|_1\|\phi\|_{k+1}+\|\phi\|_{1,\infty}|c_i|_{k+1}\right)h|w_i|_2, && (5.53b)\\
|S_3| &\le \left|\mathcal{C}_{i,h}(\mathcal{P}_ic_i-c_i;\mathcal{P}_3\phi,w_i)-\widehat{\mathcal{C}}_i(\mathcal{P}_ic_i-c_i;\phi,w_i)\right|\\
&\le \left|\mathcal{C}_{i,h}(\hat{\theta}_i;\mathcal{P}_3\phi-\phi,w_i)\right|+\left|\mathcal{C}_{i,h}(\hat{\theta}_i;\phi,w_i)-\widehat{\mathcal{C}}_i(\hat{\theta}_i;\phi,w_i)\right|\\
&\le h|\hat{\theta}_i|_1\left(|\phi|_1+2|\phi|_2\right)|w_i|_2, && (5.53c)\\
|S_4| &\le \left|\mathcal{C}_{i,h}(c_i;\mathcal{P}_3\phi-\phi,w_i)\right|\\
&\le h^{k+1}|\phi|_{k+1}|c_i|_1|w_i|_2, && (5.53d)\\
|S_5| &\le \left|\mathcal{C}_{i,h}(c_i;\phi,w_i)-\widehat{\mathcal{C}}_i(c_i;\phi,w_i)\right|\\
&\le h^{k+1}\left(|c_i|_1|\phi|_{k+1}+|c_i|_{k+1}|\phi|_2\right)|w_i|_2. && (5.53e)
\end{aligned}
$$

Substituting (5.53a)-(5.53e) into (5.52), we deduce

$$
\left|\mathcal{C}_{i,h}(\mathcal{P}_ic_i;\mathcal{P}_3\phi,w_{i,I})-\widehat{\mathcal{C}}_i(\mathcal{P}_ic_i;\phi,w_{i,I})\right| \le \left(h|\hat{\theta}_i|_1\|\phi\|_2+h^{k+1}(|c_i|_1\|\phi\|_{k+1}+\|\phi\|_{1,\infty}|c_i|_{k+1}+|c_i|_{k+1}\|\phi\|_2)\right)|w_i|_2. \quad (5.54)
$$

Finally combining (5.51a)-(5.51c), (5.54) with (5.50), we get

$$
\|\hat{\theta}_i\|_0^2 \le \left(h|\hat{\theta}_i|_1(1+\|\phi\|_2)+h^{k+1}(|c_i|_1\|\phi\|_{k+1}+(1+\|\phi\|_{1,\infty})|c_i|_{k+1}+|c_i|_{k+1}\|\phi\|_2)\right)|w_i|_2,
$$

which, together with the H^1 estimate (5.47), setting

$$
c_\phi := 1+\|\phi\|_2, \qquad \hat{C} := |c_i|_1\|\phi\|_{k+1}+(1+\|\phi\|_{1,\infty})|c_i|_{k+1}+|c_i|_{k+1}\|\phi\|_2,
$$

and using the regularity condition (5.49), implies

$$
\|\hat{\theta}_i\|_0^2 \le \left(c_\phi(Ch^{k+1}+h\|\hat{\theta}_i\|_0)+\hat{C}h^{k+1}\right)\|\hat{\theta}_i\|_0.
$$

Hence, if h is small enough, then it follows that

$$
\|\hat{\theta}_i\|_0 \le Ch^{k+1},
$$

which finishes the proof of this lemma. □

Finally, we state an optimal error estimate for $c_1^n-c_{1,h}^n$, $c_2^n-c_{2,h}^n$ and $\phi^n-\phi_h^n$ in the L^2-norm valid for the scheme (2.27).

Theorem 5.2 *Let the assumption of Theorem 3.1 be satisfied and suppose that the data satisfy*

$$C_{\mathtt{stab}}\left(\|c_{1,0}\|_0+\|c_{2,0}\|_0+\|\mathbf{u}_0\|_0\right)\leq\frac{1}{4}. \tag{5.55}$$

Also, assume that $\{c_1^n,c_2^n,\phi^n\}$ *is the solution of* (1.1) *satisfying the regularity assumptions presented in Lemma 5.9 and* $\{c_{1,h}^n,c_{2,h}^n,\phi_h^n\}$ *is the solution of* (5.41)*. Then, the following error estimation holds for* $n=1,\cdots,N$,

$$\|c_1^n-c_{1,h}^n\|_0+\|c_2^n-c_{2,h}^n\|_0+\left(\tau\sum_{j=1}^n\left[\|c_1^n-c_{1,h}^n\|_1^2+\|c_2^n-c_{2,h}^n\|_1^2\right]\right)^{1/2}\leq C(\tau+h^{k+1}).$$

Proof. We divide the proof into three steps.

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

$$c_i^n-c_{i,h}^n=c_i^n-\mathcal{P}_{i,h}c_i^n+\mathcal{P}_{i,h}c_i^n-c_{i,h}^n:=\rho_i^n+\vartheta_i^n,$$

and

$$\phi^n-\phi_h^n=\phi^n-\mathcal{P}_{3,h}\phi^n+\mathcal{P}_{3,h}\phi^n-\phi_h^n:=\rho_3^n+\vartheta_3^n,$$

where ρ_i^n and ρ_3^n are estimated in Lemmas 5.9 and 5.8, respectively. Now we estimate ϑ_i^n and ϑ_3^n. An application of Eqs. (1.3a) and (5.41) with $z_{i,h}=\vartheta_i^n$ and the definition of the projector $\mathcal{P}_{i,h}$ given in (5.42) imply

$$\begin{aligned}
&\mathcal{M}_{1,h}(\frac{\vartheta_i^n-\vartheta_i^n}{\tau},\vartheta_i^n)+\mathcal{A}_{i,h}(\vartheta_i^n,\vartheta_i^n)\\
&=\left[\mathcal{M}_{1,h}(\delta_t\mathcal{R}_{i,h}c_i^n,\vartheta_i^n)-\mathcal{M}_1(\Pi_k^0\partial_tc_i,\vartheta_i^n)\right]+\left[\widehat{\mathcal{D}}(\mathbf{u}^n;c_i^n,\vartheta_i^n)-\mathcal{D}_h(\mathbf{u}_h^n;c_{i,h}^n,\vartheta_i^n)\right]\\
&\quad+e_i\mathcal{C}_{i,h}(\mathcal{R}_{i,h}c_i^n;\phi_h^n-\mathcal{P}_{3,h}\phi^n,\vartheta_i^n)+e_i\mathcal{C}_{i,h}(\mathcal{R}_{i,h}c_i-c_{i,h}^n;\phi_h^n,\vartheta_i^n)\\
&:=R_{1,i}+R_{2,i}+R_{3,i}+R_{4,i},
\end{aligned} \tag{5.56}$$

