CONVERGENCE ANALYSIS OF A BDF2/MIXED FINITE ELEMENT DISCRETIZATION OF A DARCY–NERNST–PLANCK–POISSON SYSTEM

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Abstract. This paper presents an *a priori* error analysis of a fully discrete scheme for the numerical solution of the transient, nonlinear Darcy–Nernst–Planck–Poisson system. The scheme uses the second order backward difference formula (BDF2) in time and the mixed finite element method with Raviart–Thomas elements in space. In the first step, we show that the solution of the underlying weak continuous problem is also a solution of a third problem for which an existence result is already established. Thereby a stability estimate arises, which provides an L^{∞} bound of the concentrations / masses of the system. This bound is used as a level for a cut-off operator that enables a proper formulation of the fully discrete scheme. The error analysis works without semi-discrete intermediate formulations and reveals convergence rates of optimal orders in time and space. Numerical simulations validate the theoretical results for lowest order finite element spaces in two dimensions.

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1. INTRODUCTION

The Stokes-Nernst-Planck-Poisson (SNPP) system is a well known continuum model describing the dynamics of dilute electrolytes and dissolved charged particles in small channels (e.g., [19, 22]) and thus also within a porous medium at the pore scale. [32] used the method of two-scale convergence (e.g., [10]) in a periodic setting to derive averaged systems that are valid on an averaged scale, one of which is the subject of this paper. The main tasks of periodic homogenization is the study and the averaging of partial differential equations with rapidly oscillating coefficients, in our case, induced by an idealized, periodic microstructure. By means of a limiting process, effective partial differential equations are obtained that describe the average macroscopic behavior of the considered quantities. The derived equations contain smooth effective coefficients, which are determined by means of the solutions of auxiliary problems defined on reference cells representing the local heterogeneities of the microscale. With an equivalent system at hand, valid on a larger scale, one may conclude microscopic processes from macroscopic observations or investigate the impact of microscale phenomena on large-scale behavior.

 $Keywords \ and \ phrases. \ Stokes / Darcy-Nernst-Planck-Poisson \ system, \ mixed \ finite \ elements, \ backward \ difference \ formula, error \ analysis, \ porous \ media.$

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The SNPP system and related models are the topic of ongoing research in numerics [2,16], numerical analysis [26], analysis [5,18,33], and homogenization theory [32,23,24,34,21,2].

The considered mathematical model reads as follows: Let $\Omega \subset \mathbb{R}^d$, $d \in \{2,3\}$ be a polygonally bounded convex domain with boundary $\partial \Omega$, let $\boldsymbol{\nu}$ denote the outward unit normal, and let $J \coloneqq [0, T[$ be a time interval, where T > 0 denotes the end time. The system (1.1) that we refer to as the *Darcy-Nernst-Planck-Poisson* (*DNPP*) system reads

$$\boldsymbol{u} = -\mathbf{K}\boldsymbol{\nabla}p + \mathbf{K}\mathbf{D}^{-1}\boldsymbol{E}(c^{+} - c^{-}) \qquad \text{in} \qquad J \times \Omega, \qquad (1.1a)$$

$$\mathbf{V} \cdot \mathbf{u} = 0 \qquad \text{in} \qquad J \times \Omega, \qquad (1.1b)$$
$$\mathbf{j}^{\pm} = -\mathbf{D} \nabla c^{\pm} + \mathbf{u} c^{\pm} \pm \mathbf{E} c^{\pm} \qquad \text{in} \qquad J \times \Omega, \qquad (1.1c)$$

$$\partial_{t}c^{\pm} + \nabla \cdot j^{\pm} = r^{\pm}(t, \boldsymbol{x}, c^{+}, c^{-}) \qquad \text{in} \qquad J \times \Omega, \qquad (1.1d)$$

$$\boldsymbol{E} = -\mathbf{D}\nabla\phi \qquad \text{in} \qquad J \times \Omega, \qquad (1.1e)$$

$$\nabla \cdot \boldsymbol{E} = c^{+} - c^{-} + \sigma \qquad \text{in} \qquad J \times \Omega, \qquad (1.1f)$$

$$\boldsymbol{u} \cdot \boldsymbol{\nu} = 0 \qquad \text{on} \qquad J \times \partial\Omega, \qquad (1.1g)$$

$$c^{\pm} = 0 \qquad \text{on} \qquad J \times \partial\Omega, \qquad (1.1h)$$

$$\phi = \phi_{\mathrm{D}} \qquad \text{on} \qquad J \times \partial\Omega, \qquad (1.1h)$$

with $c^{\pm,0}$ satisfying the boundary conditions (1.1h). The notation \pm (and \mp) is used as an abbreviation in order to formulate equations for j^+ and j^- (and c^+ and c^- , respectively) in one line: all the corresponding upper signs have to be interpreted as the first equation and all the lower signs as the second equation. The averaged physical quantities in (1.1) are the *fluid velocity* \boldsymbol{u} , the *pressure* p, the *mass fluxes* j^+ , j^- of positively and negatively charged dissolved chemical species, which are represented by their *concentrations* c^+ and c^- , respectively, the *electric field* \boldsymbol{E} and the *electric potential* ϕ . Note that the pressure (pressure head) is defined only up to a constant due to the Neumann condition (1.1g). The stationary, constant coefficients \boldsymbol{D} , \boldsymbol{K} are effective (symmetric) tensors of second order, the closed-form expression of which is provided by averaging the solutions of so-called cell problems [16, 32]. These can be interpreted as diffusion and permeability tensors, respectively. Here, we consider these two coefficients given. The reaction rates $r^{\pm} = r^{\pm}(t, \boldsymbol{x}, c^+, c^-)$ depend on $(t, \boldsymbol{x}) \in J \times \Omega$ since potential source or sink terms are incorporated in this term.

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An outline of this article is as follows: In Section 2, the mixed weak formulation of the DNPP system (1.1) is introduced. The equivalence of this formulation to another weak (semi-mixed) formulation under additional mild regularity assumptions is shown. For the latter, the well-posedness and essential boundedness of the concentrations has been established in literature. This boundedness allows the definition of a cut-off operator that is used to define the discrete scheme, which is the topic of Section 3. The approximation quality of this numerical scheme is investigated in terms of an *a priori* analysis of the discretization error in Section 4. The main result of this article is given in Theorem 4.6: the estimate of the discretization errors in terms of time step size and mesh fineness. Section 5 compares numerically estimated orders of convergence with those derived from utilizing the BDF1 and BDF2 approximation in time with the lowest Raviart–Thomas elements in space.

2. Weak problem

In this section, we introduce the mixed weak formulation of the DNPP system (1.1) on which our discrete scheme will be based, *cf.* Figure 1. Subsequently, we prove that the solution of this mixed problem satisfies another weak (semi-mixed) formulation; well-posedness and essential boundedness of the concentrations has been shown in this context [18]. This boundedness allows the definition of a cut-off operator used in defining the discrete scheme.



FIGURE 1. Roadmap for proof of well-posedness of Problem 2.2 and definition of Problem 3.3.

2.1. Preliminaries

We use the standard notation for Sobolev spaces [1,14]. Let $L^p(\Omega)$ denote the space of Lebesgue-measurable functions, which *p*th power is Lebesgue-integrable on Ω . Moreover, in the quotient space $L^2(\Omega)/\mathbb{R}$ two elements of $L^2(\Omega)$ are identified if and only if their difference is constant. For $k \in \mathbb{N}_0$, let $H^k(\Omega)$ be the set of *k*-times weakly differentiable functions in $L^2(\Omega)$ with weak derivatives in $L^2(\Omega)$, equipped with the usual scalar product $(\cdot, \cdot)_{H^k(\Omega)}$, associated norm $\|\cdot\|_{H^k(\Omega)}$, and seminorm $|\cdot|_{H^k(\Omega)}$ ([13], *cf.*, p. 483). Let the space $H^{1/2}(\partial\Omega)$ contain those functions on the boundary $\partial\Omega$ for which the norm (*cf.* [11])

$$\|v\|_{H^{1/2}(\partial\Omega)}^{2} \coloneqq \int_{\partial\Omega} |v(\boldsymbol{x})|^{2} \, \mathrm{d}s_{\boldsymbol{x}} + \int_{\partial\Omega} \int_{\partial\Omega} \frac{|v(\boldsymbol{x}) - v(\boldsymbol{y})|^{2}}{|\boldsymbol{x} - \boldsymbol{y}|^{d}} \, \mathrm{d}s_{\boldsymbol{x}} \, \mathrm{d}s_{\boldsymbol{y}}$$