and a combination of Eqs. (1.3b) and (5.41b) with choosing $\psi_h=\vartheta_3^n$ gives

$$\begin{aligned}
\mathcal{A}_{3,h}(\vartheta_3^n,\vartheta_3^n)&=\mathcal{M}_{1,h}(c_1^n-c_{1,h}^n,\vartheta_3^n)-\mathcal{M}_{1,h}(c_2^n-c_{2,h}^n,\vartheta_3^n)\\
&\quad+\left[\mathcal{M}_1(c_1^n,\vartheta_3^n)-\mathcal{M}_{1,h}(c_1^n,\vartheta_3^n)\right]-\left[\mathcal{M}_1(c_2^n,\vartheta_3^n)-\mathcal{M}_{1,h}(c_2^n,\vartheta_3^n)\right].
\end{aligned}$$

The continuity of $\mathcal{M}_{1,h}(\cdot,\cdot)$ given in (2.9a), and Lemma 2.4, confirm that

$$\beta_4\|\vartheta_3^n\|_1^2\leq\left(\alpha_1(\|c_1^n-c_{1,h}^n\|_0+\|c_2^n-c_{2,h}^n\|_0)+Ch^{k+1}(\|c_1^n\|_{k+1}+\|c_2^n\|_{k+1})\right)\|\vartheta_3^n\|_1, \tag{5.57}$$

which, by Poincaré inequality, implies that

$$\|\vartheta_3^n\|_0\leq C_{\mathtt{P}}\beta_4^{-1}\left(\alpha_1(\|c_1^n-c_{1,h}^n\|_0+\|c_2^n-c_{2,h}^n\|_0)+Ch^{k+1}(\|c_1^n\|_{k+1}+\|c_2^n\|_{k+1})\right). \tag{5.58}$$

Step 2: bounding the error terms $R_{1,i}$-$R_{4,i}$. For the term $R_{1,i}$ we first notice that by adding zero in the form $\pm\mathcal{M}_{1,h}(\partial_tc_i^n,\vartheta_i^n)$, we can obtain

$$R_{1,i}=\mathcal{M}_1(\partial_tc_i^n,\vartheta_i^n)-\mathcal{M}_{1,h}(\delta_t\mathcal{P}_{i,h}c_i^n,\vartheta_i^n)=\left[\mathcal{M}_{1,h}(\partial_tc_i^n,\vartheta_i^n)-\mathcal{M}_1(\Pi_k^0\partial_tc_i^n,\vartheta_i^n)\right]+\mathcal{M}_{1,h}(\delta_t\mathcal{P}_{i,h}c_i^n-\partial_tc_i^n,\vartheta_i^n).$$

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

$$|R_{1,i}|\leq\left(Ch^{k+1}\|\partial_tc_i^n\|_{k+1}+\alpha_1\tau^{1/2}\|\partial_{tt}c_i\|_{\mathrm{L}^2(\mathrm{L}^2)}\right)\|\vartheta_i^n\|_0.$$

For the term $R_{2,i}$, after adding and subtracting some suitable terms, we can rewrite the corresponding term as

$$R_{2,i}=\underbrace{\widehat{\mathcal{D}}(\mathbf{u}^n;c_i^n,\vartheta_i^n)-\mathcal{D}_h(\mathbf{u}^n;c_i^n,\vartheta_i^n)}_{:=R_{2,i}^{(1)}}+\underbrace{\mathcal{D}_h(\mathbf{u}^n;c_i^n,\vartheta_i^n)-\mathcal{D}_h(\mathbf{u}_h^n;c_{i,h}^n,\vartheta_i^n)}_{:=R_{2,i}^{(2)}}.$$

Using Lemma 2.6, it follows that

$$|R_{2,i}^{(1)}|\leq Ch^{k+1}\left(\|\mathbf{u}^n\|_{k+1}\|c_i^n\|_2+\|c_i^n\|_{k+1}\|\mathbf{u}^n\|_2\right)|\vartheta_i^n|_1. \tag{5.59}$$

For the term $R_{2,i}^{(2)}$, we note that the definition of $\mathcal{D}_h(\cdot;\cdot,\cdot)$ implies

$$R_{2,i}^{(2)}=\mathcal{D}_h(\mathbf{u}^n;c_i^n,\vartheta_i^n)-\mathcal{D}_h(\mathbf{u}_h^n;c_{i,h}^n,\vartheta_i^n)$$

$$= \frac{1}{2}\big[(\mathbf{u}^n\, c_i^n, \nabla\vartheta_i^n)_h - \big(\mathbf{u}_h^n c_{i,h}^n, \nabla\vartheta_i^n\big)_h\big] - \frac{1}{2}\big[(\mathbf{u}^n\cdot\nabla c_i^n, \vartheta_i^n)_h - \big(\mathbf{u}_h^n\cdot\nabla c_{i,h}^n, \vartheta_i^n\big)_h\big].$$

We note that the above equation, after adding zero as

$$\begin{aligned}0 &= (\mathbf{u}_h^n\cdot\nabla\vartheta_i^n, \vartheta_i^n)_h - (\mathbf{u}_h^n\cdot\nabla\vartheta_i^n, \vartheta_i^n)_h\\ &= \big(\mathbf{u}_h^n\cdot\nabla\vartheta_i^n, c_{i,h}^n\big)_h - (\mathbf{u}_h^n\cdot\nabla\vartheta_i^n, \mathcal{P}_{i,h}c_i^n)_h - \big(\mathbf{u}_h^n\nabla c_{i,h}^n, \vartheta_i^n\big)_h + (\mathbf{u}_h^n\nabla\mathcal{P}_{i,h}c_i^n, \vartheta_i^n)_h\,,\end{aligned}$$

can be bounded as follows

$$|R_{2,i}^{(2)}| \le \frac{1}{2}\big[((\mathbf{u}^n - \mathbf{u}_h^n)\mathcal{P}_{i,h}c_i^n, \nabla\vartheta_i^n)_h - ((\mathbf{u}^n - \mathbf{u}_h^n)\cdot\nabla\mathcal{P}_{i,h}c_i^n, \vartheta_i^n)_h\big] =: \mathrm{I} + \mathrm{II}.$$

For the term II, 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

$$\begin{aligned}|\mathrm{II}| = \left|((\mathbf{u}^n - \mathbf{u}_h^n)\cdot\nabla\mathcal{P}_{i,h}c_i^n, \vartheta_i^n)_h\right| &\le \|\mathbf{\Pi}_k^0(\mathbf{u}^n - \mathbf{u}_h^n)\|_{0,4}\|\mathbf{\Pi}_{k-1}^0\nabla\mathcal{P}_{i,h}c_i^n\|_0\|\Pi_k^0\vartheta_i^n\|_{0,4}\\ &\le \|\mathbf{u}^n - \mathbf{u}_h^n\|_{0,4}\|\nabla\mathcal{P}_{i,h}c_i^n\|_0\|\vartheta_i^n\|_{0,4}.\end{aligned}$$

Using the triangle inequality and Lemma 5.9, we end up with the following upper bound for the second term on the right-hand side of the above inequality

$$\|\nabla\mathcal{P}_{i,h}c_i^n\|_0 \le \|\nabla c_i^n\|_0 + \|\nabla(\mathcal{P}_{i,h}c_i^n - c_i^n)\|_0 \le \|c_i^n\|_1,$$

which, together with the Gagliardo–Nirenberg inequality, in turn implies

$$|\mathrm{II}| \le h\|\mathbf{u}^n - \mathbf{u}_h^n\|_1\|c_i^n\|_1\|\vartheta_i^n\|_1.$$

Bounding the term I analogously to II, we can confirm that

$$|\mathrm{I}| \le h\|\mathbf{u}^n - \mathbf{u}_h^n\|_1\|c_i^n\|_1\|\vartheta_i^n\|_1.$$

Thus we arrive at the bound

$$R_{2,i}^{(2)} \le Ch\|\mathbf{u}^n - \mathbf{u}_h^n\|_1\|c_i^n\|_2\|\vartheta_i^n\|_1.$$

Inserting the above and (5.59) into (5.59), it follows

$$|R_{2,i}| \le Ch^{k+1}\left(\|\mathbf{u}^n\|_{k+1}\|c_i^n\|_2 + \|c_i^n\|_{k+1}\|\mathbf{u}^n\|_2\right)|\vartheta_i^n|_1 + Ch\|\mathbf{u}^n - \mathbf{u}_h^n\|_1\|c_i^n\|_1\|\vartheta_i^n\|_1.$$

As for the term $R_{3,i}$, Lemma 2.2, (5.46) and estimate (5.57) implies that,

$$\begin{aligned}R_{3,i} &= \mathcal{C}_{i,h}(\mathcal{R}_{i,h}c_i;\phi_h^n - \mathcal{P}_{3,h}\phi^n, \vartheta_i^n) \le \gamma_3\|\mathcal{R}_{i,h}c_i\|_\infty\|\phi_h^n - \mathcal{P}_{3,h}\phi^n\|_1|\vartheta_i^n|_1\\ &\le \|c_i\|_1\left(Ch^{k+1} + \|\vartheta_1^n\|_0 + \|\vartheta_2^n\|_0\right)|\vartheta_i^n|_1.\end{aligned}$$

As the last task in this step, we focus on the term $R_{4,i}$, that is, $\mathcal{C}_{i,h}(\mathcal{R}_{i,h}c_i - c_{i,h}^n;\phi_h^n, \vartheta_i^n)$. It is easy to see that the Gagliardo–Nirenberg inequality and Theorem 3.1 imply

$$R_{4,i} \le \|\vartheta_i^n\|_\infty\|\phi_h^n\|_1|\vartheta_i^n|_1 \le C_{\mathtt{GN}}C_{\mathtt{stab}}\left(\|c_{1,0}\|_0 + \|c_{2,0}\|_0 + \|\mathbf{u}_0\|_0\right)|\vartheta_i^n|_1^2.$$

Step 3: error estimate at a generic n-th time step. We now insert the bounds on $R_{1,i} - R_{3,i}$ in (5.56), yielding

$$\begin{aligned}\frac{1}{2\tau}\left(\|\vartheta_i^n\|_0^2 - \|\vartheta_i^{n-1}\|_0^2\right) + |\vartheta_i^n|_1^2 &\le \varpi_{1,i}\|\vartheta_i^n\|_0\\ &\quad + \left[\varpi_{2,i} + C_{\mathsf{c}}h\|\mathbf{u}^n - \mathbf{u}_h^n\|_1 + C_1(\|\vartheta_1^n\|_0 + \|\vartheta_2^n\|_0)\right]|\vartheta_i^n|_1 + C_2|\vartheta_i^n|_1^2\\ &\le \frac{1}{2}\left[\varpi_{1,i}^2 + \|\vartheta_i^n\|_0^2\right] + \frac{1}{2}|\vartheta_i^n|_1^2\\ &\quad + \frac{1}{2}\left[\varpi_{2,i} + C_1h\|\mathbf{u}^n - \mathbf{u}_h^n\|_1 + C_1(\|\vartheta_1^n\|_0 + \|\vartheta_2^n\|_0)\right]^2 + C_2|\vartheta_i^n|_1^2,\end{aligned} \tag{5.60}$$

with positive scalars

$$\varpi_{1,i} \le Ch^{k+1}\|\partial_t c_i^n\|_{k+1} + \alpha_1\tau^{1/2}\|\partial_{tt}c_i\|_{\mathrm{L}^2(\mathrm{L}^2)}, \qquad C_1 \le \|c_i^n\|_1, \qquad C_2 \le C_{\mathtt{GN}}C_{\mathtt{stab}}\left(\|c_{1,0}\|_0 + \|c_{2,0}\|_0 + \|\mathbf{u}_0\|_0\right).$$

Next, invoking the smallness assumptions (5.55) and summing on n on both sides of (5.60), where $0 \le n \le N$, we arrive at

$$\frac{1}{2\tau}\left(\|\vartheta_i^n\|_0^2 - \|\vartheta_i^0\|_0^2\right) + \sum_{j=0}^n|\vartheta_i^j|_1^2 \le \sum_{j=0}^n(\varpi_{1,i}^2 + \varpi_{2,i}^2) + C_1\sum_{j=0}^n\left(\|\vartheta_1^j\|_0^2 + \|\vartheta_2^j\|_0^2 + h^2\|\mathbf{u}^j - \mathbf{u}_h^j\|_1^2\right).$$