is finite, let $H^{-1/2}(\partial \Omega)$ denote its dual space, and let the duality pairing be denoted by $\langle \cdot, \cdot \rangle_{H^{-1/2}(\partial \Omega), H^{1/2}(\partial \Omega)}$. We define by $\mathbf{H}^k(\Omega) \coloneqq (H^k(\Omega))^d = H^k(\Omega; \mathbb{R}^d)$ the space of vector-valued functions $\mathbf{v} = (v_1, \ldots, v_d)^{\mathrm{T}} : \Omega \to \mathbb{R}^d$, whose components are in $H^k(\Omega)$ equipped with the norm and the scalar product

$$\|\boldsymbol{v}\|_{\boldsymbol{H}^{k}(\Omega)}^{2} \coloneqq \sum_{i=1}^{d} \|v_{i}\|_{H^{k}(\Omega)}^{2} \quad \text{and} \quad (\boldsymbol{v}, \boldsymbol{w})_{\boldsymbol{H}^{k}(\Omega)} \coloneqq \sum_{i=1}^{d} (v_{i}, w_{i})_{H^{k}(\Omega)}, \quad (2.1)$$

respectively. Furthermore, let $\boldsymbol{H}^{\operatorname{div}}(\Omega) \coloneqq \{\boldsymbol{v} \in \boldsymbol{L}^{2}(\Omega); \boldsymbol{\nabla} \cdot \boldsymbol{v} \in L^{2}(\Omega)\}$. With the scalar product $(\boldsymbol{v}_{1}, \boldsymbol{v}_{2})_{\boldsymbol{H}^{\operatorname{div}}(\Omega)} = (\boldsymbol{v}_{1}, \boldsymbol{v}_{2})_{\boldsymbol{L}^{2}(\Omega)} + (\boldsymbol{\nabla} \cdot \boldsymbol{v}_{1}, \boldsymbol{\nabla} \cdot \boldsymbol{v}_{2})_{\boldsymbol{L}^{2}(\Omega)}$ and the induced norm $\|\cdot\|^{2}_{\boldsymbol{H}^{\operatorname{div}}(\Omega)} = (\cdot, \cdot)_{\boldsymbol{H}^{\operatorname{div}}(\Omega)}$, the space $\boldsymbol{H}^{\operatorname{div}}(\Omega)$ is a Hilbert space. For $L^{2}(\Omega)$ or $\boldsymbol{L}^{2}(\Omega)$ we simply write $\|\cdot\|$ and (\cdot, \cdot) .

We continue with the definition of spaces containing time-dependent functions. With V being a Banach space, the space $L^p(J; V)$ consists of Bochner-measurable, V-valued functions $v : J \ni t \mapsto v(t) \in V$ such that the norm

$$\|v\|_{L^{p}(J;V)} \coloneqq \left\{ \begin{array}{ll} \left(\int_{J} \|v(t)\|_{V}^{p} \, \mathrm{d}t\right)^{1/p}, & 1 \le p < \infty \\ \mathrm{ess} \sup_{t \in J} \|v(t)\|_{V}, & p = \infty \end{array} \right\}$$

is finite, which makes $L^p(J; V)$ a Banach space. For the case of $V = L^p(\Omega)$, we identify $L^p(J \times \Omega) = L^p(J; V)$. For $k \in \mathbb{N}_0$, let $H^k(J; V)$ be the set of functions in $L^2(J; V)$ that are k-times weakly differentiable with respect to time with weak derivatives $\partial_t^k v$ in $L^2(J; V)$. Its norm is given by

$$\|v\|_{H^k(J;V)}^2 \coloneqq \sum_{j=0}^k \int_J \|\partial_t^k v(t)\|_V^2 dt.$$

The notation $v(t, \boldsymbol{x})$ is identified with $v(t)(\boldsymbol{x})$.

We recall the trace operator $\gamma_0 : H^1(\Omega) \ni w \mapsto w|_{\partial\Omega} \in H^{1/2}(\partial\Omega)$ and the normal trace operator $\gamma_{\boldsymbol{\nu}} : H^{\operatorname{div}}(\Omega) \ni \boldsymbol{v} \mapsto \boldsymbol{v} \cdot \boldsymbol{\nu}|_{\partial\Omega} \in H^{-1/2}(\partial\Omega)$, which are both linear, continuous, and surjective. We also recall Green's formula: let $\boldsymbol{v} \in \boldsymbol{H}^{\operatorname{div}}(\Omega)$, then $\boldsymbol{v} \cdot \boldsymbol{\nu}|_{\partial\Omega} \in H^{-1/2}(\partial\Omega)$ and there holds

$$\forall w \in H^{1}(\Omega), \quad (\nabla \cdot \boldsymbol{v}, w) + (\boldsymbol{v}, \nabla w) = \langle \boldsymbol{v} \cdot \boldsymbol{\nu}, w \rangle_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)}.$$
(2.2)

If, in addition, $\boldsymbol{v} \cdot \boldsymbol{\nu}|_{\partial \Omega} \in L^2(\partial \Omega)$ the duality pairing in (2.2) can be identified by $\int_{\partial \Omega} \boldsymbol{v} \cdot \boldsymbol{\nu} \, w = (\boldsymbol{v} \cdot \boldsymbol{\nu}, \, w)_{L^2(\partial \Omega)}$. We define the following *constrained ansatz spaces*:

$$\boldsymbol{H}_{a}^{\mathrm{div}}(\Omega) := \left\{ \boldsymbol{v} \in \boldsymbol{H}^{\mathrm{div}}(\Omega); \, \boldsymbol{v} \cdot \boldsymbol{\nu} = a \quad \mathrm{on} \quad \partial \Omega \right\}, \ \ \boldsymbol{H}_{b}^{1}(\Omega) := \left\{ w \in H^{1}(\Omega); \, w = b \quad \mathrm{on} \quad \partial \Omega \right\},$$

where $a \in H^{-1/2}(\partial \Omega)$ and $b \in H^{1/2}(\partial \Omega)$. The spaces $H_0^{\text{div}}(\Omega)$ and $H_0^1(\Omega)$ therefore consist of functions with vanishing normal trace and vanishing trace, respectively.

We make frequent use of the identity $(a + b)^2 \leq 2a^2 + 2b^2$ and the inequality $ab \leq \frac{\delta}{2}a^2 + \frac{1}{2\delta}b^2$ for positive numbers $a, b, and \delta > 0$. Furthermore, we tacitly apply the Hölder and Cauchy–Schwarz inequalities.

2.2. Continuous formulation

The hypotheses imposed on the data of system (1.1) are as follows:

Hypotheses 2.1 (Hypotheses on the data).

(H1) The inverse of the (constant) coefficient $\mathbf{D} \in \mathbb{R}^{d,d}$ is symmetric, positive definite, and bounded, i.e., there exist strictly positive constants D_{α} , D_{∞} , such that

$$\begin{aligned} \forall \boldsymbol{\xi} \in \mathbb{R}^d, & \boldsymbol{\xi} \cdot \mathbf{D}^{-1} \, \boldsymbol{\xi} \, \geq \, D_\alpha \, |\boldsymbol{\xi}|^2, \\ \forall \boldsymbol{\xi}_1, \boldsymbol{\xi}_2 \in \mathbb{R}^d, & \boldsymbol{\xi}_1 \cdot \mathbf{D}^{-1} \, \boldsymbol{\xi}_2 \, \leq \, D_\infty \, |\boldsymbol{\xi}_1| \, |\boldsymbol{\xi}_2|. \end{aligned}$$

- (H2) Hypothesis (H1) holds for the (constant) coefficient K with the constants K_{α} , K_{∞} .
- (H3) The (possibly nonlinear) coefficients r^{\pm} are globally Lipschitz continuous in (c^+, c^-) .
- (H4) The initial data $c^{\pm,0}$ are bounded and nonnegative, i.e., $c^{\pm,0} \in L^{\infty}(\Omega)$ and $c^{\pm,0}(\mathbf{x}) \geq 0$ for a.e. $\mathbf{x} \in \Omega$.
- (H5) The coefficient $\phi_{\rm D}$ is bounded in $H^1(J; H^{1/2}(\partial \Omega))$.
- (H6) The coefficient σ is bounded in $L^{\infty}(J \times \Omega)$.