Summing up these inequalities and employing Theorem 5.1 and the estimate (5.58) and Gronwall's inequality, it finally gives

$$\|\vartheta_1^n\|_0^2 + \|\vartheta_2^n\|_0^2 + \tau\sum_{j=0}^n\left(|\vartheta_1^j|_1^2 + |\vartheta_2^j|_1^2\right) \le \tau\sum_{j=0}^n\left(\varpi_{1,1}^2 + \varpi_{1,2}^2\right) + C(h^{k+1} + \tau).$$

The sought result follows from a similar procedure as in Theorem 5.1 and employing Lemma 5.9. □

6 Numerical Results

In this section, we provide numerical experiments to show the performance of the proposed VEM for coupled PNP/NS equations. In all examples, we use the virtual spaces $(\mathbf{Z}_h, \mathring{Z}_h)$ for concentrations and electrostatic potential and the pair $(\mathbf{X}_h, Y_h)$ for velocity and pressure, specified by the polynomial degree $k = 2$, unless otherwise stated. The nonlinear fully-discrete system is linearized using a Picard algorithm and the fixed-point iterations are terminated when the ℓ^2-norm of the global incremental discrete solutions drop below a fixed tolerance of 1e-08.

6.1 Example 1: Accuracy assessment

First we apply the fully discrete VEM to validate the theoretical convergence results shown in Theorems 5.1 and 5.2. For this we consider the following closed-form solutions to the coupled PNP/NS problem

$$\begin{cases} c_1(x,y,t) = \sin(2\pi x)\sin(2\pi y)\sin(t), \qquad c_2(x,y,t) = \sin(3\pi x)\sin(3\pi y)\sin(2t), \\ \phi(x,y,t) = \sin(\pi x)\sin(\pi y)(1-\exp(-t)), \\ \mathbf{u}(x,y,t) = \begin{pmatrix} -0.5\exp(t)\cos(x)^2\cos(y)\sin(y) \\ 0.5\exp(t)\cos(y)^2\cos(x)\sin(x) \end{pmatrix}, \quad p(x,y,t) = \exp(t)(\sin(x)-\sin(y)), \end{cases} \tag{6.1}$$

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). The model parameters are taken as $\kappa_1, \kappa_2, \epsilon = 1$.

The magnitude of approximate errors (computed with the aid of suitable projections) and the associated convergence rates generated on a sequence of successively refined grids (uniform hexagon meshes) are displayed in Fig. 6.1 by setting $\tau = h$ and $\tau = h^2$. One can see the second-order convergence for the total errors of all individual variables in the L^2- and energy norms, 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 Fig. 6.1 show samples of coarse-mesh approximate solutions together with absolute errors.

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

Now we investigate the dynamics of the system on the unit square with an initial value as follows (see [25, 26, 46])

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

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

and $\mathbf{u}_0 = \mathbf{0}$. The discontinuity of the initial concentrations represents an interface between the the electrolyte and the solid surfaces where electroosmosis (transport of ions from the electrolyte towards the solid surface) is expected to occur. We consider a fixed time step of $\tau =$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., [25, 26, 46] (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 4.1 and 4.2.

6.3 Example 3: Application to water desalination

The desalination of alternative waters, such as brackish and seawater, municipal 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 [55]. 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

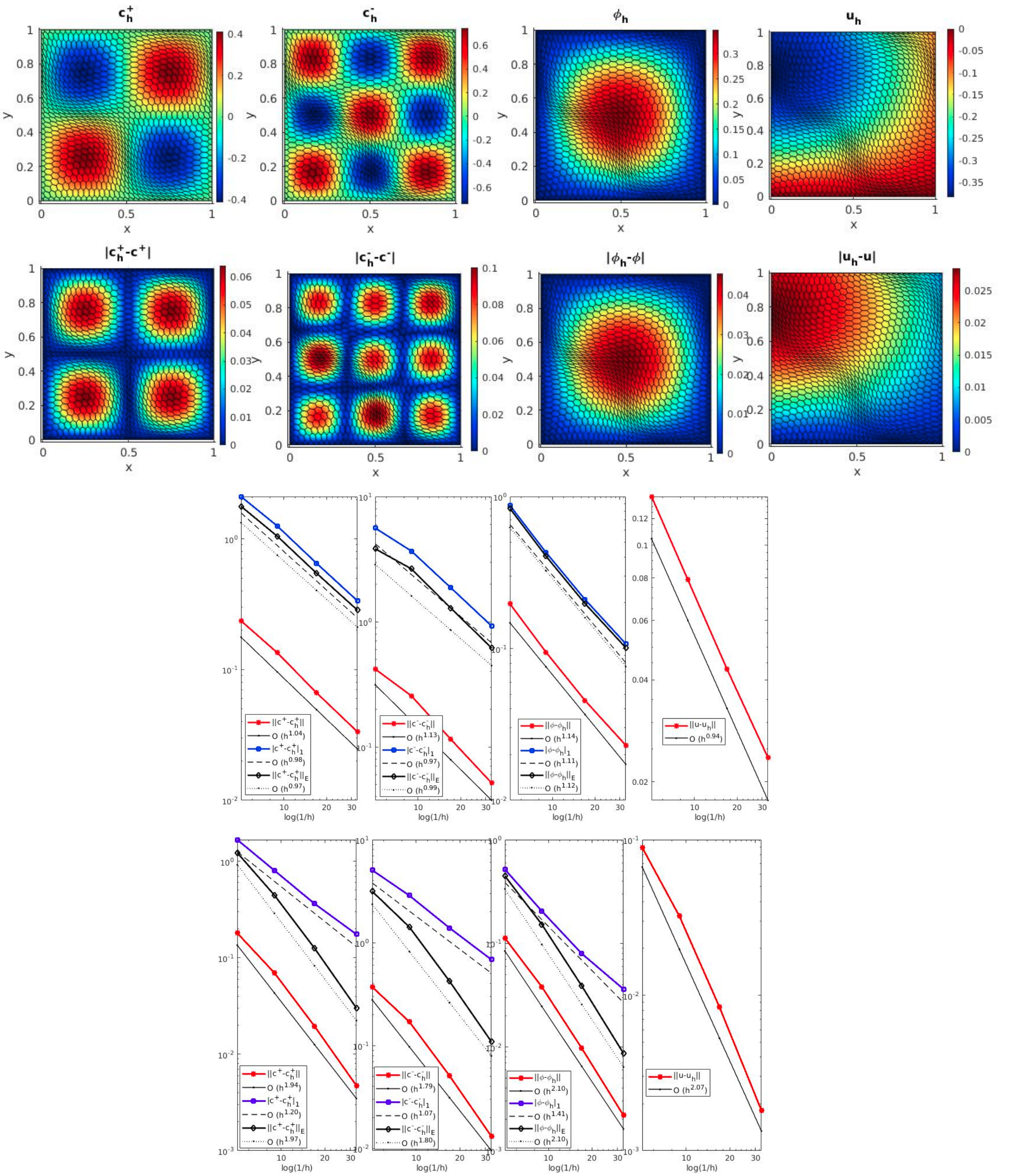

Fig. 6.1 Example 1. Snapshots of numerical solutions $\{c_{1,h}^n, c_{2,h}^n, \phi_h^n, \mathbf{u}_{1,h}^n\}$ and its absolute error (first two rows), and error history for the verification of convergence with $\tau = h$ (third row) and $\tau = h^2$ (bottom).

increases. Finally, an ion-free dilute solution and a concentrated solution as saline or concentrated 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 used in [21] (see also [38, 52]), consisting 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 $\Omega = (0,4)\times(0,1)$

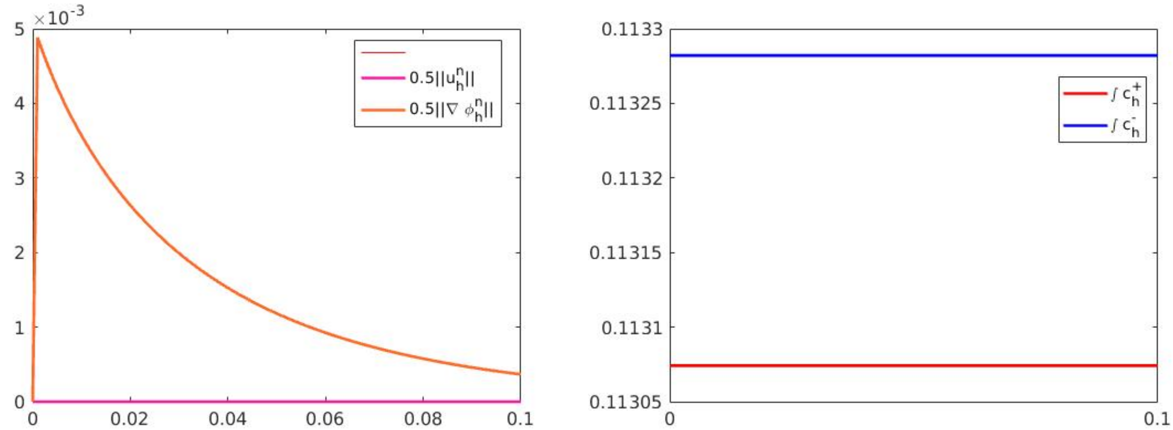

Fig. 6.2 Example 2. Evolution of electric (and kinetic) energy (left) and global masses (right) with τ = 1e-3.

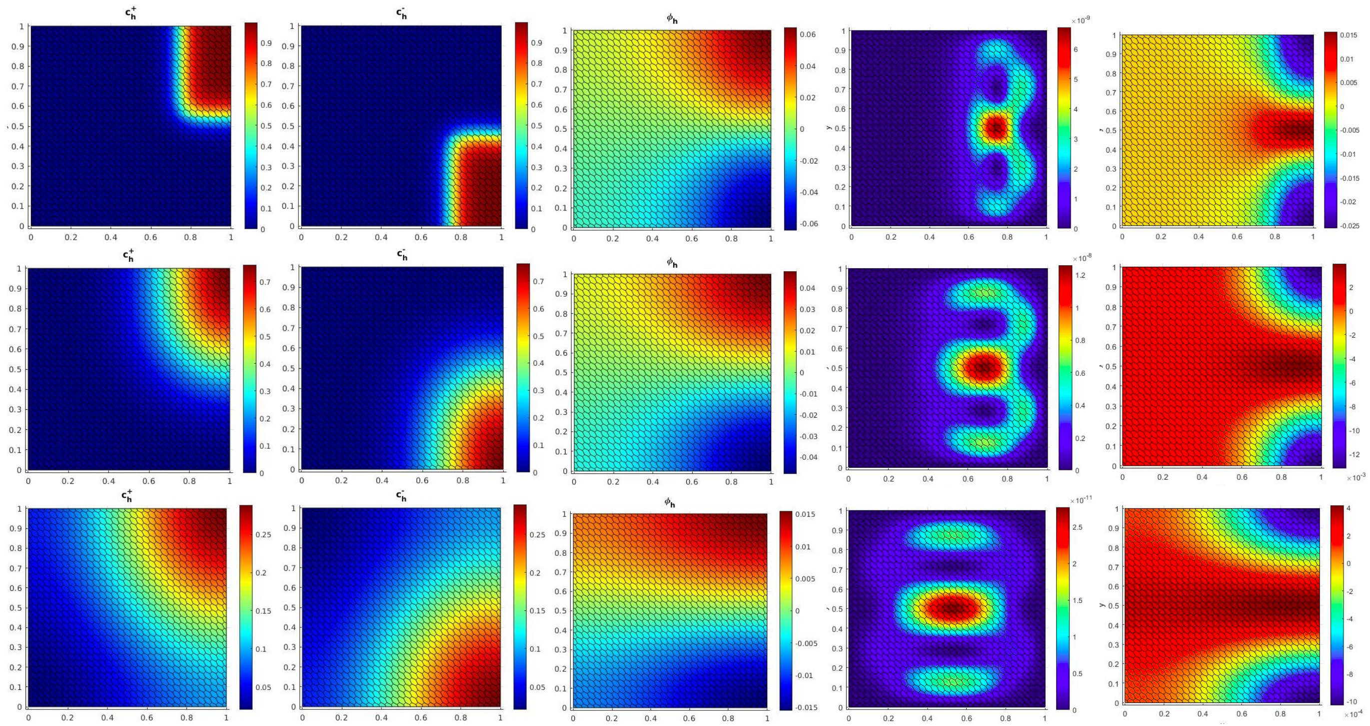

Fig. 6.3 Example 2. Snapshots of the approximate solutions $\{c^n_{1,h}, c^n_{2,h}, \phi^n_h, |\mathbf{u}^n_h|, p^n_h\}$ obtained with the proposed VEM, and shown at times t_F =2e-03 (top row), t_F =2e-02 (middle) and t_F =1e-01 (bottom).