With (1.1) being a model obtained by periodic homogenization, the coefficients **D** and **K** have closed-form expressions and can be obtained by solving auxiliary problems on a reference cell [16, 32]. The symmetry and positive definiteness of these upscaled tensors as postulated in (H1) and (H2) is naturally satisfied [10]. Note that the symmetry and positive definiteness of the matrices in hypotheses (H1) and (H2) imply the symmetry and positive definiteness of their inverses (cf. [20], Thm. 4.135). Hypothesis (H3) is reasonable, since on the one hand, rates obeying the law of mass action are polynomials in c^+ and c^- , and on the other hand, c^{\pm} is nonnegative and essentially bounded, as shown below. The continuity in time of ϕ_D , *i.e.* $\phi_D \in C(J; H^{1/2}(\partial \Omega)) \subset$ $H^1(J; H^{1/2}(\partial \Omega))$ as implicitly postulated in (H5), will be required in the discrete problem in order to make a point-wise evaluation at $t_n \in J$ meaningful. In the homogenization context, σ is also an effective coefficient, the boundedness of which as postulated in (H6) directly follows from the boundedness of its associated pore-scale quantity.

The error analysis of this article deals with the discretization of the following *mixed weak continuous problem* that is derived by multiplication of the flux equations of (1.1) by the inverse tensors and using the Green formula (2.2):

Problem 2.2 (Mixed weak continuous DNPP problem).

Let **D**, **K**, r^{\pm} , $c^{\pm,0}$, $\phi_{\rm D}$, σ be given and let (H1)-(H6) hold. Seek $(\boldsymbol{u}, p, \boldsymbol{j}^+, c^+, \boldsymbol{j}^-, c^-, \boldsymbol{E}, \phi)$ with $\boldsymbol{u} \in L^2(J; \boldsymbol{H}_0^{\operatorname{div}}(\Omega)), \ p \in L^2(J; L^2(\Omega)/\mathbb{R}), \ \boldsymbol{j}^{\pm} \in L^2(J; \boldsymbol{H}^{\operatorname{div}}(\Omega)), \ c^{\pm} \in L^{\infty}(J \times \Omega) \cap H^1(J; L^2(\Omega)),$

$$\boldsymbol{E} \in L^{\infty}(J; \boldsymbol{H}^{\operatorname{div}}(\Omega)), \ \phi \in L^{\infty}(J; L^{2}(\Omega)) \ \text{such that for a.e. } t \in J, \ \forall \boldsymbol{v} \in \boldsymbol{H}^{\operatorname{div}}(\Omega), \ \forall \boldsymbol{y} \in \boldsymbol{H}_{0}^{\operatorname{div}}(\Omega), \ w \in L^{2}(\Omega), \\ -\left(\boldsymbol{\mathsf{K}}^{-1}\boldsymbol{u}(t), \ \boldsymbol{y}\right) + \left(\boldsymbol{\nabla} \cdot \boldsymbol{y}, \ p(t)\right) = -\left(\boldsymbol{\mathsf{D}}^{-1}\boldsymbol{E}(t)\left(c^{+}(t) - c^{-}(t)\right), \ \boldsymbol{y}\right),$$
(2.3a)

$$(\nabla \cdot u(t), w) = 0,$$
 (2.3b)

$$-\left(\mathbf{D}^{-1}\boldsymbol{j}^{\pm}(t),\,\boldsymbol{v}\right)+\left(\boldsymbol{\nabla}\cdot\boldsymbol{v}\,,\,c^{\pm}(t)\right)+\left(\mathbf{D}^{-1}\left(\boldsymbol{u}(t)\pm\boldsymbol{E}(t)\right)c^{\pm}(t)\,,\,\boldsymbol{v}\right)\ =\ 0,\tag{2.3c}$$

$$(\partial_t c^{\pm}(t), w) + (\nabla \cdot \boldsymbol{j}^{\pm}(t), w) = (r^{\pm}(t, \boldsymbol{x}, c^{+}(t), c^{-}(t)), w),$$

$$- (\mathbf{D}^{-1}\boldsymbol{E}(t), \boldsymbol{v}) + (\nabla \cdot \boldsymbol{v}, \phi(t)) = \langle \boldsymbol{v} \cdot \boldsymbol{\nu}, \phi_{\mathrm{D}}(t) \rangle_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)},$$

$$(2.3d)$$

$$(2.3e)$$

$$, \boldsymbol{v}) + (\boldsymbol{\nabla} \cdot \boldsymbol{v}, \phi(t)) = \langle \boldsymbol{v} \cdot \boldsymbol{\nu}, \phi_{\mathrm{D}}(t) \rangle_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)}, \qquad (2.3e)$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{E}(t), w) = \left(c^+(t) - c^-(t) + \sigma(t), w \right)$$
(2.3f)

with c^{\pm} satisfying $\forall w \in L^2(\Omega)$, $(c^{\pm}(0) - c^{\pm,0}, w) = 0$.

System (2.3) is the dual mixed formulation of the DNPP system (1.1). At this point it is not clear whether Problem 2.2 is well-posed. To handle this situation, we first introduce another weak problem for which wellposedness has been shown in [18] and subsequently prove the equivalence of both problems. The second weak problem derives from the *semi-mixed* formulation of (1.1c), (1.1d), (1.1e), (1.1f) and reads as follows:

Problem 2.3 (Semi-mixed weak continuous DNPP problem).

Let **D**, **K**, r^{\pm} , $c^{\pm,0}$, $\phi_{\rm D}$, σ be given and let (H1)–(H6) hold. Seek $(\boldsymbol{u}, p, c^+, c^-, \phi)$ with $\boldsymbol{u} \in L^2(J; \boldsymbol{H}_0^{\operatorname{div}}(\Omega))$, $p \in L^2(J; L^2(\Omega)/\mathbb{R})$, $c^{\pm} \in L^{\infty}(J \times \Omega) \cap L^2(J; H_0^1(\Omega)) \cap H^1(J; H^{-1}(\Omega))$, $\phi \in L^{\infty}(J; H^2(\Omega) \cap H_{\phi_{\rm D}}^1(\Omega))$ such that for a.e. $t \in J, \forall \boldsymbol{y} \in \boldsymbol{H}_0^{\operatorname{div}}(\Omega), \forall w \in L^2(\Omega), \forall z \in H_0^1(\Omega),$

$$-(\mathbf{K}^{-1}\boldsymbol{u}(t),\boldsymbol{y}) + (\boldsymbol{\nabla}\cdot\boldsymbol{y},\boldsymbol{p}(t)) = ((c^{+}(t) - c^{-}(t))\boldsymbol{\nabla}\phi,\boldsymbol{y}), \qquad (2.4a)$$

$$(\boldsymbol{\nabla} \cdot \boldsymbol{u}(t), w) = 0, \tag{2.4b}$$

$$\left\langle \partial_t c^{\pm}(t), z \right\rangle_{H^{-1}(\Omega), H^1_0(\Omega)} + \left(\mathbf{D} \, \boldsymbol{\nabla} c^{\pm}(t), \, \boldsymbol{\nabla} z \right) - \left(\boldsymbol{u}(t) \, c^{\pm}(t), \, \boldsymbol{\nabla} z \right) \pm \left(c^{\pm}(t) \, \mathbf{D} \, \boldsymbol{\nabla} \phi(t), \, \boldsymbol{\nabla} z \right)$$
(2.4c)

$$\pm (c^{\pm}(t) \mathbf{D} \nabla \phi(t), \nabla z) = (r^{\pm}(t, \boldsymbol{x}, c^{+}(t), c^{-}(t)), z), -(\nabla \cdot \mathbf{D} \nabla \phi(t), w) = (c^{+}(t) - c^{-}(t) + \sigma(t), w)$$
(2.4d)

with c^{\pm} satisfying $\forall w \in L^2(\Omega)$, $(c^{\pm}(0) - c^{\pm,0}, w) = 0$.

We summarize the most important results of [18] in the following theorem, which, in particular, provides an explicit bound for $\sum_{i \in \{+,-\}} \|c^{\pm}\|_{L^{\infty}(J \times \Omega)}$ that is required for the definition of the discrete scheme of Problem 2.2:

Theorem 2.4 (Well-posedness, nonnegativity, and explicit bound). Let (u, p, c^+, c^-, ϕ) be the solution of Problem 2.3 and let (H1)-(H6) hold. Then the following statements hold:

- (i) The solution $(\boldsymbol{u}, p, c^+, c^-, \phi)$ uniquely exists.
- (ii) The partial solutions c^{\pm} are nonnegative, i.e., $c^{\pm}(t, \mathbf{x}) \geq 0$ for a.e. $(t, \mathbf{x}) \in J \times \Omega$.
- (iii) The following estimate holds for arbitrary end time $T \in [0, \infty[$:

$$\sum_{i \in \{+,-\}} \|c^i\|_{L^{\infty}(J \times \Omega)} \leq C(c^{\pm,0}, \sigma, \Omega, T),$$
(2.5)

with $C(c^{\pm,0},\sigma,\Omega,T) > 0$ depending only on $\|c^{\pm,0}\|_{L^{\infty}(\Omega)}$, on $\|\sigma\|_{L^{\infty}(J\times\Omega)}$, on coefficients of the Sobolev embedding theorem, and on the end time T.

Proof. (See [18], Thms. 3.4, 3.10, 3.11 and Rems. 2.2, 3.7). Item (iii) can be deduced as follows: from [18], Theorem 3.5, we have

$$\sum_{i \in \{+,-\}} \|c^i\|_{L^{\infty}(J \times \Omega)} \leq C_{\mathcal{M}} \sum_{i \in \{+,-\}} \|c^i\|_{L^2(J \times \Omega)} + 4 \sum_{i \in \{+,-\}} \|c^{i,0}\|_{L^{\infty}(\Omega)}$$

with a constant $C_{\rm M} > 0$ depending only on $\|\sigma\|_{L^{\infty}(J \times \Omega)}$ and on coefficients of the Sobolev embedding theorem. Application of Gronwall's lemma to the parabolic estimate ([18], Rem. 3.6)

$$d_t \sum_{i \in \{+,-\}} \|c^i(t)\| + \sum_{i \in \{+,-\}} \|\nabla c^i(t)\| \le \frac{2}{D_\alpha} \|\sigma\|_{L^{\infty}(J \times \Omega)} \sum_{i \in \{+,-\}} \|c^i(t)\|$$

yields

$$\forall t \in J, \quad \sum_{i \in \{+,-\}} \|c^{i}(t)\| \leq \exp\left(\frac{2T\|\sigma\|_{L^{\infty}(J \times \Omega)}}{D_{\alpha}}\right) \sum_{i \in \{+,-\}} \|c^{i,0}\|_{T^{\infty}(J \times \Omega)}$$

which, inserted in the first equation, closes the proof.

In the next two propositions, we show that the solution of the mixed weak continuous DNPP problem solves the semi-mixed version and *vice versa* under additional mild regularity assumptions for c^{\pm} . We conclude that Theorem 2.4, in particular the essential boundedness of the concentrations (iii), holds for the solution of the mixed continuous problem. The idea stems from the paper of [28].

Proposition 2.5 (Solution of Problem 2.2 solves Problem 2.3).

Let $(\boldsymbol{u}, p, \boldsymbol{j}^+, c^+, \boldsymbol{j}^-, c^-, \boldsymbol{E}, \phi)$ be a solution of Problem 2.2. Then the partial solution $(\boldsymbol{u}, p, c^+, c^-, \phi)$ is a solution of Problem 2.3. In particular, $c^{\pm} \in L^2(J; H^1_0(\Omega))$ and $\phi \in L^{\infty}(J; H^2(\Omega) \cap H^1_{\phi_{\mathcal{D}}}(\Omega))$ holds.

In what follows, we denote by $\mathcal{D}(\Omega)$ the space of infinitely differentiable functions with compact support on Ω , and by $\mathcal{D}'(\Omega)$ the space of distributions (*cf.*, [13], Sect. B.2).

Proof of Proposition 2.5. Testing (2.3e) with $\boldsymbol{v} \in \mathcal{D}(\Omega)^d \subset \boldsymbol{H}^{\operatorname{div}}(\Omega)$ yields

$$\forall \boldsymbol{v} \in \mathcal{D}(\Omega)^d, \quad \left(\mathbf{D}^{-1} \boldsymbol{E}(t) \,, \, \boldsymbol{v} \right) \stackrel{=}{\underset{(2.3e)}{=}} \left(\phi(t) \,, \, \boldsymbol{\nabla} \cdot \boldsymbol{v} \right) = -\langle \boldsymbol{\nabla} \phi(t) \,, \, \boldsymbol{v} \rangle_{\mathcal{D}'(\Omega)^d, \mathcal{D}(\Omega)^d}, \tag{2.6}$$

which is the defining equation for $\nabla \phi(t)$, *i.e.*, $\nabla \phi(t)$ in the distributional sense is a function: $\forall t \in J$, $-\nabla \phi(t) = \mathbf{D}^{-1} \mathbf{E}(t)$. Since $\|\mathbf{D}^{-1} \mathbf{E}\|_{L^{\infty}(J; \mathbf{L}^{2}(\Omega))} < \infty$ due to $\mathbf{E} \in L^{\infty}(J; \mathbf{L}^{2}(\Omega))$ and (H1), it follows that $\nabla \phi \in L^{\infty}(J; \mathbf{L}^{2}(\Omega))$. From $\phi \in L^{\infty}(J; L^{2}(\Omega))$ given, we consequently infer that $\phi \in L^{\infty}(J; H^{1}(\Omega))$. Owing to $\mathcal{D}(\Omega) \subset L^{2}(\Omega)$ dense (cf. [13], Thm. B.14 and [39], Cor. 1.1.1), the variational equation

$$\forall \boldsymbol{v} \in \boldsymbol{L}^{2}(\Omega), \quad \left(\boldsymbol{\mathsf{D}}^{-1}\boldsymbol{E}(t), \, \boldsymbol{v}\right) = -(\boldsymbol{\nabla}\phi(t), \, \boldsymbol{v}) \tag{2.7}$$

holds. Next, we show that $\phi(t) = \phi_{\rm D}(t)$ on $\partial \Omega$ for *a.e.* $t \in J$, which was demanded implicitly in Problem 2.3 by the constrained ansatz space $H^1_{\phi_{\rm D}}(\Omega)$ and explicitly in Problem 2.2 by a boundary integral: using the fact that (2.7) also holds for $\boldsymbol{v} \in \boldsymbol{H}^{\rm div}(\Omega) \subset \boldsymbol{L}^2(\Omega)$ and application of Green's formula yields

$$\begin{aligned} \forall \boldsymbol{v} \in \boldsymbol{H}^{\mathrm{div}}(\Omega), \quad \langle \boldsymbol{v} \cdot \boldsymbol{\nu}, \phi(t) \rangle_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)} &= (\phi(t), \, \boldsymbol{\nabla} \cdot \boldsymbol{v}) + (\boldsymbol{\nabla}\phi(t), \, \boldsymbol{v}) \\ &= (\phi(t), \, \boldsymbol{\nabla} \cdot \boldsymbol{v}) - \left(\boldsymbol{\mathsf{D}}^{-1}\boldsymbol{E}(t), \, \boldsymbol{v}\right) = \langle \boldsymbol{v} \cdot \boldsymbol{\nu}, \, \phi_{\mathrm{D}}(t) \rangle_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)}. \end{aligned}$$

In order to prove that $\phi(t)$ is also in $H^2(\Omega)$, we test (2.3f) with $w \in \mathcal{D}(\Omega) \subset L^2(\Omega)$:

$$\begin{aligned} \forall w \in \mathcal{D}(\Omega), \quad \left(c^{+}(t) - c^{-}(t) + \sigma(t), w\right) &= \left(\boldsymbol{\nabla} \cdot \boldsymbol{E}(t), w\right) \\ &= -(\boldsymbol{E}(t), \, \boldsymbol{\nabla} w) = \left(\boldsymbol{D} \boldsymbol{\nabla} \phi(t), \, \boldsymbol{\nabla} w\right) = -\langle \boldsymbol{\nabla} \cdot \boldsymbol{D} \boldsymbol{\nabla} \phi(t), w \rangle_{\mathcal{D}'(\Omega), \mathcal{D}(\Omega)}, \end{aligned}$$

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which shows that the distributional divergence of $\mathbf{D}\nabla\phi(t)$ is a function. Because c^{\pm} and σ are element of $L^{\infty}(J; L^2(\Omega))$ from assumption and due to (H6), respectively, we conclude—taking the previous considerations into account—that $\phi \in L^{\infty}(J; H^2(\Omega) \cap H^1_{\phi_{\mathbf{D}}}(\Omega))$. Thus $\phi(t)$ is a partial solution of (2.4d) for *a.e.* $t \in J$.

into account—that $\phi \in L^{\infty}(J; H^2(\Omega) \cap H^1_{\phi_{\mathrm{D}}}(\Omega))$. Thus $\phi(t)$ is a partial solution of (2.4d) for *a.e.* $t \in J$. With (2.7) and the fact that $c^{\pm} \in L^{\infty}(J \times \Omega)$, the mixed variational subsystems (2.4a), (2.4b) and (2.3a), (2.3b) coincide. Hence, $(\boldsymbol{u}(t), p(t)) \in \boldsymbol{H}_0^{\mathrm{div}}(\Omega) \times L^2(\Omega)/\mathbb{R}$ is also a partial solution of (2.4a), (2.4b).