and consider the NS momentum balance equation using the following non-dimensionalization

$$\frac{1}{S_c}\left(\mathbf{u}_t + (\mathbf{u}\cdot\boldsymbol{\nabla})\mathbf{u}\right) - \boldsymbol{\Delta}\mathbf{u} + \nabla p + \frac{\kappa}{\epsilon}(c_1 - c_2)\nabla\phi = \mathbf{0}.$$

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:

$$c_1(x, y, 0) = \alpha\ \mathrm{rand}(x, y)(2 - y), \qquad c_2(x, y, 0) = \alpha\ \mathrm{rand}(x, y)y,$$

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 $\partial\Omega_{lr}$

$$\begin{cases} c_1 = \alpha, \quad c_2 = \alpha, \quad \phi = \beta, \quad \mathbf{u} = \mathbf{0}, & \text{on } \partial\Omega_{top}, \\ c_1 = 2\alpha, \quad \nabla c_2\cdot\mathbf{n} = 0, \quad \phi = 0, \quad \mathbf{u} = \mathbf{0}, & \text{on } \partial\Omega_{bot}, \\ u(4, y, t) = u(0, y, t), \quad \forall u \in \{c_1, c_2, \phi, \mathbf{u}\}, & \text{on } \partial\Omega_{lr}. \end{cases}$$

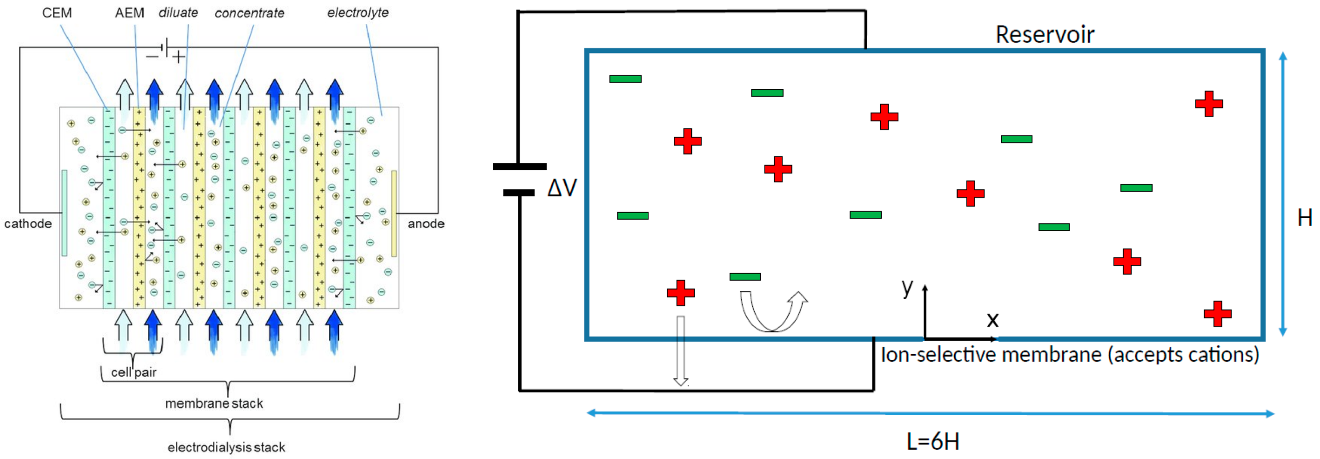

Fig. 6.4 Example 3. Schematic of an electrodialysis stack [29] (left) and simplified configuration of a 2D problem with ion-selective membrane as in [21] (right).

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

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

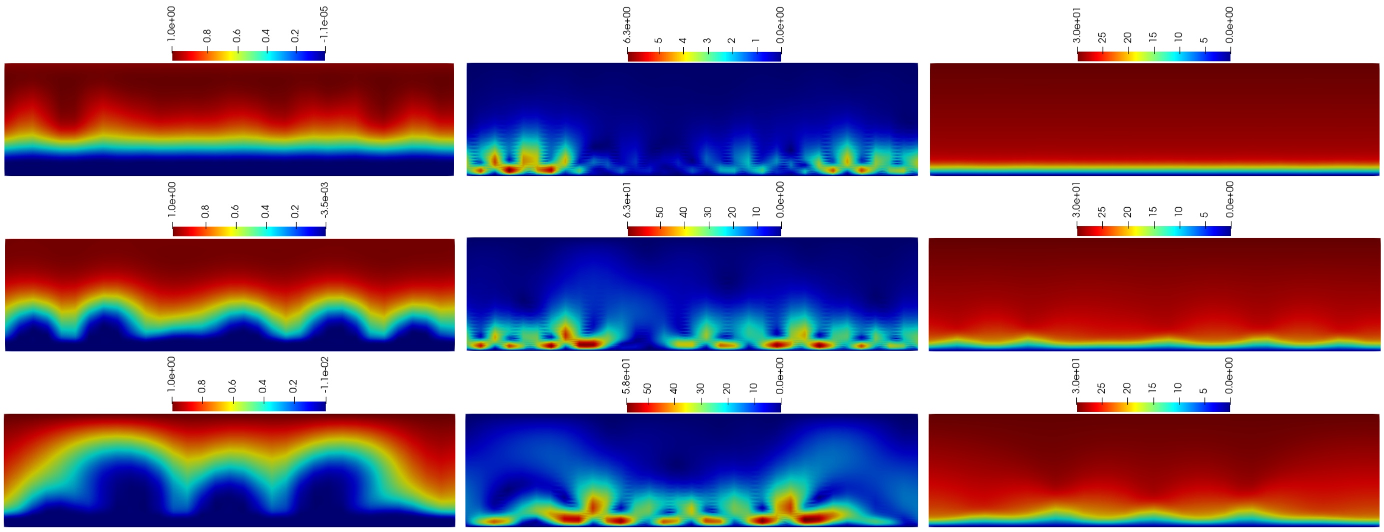

Fig. 6.5 Example 3A. Snapshots of numerical solutions $c_{2,h}$ (left), $|\mathbf{u}_h|$ (middle) and ϕ_h (right) using the proposed VEM at times t_F =3e-03, t_F =2e-02, and t_F =8e-02 with voltage $V = 30$.