It remains to show that $c^{\pm}(t)$ are partial solutions of (2.4c). We test (2.3c) with $v \in \mathcal{D}(\Omega)^d \subset H^{\text{div}}(\Omega)$:

$$\forall \boldsymbol{v} \in \mathcal{D}(\Omega)^{d}, \quad \left(\mathbf{D}^{-1} \Big(\boldsymbol{j}^{\pm}(t) - \big(\boldsymbol{u}(t) \pm \boldsymbol{E}(t) \big) \boldsymbol{c}^{\pm}(t) \Big), \, \boldsymbol{v} \right) \underset{(2.3c)}{=} \left(\boldsymbol{c}^{\pm}(t), \, \boldsymbol{\nabla} \cdot \boldsymbol{v} \right) = - \left\langle \boldsymbol{\nabla} \boldsymbol{c}^{\pm}(t), \, \boldsymbol{v} \right\rangle_{\mathcal{D}'(\Omega)^{d}, \mathcal{D}(\Omega)^{d}}, \tag{2.8}$$

i.e., $\nabla c^{\pm}(t)$ in the distributional sense is a function. It holds $\nabla c^{\pm}(t) \in L^2(\Omega)$ and thus $c^{\pm}(t) \in H^1(\Omega)$ for *a.e.* $t \in J$ due to (H1) and $c^{\pm}(t) \in L^{\infty}(\Omega)$ for *a.e.* $t \in J$. In particular, (2.8) also holds in the $L^2(\Omega)$ sense. With this result, $c^{\pm} \in L^2(J; H^1(\Omega))$ can be shown:

$$\begin{aligned} \|c^{\pm}\|_{L^{2}(J;H^{1}(\Omega))}^{2} &= \|c^{\pm}\|_{L^{2}(J\times\Omega)}^{2} + \int_{J} \left\| \mathbf{D}^{-1} \left(\boldsymbol{j}^{\pm} - (\boldsymbol{u} \pm \boldsymbol{E}) c^{\pm} \right) (s) \right\|^{2} \mathrm{d}s \\ &\leq \|c^{\pm}\|_{L^{2}(J\times\Omega)}^{2} + 2\|\mathbf{D}^{-1}\|_{\mathbf{L}^{\infty}(\Omega)}^{2} \left(\|\boldsymbol{j}^{\pm}\|_{\boldsymbol{L}^{2}(J\times\Omega)}^{2} + \|\boldsymbol{u} \pm \boldsymbol{E}\|_{\boldsymbol{L}^{2}(J\times\Omega)}^{2} \|c^{\pm}(t)\|_{L^{\infty}(J\times\Omega)}^{2} \right) < \infty. \end{aligned}$$

It remains to show that c^{\pm} satisfies the homogeneous Dirichlet boundary conditions: Testing (2.8) with $v \in H^{\text{div}}(\Omega) \subset L^2(\Omega)$ and using Green's formula yields

$$\forall \boldsymbol{v} \in \boldsymbol{H}^{\operatorname{div}}(\Omega), \quad \left\langle \boldsymbol{v} \cdot \boldsymbol{\nu}, \, c^{\pm}(t) \right\rangle_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)} = 0,$$

i.e. $c^{\pm}(t) \in H_0^1(\Omega)$ holds for a.e. $t \in J$.

Equation (2.3c) also holds for $\boldsymbol{v} \in \mathcal{D}(\Omega)^d \subset \boldsymbol{H}_0^{\text{div}}(\Omega)$. We test (2.3c) with $\boldsymbol{v} = \boldsymbol{\mathsf{D}}^{\mathrm{T}} \boldsymbol{\nabla} w$, where $w \in \mathcal{D}(\Omega)$, use (H1), and apply Green's formula to the first and the second term:

$$\forall w \in \mathcal{D}(\Omega), \quad \left(\boldsymbol{\nabla} \cdot \boldsymbol{j}^{\pm}(t), w\right) = \left(\boldsymbol{\mathsf{D}}\boldsymbol{\nabla}c^{\pm}(t), \boldsymbol{\nabla}w\right) - \left((\boldsymbol{u}(t) \pm \boldsymbol{E}(t))c^{\pm}(t), \boldsymbol{\nabla}w\right).$$
(2.9)

Note that the second scalar product is meaningful due to the above shown regularity. Since $\mathcal{D}(\Omega) \subset L^2(\Omega)$, we may substitute (2.9) into (2.3d):

$$\forall w \in \mathcal{D}(\Omega), \quad \left(\partial_t c^{\pm}(t), w\right) + \left(\mathbf{D}\boldsymbol{\nabla} c^{\pm}(t), \boldsymbol{\nabla} w\right) - \left(\left(\boldsymbol{u}(t) \pm \boldsymbol{E}(t)\right)c^{\pm}(t), \boldsymbol{\nabla} w\right) = \left(r^{\pm}(t), w\right)$$
(2.10)

for a.e. $t \in J$. Since $\mathcal{D}(\Omega) \subset H_0^1(\Omega)$ dense with respect to $\|\cdot\|_{H^1(\Omega)}$ ([14], Sect. 5.2.2), (2.10) also holds for $w \in H_0^1(\Omega)$. Using that $\mathbf{E}(t) = -\mathbf{D}\nabla\phi(t)$ holds in $\mathbf{L}^2(\Omega)$ for a.e. $t \in J$, as shown above, and noting that

$$\forall w \in H_0^1(\Omega), \quad \left(\partial_t c^{\pm}(t), w\right) = \left\langle \partial_t c^{\pm}(t), w \right\rangle_{H^{-1}(\Omega), H_0^1(\Omega)}$$

since $\partial_t c^{\pm}(t) \in L^2(\Omega)$ by the definition of Problem 2.2 and $(H_0^1(\Omega), L^2(\Omega), H^{-1}(\Omega))$ is a Gelfand triple, it follows that the partial solutions $c^{\pm}(t)$ of Problem 2.2 solve the semi-mixed variational equation (2.4c) of Problem 2.3.

For the reverse direction of Proposition 2.5—*i.e.* the solution of Problem 2.2 solves Problem 2.3—we need to ask for additional regularity on the concentrations c^{\pm} :

Hypotheses 2.6 (Hypothesis on the concentrations).

(H7) The partial solution c^{\pm} of Problem 2.3 is bounded in $L^2(J; H^2(\Omega))$.

If Hypothesis (H7) follows naturally from Problem 2.3 is unclear at this point. The smoothness as of (H7) is contained in (H9) in the case of optimal convergence for c^{\pm} in the numerical scheme except for lowest-order elements.

Proposition 2.7 (Solution of Problem 2.3 solves Problem 2.2). Let (u, p, c^+, c^-, ϕ) be a solution of Problem 2.3 and let

$$m{j}^{\pm}\ \coloneqq\ -{\sf D}m{
abla} c^{\pm}+m{u} c^{\pm}\pm m{E} c^{\pm}\ ,\qquad m{E}\ \coloneqq\ -{\sf D}m{
abla} \phi$$

in the $L^{\infty}(J; \mathbf{L}^{2}(\Omega))$ sense, and let (H7) hold. Then $(\mathbf{u}, p, \mathbf{j}^{+}, c^{+}, \mathbf{j}^{-}, c^{-}, \mathbf{E}, \phi)$ is a solution of Problem 2.2. In particular, $c^{\pm} \in H^{1}(J; L^{2}(\Omega))$.