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 patterns, 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 [38, 39] and it is fact similar to the encountered in fluid mechanics vortex fusion.

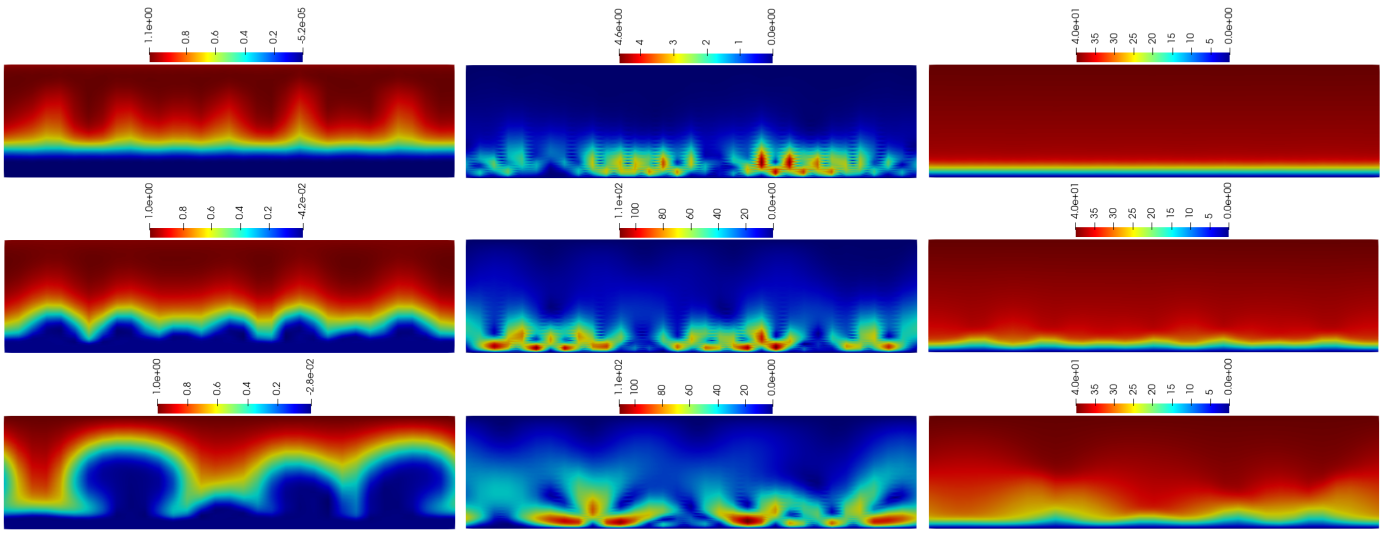

Fig. 6.6 Example 3A. Snapshots of numerical solutions $c_{2,h}$ (left), $\mathbf{u}_h$ (middle) and ϕ_h (right) using the proposed VEM at times t_F =3e-03, t_F =2e-02, and t_F =8e-02 with voltage $V = 40$.

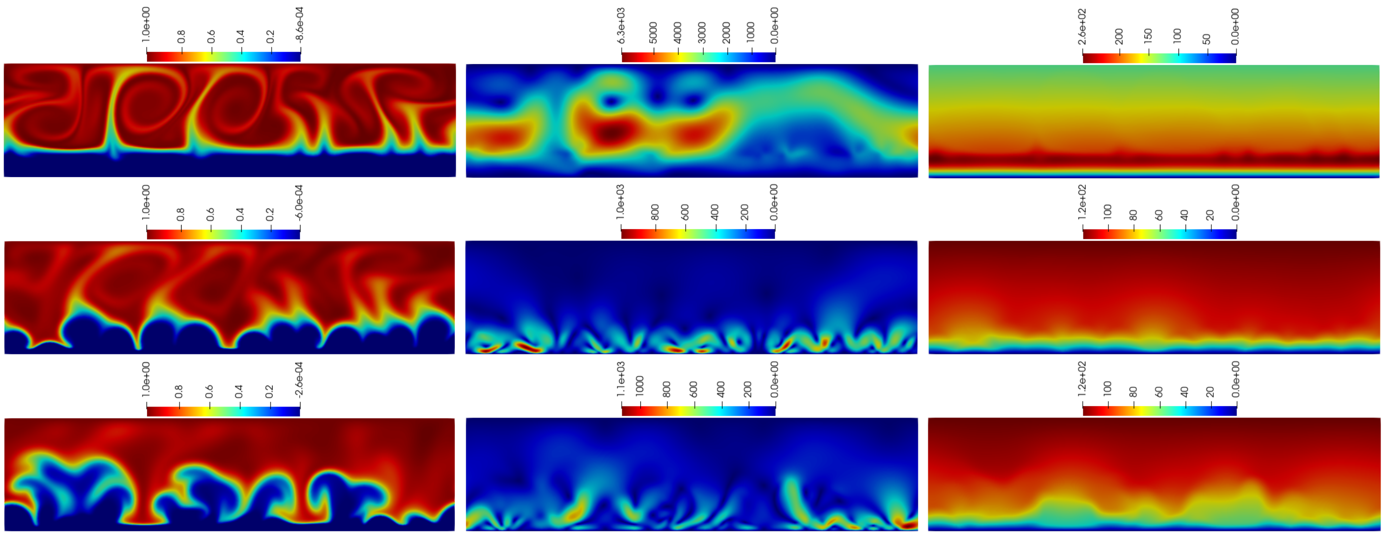

Fig. 6.7 Example 3A. Snapshots of numerical solutions $c_{2,h}$ (left), $\mathbf{u}_h$ (middle) and ϕ_h (right) using the proposed VEM at times t_F =3e-03, t_F =2e-02, and t_F =8e-02 with voltage $V = 120$.

Example 3B: Effect of salt concentration. Finally, we considered a fixed applied voltage of $V = 120$. A NaCl concentration of 10 was simulated, representing slightly brackish water; and we have also increased 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 case of concentration 100, similar findings can be obtained (see Fig. 6.8, right column). Based on this, it can be concluded that, in addition to voltage, the start of the instability depends also on the ion concentration.