Proof. The regularity $\boldsymbol{E} \in L^{\infty}(J; \boldsymbol{H}^{\text{div}}(\Omega))$ follows immediately from that of ϕ and (H1). Substituting the definition of the flux \boldsymbol{E} into (2.4d) yields (2.3f). Testing the definition of \boldsymbol{E} pointwise in $t \in J$ with $\boldsymbol{v} \in \boldsymbol{H}^{\text{div}}(\Omega) \subset \boldsymbol{L}^{2}(\Omega)$ yields

$$\forall \boldsymbol{v} \in \boldsymbol{H}^{\mathrm{div}}(\varOmega), \quad \left(\boldsymbol{\mathsf{D}}^{-1}\boldsymbol{E}(t),\,\boldsymbol{v}\right) = -(\boldsymbol{\nabla}\phi(t),\,\boldsymbol{v}) = \left(\phi(t),\,\boldsymbol{\nabla}\cdot\boldsymbol{v}\right) - \left\langle\boldsymbol{v}\cdot\boldsymbol{\nu},\,\phi(t)\right\rangle_{H^{-1/2}(\partial\varOmega),H^{1/2}(\partial\varOmega)}$$

where (H1) and Green's formula was used. This gives (2.3e) since $\phi(t) \in H^1_{\phi_D}(\Omega)$. Equations (2.3a), (2.3b) are identical to (2.4a), (2.4b) when inserting \boldsymbol{E} . It remains to derive (2.3c), (2.3d) and to show that $c^{\pm} \in H^1(J; L^2(\Omega))$. The regularity of \boldsymbol{j}^{\pm} follows immediately from that of c^{\pm} , \boldsymbol{u} , \boldsymbol{E} , (H1), and (H7). Testing the definition of \boldsymbol{j}^{\pm} with $\boldsymbol{v} \in \boldsymbol{H}^{\text{div}}(\Omega) \subset \boldsymbol{L}^2(\Omega)$ and using (H1) yields (2.3c). Inserting the definitions of \boldsymbol{j}^{\pm} and \boldsymbol{E} into (2.4c) yields

$$\begin{aligned} \forall z \in H_0^1(\Omega), \quad \left\langle \partial_t c^{\pm}(t) \,, \, z \right\rangle_{H^{-1}(\Omega), H_0^1(\Omega)} &- \left(r^{\pm}(t) \,, \, z \right) \\ &= \left. - \left(\boldsymbol{\nabla} \cdot \boldsymbol{j}^{\pm}(t) \,, \, z \right) - \left\langle \boldsymbol{j}^{\pm} \cdot \boldsymbol{\nu} \,, \, z \right\rangle_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)}, \end{aligned}$$

where the last term vanishes due to $z \in H_0^1(\Omega)$. Testing the above equation with $v \in \mathcal{D}(\Omega) \subset H_0^1(\Omega)$ yields

$$\forall v \in \mathcal{D}(\Omega), \quad \left\langle \partial_t c^{\pm}(t), z \right\rangle_{\mathcal{D}'(\Omega), \mathcal{D}(\Omega)} = \left\langle r^{\pm}(t), z \right\rangle_{\mathcal{D}'(\Omega), \mathcal{D}(\Omega)} - \left\langle \boldsymbol{\nabla} \cdot \boldsymbol{j}^{\pm}(t), z \right\rangle_{\mathcal{D}'(\Omega), \mathcal{D}(\Omega)},$$

i.e. $\partial_t c^{\pm}(t) = r^{\pm}(t) - \nabla \cdot \boldsymbol{j}^{\pm}(t)$ in the distributional sense. Since $\mathcal{D}(\Omega) \subset L^2(\Omega)$ dense and $r^{\pm}(t) - \nabla \cdot \boldsymbol{j}^{\pm}(t) \in L^2(\Omega)$, it follows $\partial_t c^{\pm}(t) \in L^2(\Omega)$ and we obtain (2.3d).

From Proposition 2.5 and 2.7 it follows immediately the following corollary stating the well-posedness of Problem 1:

Corollary 2.8. Let (H7) hold. Then Theorem 2.4 holds true for the solution $(\boldsymbol{u}, p, \boldsymbol{j}^+, c^+, \boldsymbol{j}^-, c^-, \boldsymbol{E}, \phi)$ of Problem 2.2.

3. Numerical scheme

This section defines the numerical setting and scheme for the *a priori* error analysis in Section 4. We set up the Raviart–Thomas spaces of arbitrary order and outline their main properties as well as properties of associated projectors in Section 3.1. Furthermore, the BDF stencils used for time discretization are defined. Section 3.2 introduces the cut-off operator used to define the discrete scheme approximating Problem 2.2.

3.1. Preliminaries

Let \mathcal{T}_h be a regular family of decompositions ([9], (H1), p. 131) into closed d-simplices T of characteristic size h such that $\overline{\Omega} = \cup T$.

We denote by $\mathbb{P}_k(T)$ the space of polynomials of degree at most k on a triangle $T \in \mathcal{T}_h$ and define by

$$\mathbb{RT}_k(T) \coloneqq \mathbb{P}_k(T)^d \oplus \boldsymbol{x} \mathbb{P}_k(T) = \left\{ \boldsymbol{v}_h : T \to \mathbb{R}^d; \ \boldsymbol{v}_h(\boldsymbol{x}) = a\boldsymbol{x} + \boldsymbol{b}, \ a \in \mathbb{P}_k(T), \ \boldsymbol{b} \in \mathbb{P}_k(T)^d \right\}$$

the local Raviart-Thomas space of order $k \in \mathbb{N}_0$ [36, 31, 25]. We define by $\mathbb{P}_k(\mathcal{T}_h) := \{w_h : \Omega \to \mathbb{R}; \forall T \in \mathcal{T}_h, w_h|_T \in \mathbb{P}_k(T)\}$ the global polynomial spaces on the triangulation \mathcal{T}_h . Clearly, $\mathbb{P}_k(\mathcal{T}_h) \subset L^2(\Omega)$. The global

Raviart-Thomas space of order k is defined by $\mathbb{RT}_k(\mathcal{T}_h) := H^{\operatorname{div}}(\Omega) \cap \prod_{T \in \mathcal{T}_h} \mathbb{RT}_k(T)$. The inclusion $\mathbb{RT}_k(\mathcal{T}_h) \subset \mathbb{RT}_k(\Omega)$ $H^{\text{div}}(\Omega)$ ensures that the normal components of v_h are continuous across the interior edges. Note that in general these functions are not continuous in each component.

Let the projectors $\boldsymbol{\Pi}_{h}^{k}: \boldsymbol{H}^{\text{div}}(\Omega) \cap \prod_{T \in \mathcal{T}_{h}} \boldsymbol{H}^{1}(T) \ni \boldsymbol{v} \mapsto \boldsymbol{\Pi}_{h}^{k} \boldsymbol{v} \in \mathbb{RT}_{k}(\mathcal{T}_{h}) \text{ and } P_{h}^{k}: L^{2}(\Omega) \ni \boldsymbol{w} \mapsto P_{h}^{k} \boldsymbol{w} \in \mathbb{P}_{k}(\mathcal{T}_{h})$ be the global interpolation operators due to Raviart and Thomas [12,6]. The projectors fulfill the following well-known properties [12, 31, 8, 6, 27]:

- (P1) $\nabla \cdot \boldsymbol{\Pi}_{h}^{k} = P_{h}^{k} \nabla \cdot \text{ and } \nabla \cdot \mathbb{RT}_{k}(\mathcal{T}_{h}) = \mathbb{P}_{k}(\mathcal{T}_{h}).$ (P2) For $w \in L^{2}(\Omega)$ given, $\forall w_{h} \in \mathbb{P}_{k}(\mathcal{T}_{h}), (P_{h}^{k}w, w_{h}) = (w, w_{h}).$
- (P3) For $\boldsymbol{v} \in \boldsymbol{H}^{\operatorname{div}}(\Omega) \cap \prod_{T \in \mathcal{T}_h} \boldsymbol{H}^1(T)$ given, $\forall w_h \in \mathbb{P}_k(\mathcal{T}_h), \left(\boldsymbol{\nabla} \cdot \boldsymbol{\Pi}_h^k \boldsymbol{v}, w_h\right) = (\boldsymbol{\nabla} \cdot \boldsymbol{v}, w_h).$ (P4) Given $w_h \in \mathbb{P}_k(\mathcal{T}_h)$, there exists $\boldsymbol{v}_h \in \mathbb{RT}_k(\mathcal{T}_h)$ such that $\boldsymbol{\nabla} \cdot \boldsymbol{v}_h = w_h$ and $\|\boldsymbol{v}_h\|_{\boldsymbol{H}^{\operatorname{div}}(\Omega)} \leq C_{\Omega} \|w_h\|$ holds with a constant C_{Ω} depending only on Ω .
- (P5) For any $\boldsymbol{v} \in \boldsymbol{H}^{l}(\Omega)$ and $w \in H^{l}(\Omega)$, for $l \in \{1, \dots, k+1\}$,

$$\|(\boldsymbol{\Pi}_h^k - \boldsymbol{I})\boldsymbol{v}\| \lesssim h^l \, |\boldsymbol{v}|_{\boldsymbol{H}^l(\Omega)}, \qquad \|(P_h^k - \boldsymbol{I})\boldsymbol{w}\| \lesssim h^l \, |\boldsymbol{w}|_{H^l(\Omega)}.$$

Here and in the following, the symbol \lesssim indicates inequalities that are valid up to a multiplicative constant which is independent of the discretization parameters τ and h.