7 Concluding remarks

In this paper we have proposed and analyzed a virtual element method (VEM) for the numerical approximation of the coupled Poisson–Nernst–Planck (PNP)/Navier–Stokes (NS) equations in the context of applications such as the desalination of water, microfluidic processes, and other electrochemical systems. The VEM formulation advanced here leads to a nonlinear system, in which the existence and uniqueness of the discrete solution are examined using tools of nonlinear functional analysis, including fixed point strategies. More precisely, we have defined an appropriate fixed point operator and have established its well-definedness, its compactness, and its Lipschitz-continuity under smallness data assumptions. Banach's fixed point theorem then gives the unique solvability of the corresponding discrete system. We have also rigorously derived a priori estimates for the discrete solution, which represent a key step in writing error estimates. On the other hand, we have proved that the approximate solution features the properties of discrete mass conservation and free energy dissipation. These properties have also been verified by our computational simulations. Then we carried out an error analysis under the natural smoothness assumption on the solution. This analysis does not require any conditions on the time step and spatial mesh size. Moreover, considering only the Navier–Stokes subsystem, we

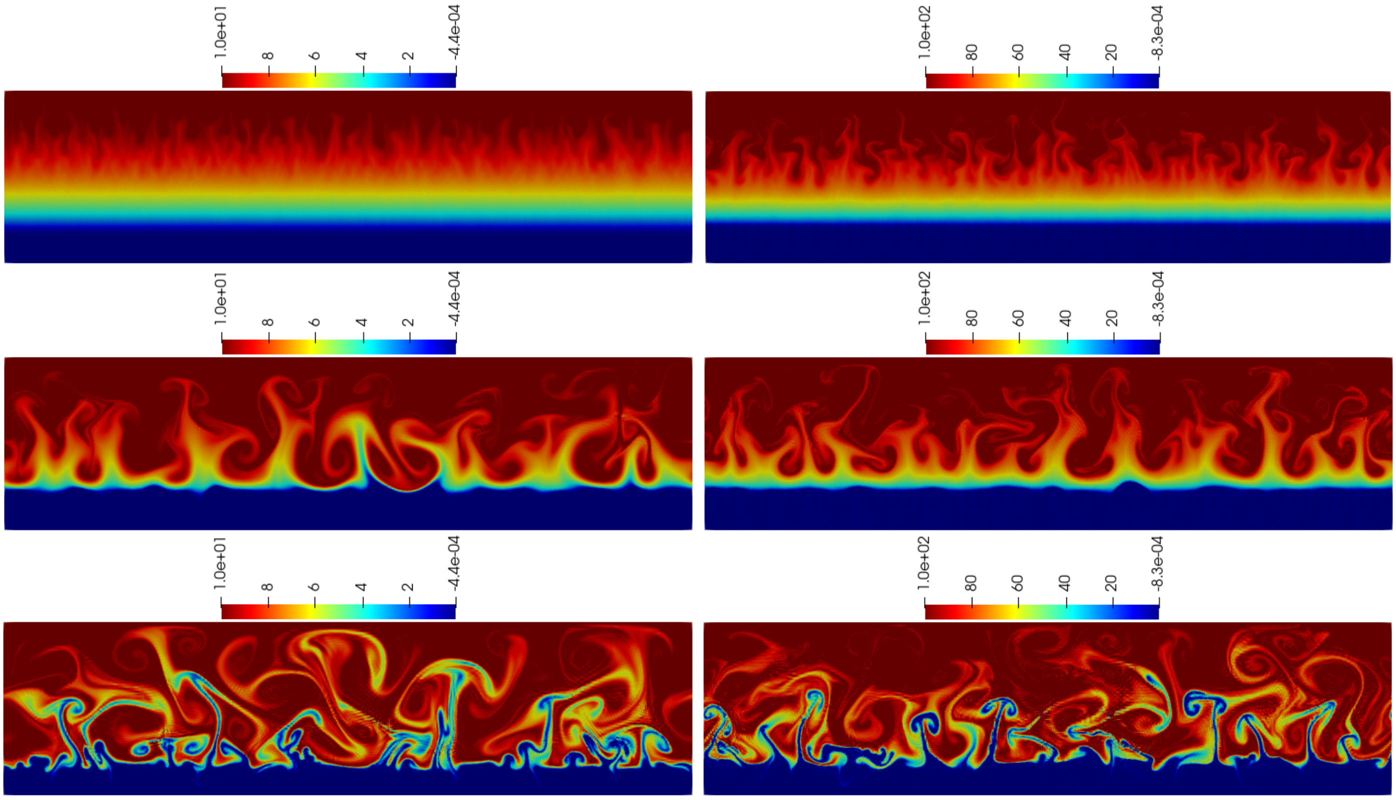

Fig. 6.8 Example 3B. Snapshots of numerical solutions $c_{2,h}$ with voltage $V = 120$, for NaCl=10 at times t_F =5e-07, t_F =2e-06, and t_F =5e-06 (left); and for NaCl = 100 t_F =5e-07, t_F =1e-06, and t_F =2e-06 (right).

have extended the error analysis for FEMs applied to Navier–Stokes equations considered in [61] to the VEM framework. Owing to inverse and Gagliardo–Nirenberg inequalities, we arrive at optimal error estimation in the L^2-norm, which differs from, e.g., [6]. Regarding the PNP equations we derived optimal error estimates for concentrations and potential (again in the L^2-norm) thanks to suitable projection operators as well as a prior estimate of the solution. These results improve the sub-optimal error analysis presented in the recent works [42, 59]. Finally, our numerical results have confirmed the theoretical analysis of convergence and they have shown that the proposed VEM performs well when simulating PNP-NS equations with physically realistic parameters.

We conclude this section by mentioning some of the limitations of the present work as well as possible extensions. First, we note that in the numerical experiments, for some time instances we observe concentrations that go slightly below zero. One remedy to obtain only physical concentration values would be to consider pressure-robust variants of the scheme, such as those introduced in [23, 24] in the context of electrically charged flows. Also from the viewpoint of the numerical simulations, we did not verify that the ℓ^∞-norm of the divergence of the projected discrete velocity is zero and it will be done in a forthcoming study. Regarding the analysis of the proposed VE discretization, small data assumptions were necessary to establish the unique solvability of the discrete problem. We are currently investigating an alternative proof that circumvents these assumptions. Model extensions that we plan to undertake include the case of concentration-dependent viscosity and concentration-dependent dielectric diffusion as in, e.g., [40], and to extend the present VEM formulation in its usual form to the formulation of the set of equations in fully mixed form (using stress, strain rate, concentration fluxes, and electric field as additional field variables) following [17, 18].

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