Let $0 =: t_0 < t_1 < \ldots < t_N := T$ be an equidistant decomposition of the time interval J and let $\tau := T/N$ denote the time step size. For discrete functions $v_h^n \in \mathbb{P}_k(\mathcal{T}_h)$, the first and the second order backward difference quotient is defined by

$$\overline{\partial}_1 v_h^n \coloneqq \frac{1}{\tau} \left(v_h^n - v_h^{n-1} \right), \quad \overline{\partial}_2 v_h^n \coloneqq \frac{3}{2} \overline{\partial}_1 v_h^n - \frac{1}{2} \overline{\partial}_1 v_h^{n-1} = \frac{1}{\tau} \left(\frac{3}{2} v_h^n - 2 v_h^{n-1} + \frac{1}{2} v_h^{n-2} \right) \tag{3.1}$$

for admissible n. This notation applies to continuous functions analogously.

We use the following notation associated with the *discretization error* of v and of w, respectively, at the time $t_n \in J$:

$$\boldsymbol{\eta}_{\boldsymbol{v}}^n \coloneqq \boldsymbol{v}_h^n - \boldsymbol{v}(t_n), \qquad \boldsymbol{\eta}_w^n \coloneqq \boldsymbol{w}_h^n - \boldsymbol{w}(t_n)$$
(3.2)

for time and space continuous, vector-valued functions v and corresponding fully discrete approximations $v_h^h \in$ $\mathbb{RT}_k(\mathcal{T}_h)$ and for time and space continuous, scalar-valued functions w and corresponding fully discrete approximations $w_h^n \in \mathbb{P}_k(\mathcal{T}_h)$, respectively. In the analysis that follows, we make frequent use of the identities $\boldsymbol{\eta}_{\boldsymbol{v}}^{n} = \boldsymbol{\Pi}_{h}^{k} \boldsymbol{\eta}_{\boldsymbol{v}}^{n} + (\boldsymbol{\Pi}_{h}^{k} - \boldsymbol{I}) \boldsymbol{v} \text{ and } \boldsymbol{\eta}_{w}^{n} = P_{h}^{k} \boldsymbol{\eta}_{w}^{n} + (P_{h}^{k} - \boldsymbol{I}) \boldsymbol{w}.$

3.2. Fully discrete formulation

In the formulation of the fully discrete counterpart of Problem 2.2, we make use of the following *cut-off* operator [35, 4]:

Definition 3.1 (Cut-off operator). For $w \in L^p(\Omega)$, $1 \leq p \leq \infty$ and fixed $M \in \mathbb{R}^+$, let $\mathcal{M}: L^p(\Omega) \ni w \mapsto \mathcal{M}(w) \in L^{\infty}(\Omega)$ be an operator such that for *a.e.* $x \in \Omega, \mathcal{M}(w)(x) = \min\{|w(x)|, M\}$ holds.

Lemma 3.2 (Properties of the cut-off operator). Let $1 \le p \le \infty$. The following statements hold:

- (i) $\forall w \in L^p(\Omega), \|\mathcal{M}(w)\|_{L^{\infty}(\Omega)} \leq M.$
- (ii) Let $w \in L^{\infty}(\Omega)$. If M satisfies $||w||_{L^{\infty}(\Omega)} \leq M$, then $\mathcal{M}(w) = |w|$.
- (iii) The operator $\mathcal{M}(\cdot)$ is globally Lipschitz continuous on $L^p(\Omega)$ with a Lipschitz constant equal to one, i.e., $\forall v, w \in L^p(\Omega), \ \|\mathcal{M}(v) - \mathcal{M}(w)\|_{L^p(\Omega)} \le \|v - w\|_{L^p(\Omega)}.$

Proof. The properties (i) and (ii) are obvious. Property (iii) follows from the pointwise Lipschitz continuity $|\mathcal{M}(v)(x) - \mathcal{M}(w)(x)| \le |v(x) - w(x)|$ for a.e. $x \in \Omega$ taking the essential supremum on both sides for $p = \infty$ and taking both sides to the power p and integration over Ω for $1 \leq p \leq \infty$.

The cut-off operator \mathcal{M} is a crucial tool in the error analysis that follows. However, the associated numerical scheme is not defined properly as long as the cut-off level M is not fixed in terms of data, *i.e.* not depending on the solution itself. Especially, it has to be ensured that M is chosen sufficiently large such that the property (ii) of Lemma 3.2 holds for the partial solutions $c^{\pm}(t)$. This means, in particular, that an $L^{\infty}(\Omega)$ a priori estimate is necessary providing an $L^{\infty}(\Omega)$ bound depending only on the data. To this end, we show that solutions of Problem 2.2 also solve Problem 2.3 in order to allow the exploitation of the estimate (iii) of Theorem 2.4 yielding the demanded explicit bound. The so obtained validity of Theorem 2.4 yields furthermore the existence and uniqueness of solutions of Problem 2.2 and also the nonnegativity of concentrations.

We continue with the formulation of the fully discrete problem. We assume that the (stationary) upscaled coefficients, namely **D**, **K**, and σ and the data $\phi_{\rm D}$ are sufficiently precisely precomputed such that a discretization error in these coefficients is negligible. Owing to Corollary 2.8, the use of the cut-off operator \mathcal{M} according to Definition 3.1 is now admissible for the definition of the *fully discrete weak problem*:

Problem 3.3 (Mixed weak discrete DNPP problem). Let $q \in \{1, 2\}$, $k \in \mathbb{N}_0$. Let \mathbf{D} , \mathbf{K} , r^{\pm} , $\phi_{\mathbf{D}}$, σ , $c_h^{\pm,0}$, $c_h^{\pm,q-1}$ be given. For $n \in \{q, \dots, N\}$, seek $(\boldsymbol{u}_h^n, p_h^n, \boldsymbol{j}_h^{\pm,n}, c_h^{\pm,n}, \boldsymbol{j}_h^{-,n}, c_h^{-,n}, \boldsymbol{E}_h^n, \phi_h^n) \in (\mathbb{RT}_k(\mathcal{T}_h) \times \mathbb{P}_k(\mathcal{T}_h))^4$ such that $\forall \boldsymbol{v}_h \in \mathbb{RT}_k(\mathcal{T}_h), w_h \in \mathbb{P}_k(\mathcal{T}_h),$

$$-(\mathbf{K}^{-1}\boldsymbol{u}_{h}^{n},\boldsymbol{v}_{h}) + (\boldsymbol{\nabla}\cdot\boldsymbol{v}_{h},p_{h}^{n}) = -(\mathbf{D}^{-1}\boldsymbol{E}_{h}^{n}\mathcal{M}(c_{h}^{+,n}-c_{h}^{-,n}),\boldsymbol{v}_{h}), \qquad (3.3a)$$
$$(\boldsymbol{\nabla}\cdot\boldsymbol{u}_{h}^{n},\boldsymbol{w}_{h}) = 0, \qquad (3.3b)$$

$$\cdot \boldsymbol{u}_h^n, w_h) = 0, \tag{3.3b}$$

$$-\left(\mathbf{D}^{-1}\boldsymbol{j}_{h}^{\pm,n},\boldsymbol{v}_{h}\right)+\left(\boldsymbol{\nabla}\cdot\boldsymbol{v}_{h},\boldsymbol{c}_{h}^{\pm,n}\right)+\left(\mathbf{D}^{-1}(\boldsymbol{u}_{h}^{n}\pm\boldsymbol{E}_{h}^{n})\mathcal{M}(\boldsymbol{c}_{h}^{\pm,n}),\boldsymbol{v}_{h}\right)=0,$$
(3.3c)

$$(\partial_{q}c_{h}^{\pm,n}, w_{h}) + (\nabla \cdot \boldsymbol{j}_{h}^{\pm,n}, w_{h}) = (r^{\pm}(t_{n}, \boldsymbol{x}, c_{h}^{\pm,n}, c_{h}^{\pm,n}), w_{h}),$$
(3.3d)

$$-(\mathbf{D}^{-1}\boldsymbol{E}_{h}^{n},\boldsymbol{v}_{h})+(\mathbf{\nabla}\cdot\boldsymbol{v}_{h},\phi_{h}^{n}) = (\boldsymbol{v}_{h}\cdot\boldsymbol{\nu},\phi_{\mathrm{D}}(t_{n}))_{L^{2}(\partial\Omega)},$$
(3.3e)

$$(\nabla \cdot E_h^n, w_h) = (c_h^{+,n} - c_h^{-,n} + \sigma(t_n), w_h), \qquad (3.3f)$$

where the cut-off level M for the cut-off operator \mathcal{M} is set equal to the right-hand side of (2.5).

The cutting off of the terms in (3.3a), (3.3c) is necessary here in order to bound the respective scalar products uniformly in h. Note that it would also be possible to cut off the fluxes u_h^n and E_h^n . However, we could not access analytical results that provide $L^{\infty}(\Omega)$ a priori estimates for u or E.

4. A priori error analysis

This section addresses the approximation quality investigation of the numerical scheme presented in Problem 3.3 in terms of an *a priori* analysis of the discretization error. In Propositions 4.2, 4.3, and 4.5 the discretization errors of the partial solutions is bounded by data and the discretization errors of other partial solutions. Those propositions are combined in Theorem 4.6, which is the main result of this paper.

In the context of *a priori* error analysis it is admissible to make further assumptions on the regularity of the solution that is to be approximated:

Hypotheses 4.1 (Hypotheses on the solution of Problem 2.2).

Let $l_1, \ldots, l_6 \in \{1, \ldots, k+1\}$ be fixed integers (k and q as in Problem 3.3).

- (H8) For the partial solution (\boldsymbol{u}, p) it holds that $\boldsymbol{u} \in L^2(J; \boldsymbol{L}^{\infty}(\Omega)) \cap H^1(J; \boldsymbol{H}^{l_1}(\Omega)), p \in H^1(J; H^{l_2}(\Omega)).$
- (H9) For the partial solutions (j^{\pm}, c^{\pm}) it holds that $j^{\pm} \in H^{1}(J; H^{l_{3}}(\Omega)), c^{\pm} \in H^{q+1}(J; L^{2}(\Omega)) \cap H^{1}(J; H^{l_{4}}(\Omega)).$
- (H10) For the partial solution (E, ϕ) it holds that $E \in L^2(J; L^{\infty}(\Omega)) \cap H^1(J; H^{l_5}(\Omega)), \phi \in H^1(J; H^{l_6}(\Omega)).$

The H^1 regularity in time was postulated as the definition of the discretization error (3.2) requires a point-wise evaluation in time.

Proposition 4.2. Let $(\mathbf{E}, \phi, c^+, c^-)$ and $(\mathbf{E}_h^n, \phi_h^n, c_h^+, c_h^-)$ be partial solutions of Problem 2.2 and Problem 3.3, respectively. Then, if in addition the regularity requirements of (H7) and (H10) are satisfied, for $n \in \{q, \ldots, N\}$,

$$\|\boldsymbol{\eta}_{\boldsymbol{E}}^{n}\|^{2} + \|\boldsymbol{\eta}_{\phi}^{n}\|^{2} \lesssim h^{2l_{5}} |\boldsymbol{E}(t_{n})|_{\boldsymbol{H}^{l_{5}}(\Omega)}^{2} + h^{2l_{6}} |\phi(t_{n})|_{H^{l_{6}}(\Omega)}^{2} + \sum_{i \in \{+,-\}} \|\boldsymbol{\eta}_{c^{i}}^{n}\|^{2}.$$

$$(4.1)$$

The errors η_v , η_w have been defined in (3.2).

Proof. Subtraction of (2.3e), (2.3f) from (3.3e), (3.3f) yields the error equations

$$\left(\mathbf{D}^{-1}\boldsymbol{\eta}_{\boldsymbol{E}}^{n},\boldsymbol{v}_{h}\right) = \left(\boldsymbol{\nabla}\cdot\boldsymbol{v}_{h},\boldsymbol{\eta}_{\phi}^{n}\right) \stackrel{(\mathrm{P1}),(\mathrm{P2})}{=} \left(\boldsymbol{\nabla}\cdot\boldsymbol{v}_{h},P_{h}^{k}\boldsymbol{\eta}_{\phi}^{n}\right),\tag{4.2a}$$

$$\left(\boldsymbol{\nabla}\cdot\boldsymbol{\eta}_{\boldsymbol{E}}^{n},w_{h}\right) = \left(\eta_{c^{+}}^{n},w_{h}\right) - \left(\eta_{c^{-}}^{n},w_{h}\right) \stackrel{(\mathbf{P3})}{=} \left(\boldsymbol{\nabla}\cdot\boldsymbol{\Pi}_{h}^{k}\boldsymbol{\eta}_{\boldsymbol{E}}^{n},w_{h}\right)$$
(4.2b)

for all $\boldsymbol{v}_h \in \mathbb{RT}_k(\mathcal{T}_h)$ and for all $w_h \in \mathbb{P}_k(\mathcal{T}_h)$. The choice of $\boldsymbol{v}_h = \boldsymbol{\Pi}_h^k \boldsymbol{\eta}_E^n \in \mathbb{RT}_k(\mathcal{T}_h)$ and $w_h = P_h^k \boldsymbol{\eta}_\phi^n \in \mathbb{P}_k(\mathcal{T}_h)$, subtraction of the resulting equations, and (H1) yields

$$D_{\alpha} \|\boldsymbol{\eta}_{\boldsymbol{E}}^{n}\|^{2} \leq \left(\mathbf{D}^{-1}\boldsymbol{\eta}_{\boldsymbol{E}}^{n}, (\boldsymbol{\Pi}_{h}^{k}-\boldsymbol{I})\boldsymbol{E}(t_{n})\right) + \left(\eta_{\phi}^{n}-(P_{h}^{k}-I)\phi(t_{n}), \eta_{c^{+}}^{n}-\eta_{c^{-}}^{n}\right) \leq \frac{\delta}{2}\|\boldsymbol{\eta}_{\boldsymbol{E}}^{n}\|^{2} \\ + \frac{1}{2\delta}D_{\infty}^{2}\|(\boldsymbol{\Pi}_{h}^{k}-\boldsymbol{I})\boldsymbol{E}(t_{n})\|^{2} + \delta\|\eta_{\phi}^{n}\|^{2} + \delta\|(P_{h}^{k}-I)\phi(t_{n})\|^{2} + \frac{1}{\delta}\sum_{i\in\{+,-\}}\|\eta_{c^{i}}^{n}\|^{2}$$
(4.3)

with $0 < \delta < 2D_{\alpha}$. Having the estimate (4.3) for $\|\boldsymbol{\eta}_{\boldsymbol{E}}^{n}\|$ at hand, an estimate for $\|\boldsymbol{\eta}_{\phi}^{n}\|$ needs to be derived: according to (P4), we may choose $\boldsymbol{v}_{h} \in \mathbb{RT}_{k}(\mathcal{T}_{h})$ in (4.2a) such that $\boldsymbol{\nabla} \cdot \boldsymbol{v}_{h} = P_{h}^{k} \boldsymbol{\eta}_{\phi}^{n} \in \mathbb{P}_{k}(\mathcal{T}_{h})$:

$$\left(P_h^k\eta_\phi^n\,,\,\eta_\phi^n
ight) \ = \ \left(\boldsymbol{\nabla}\cdot\boldsymbol{v}_h\,,\,\eta_\phi^n
ight) \stackrel{(4.2a)}{=} \left(\boldsymbol{\mathsf{D}}^{-1}\boldsymbol{\eta}_{\boldsymbol{E}}^n\,,\,\boldsymbol{v}_h
ight).$$

With (H1) and $\|\boldsymbol{v}_h\| \leq \|\boldsymbol{v}_h\|_{\boldsymbol{H}^{\operatorname{div}}(\Omega)} \overset{(\mathrm{P4})}{\leq} C_{\Omega} \|P_h^k \eta_{\phi}^n\|$ it follows

$$\begin{aligned} \|\eta_{\phi}^{n}\|^{2} &= \left(\mathbf{D}^{-1}\,\boldsymbol{\eta}_{E}^{n},\,\boldsymbol{v}_{h}\right) + \left(\left(P_{h}^{k}-I\right)\phi(t_{n}),\,\eta_{\phi}^{n}\right) \,\leq\, C_{\Omega}D_{\infty}\|\boldsymbol{\eta}_{E}^{n}\|\,\|P_{h}^{k}\eta_{\phi}^{n}\| + \|(P_{h}^{k}-I)\phi(t_{n})\|\,\|\eta_{\phi}^{n}\| \\ &\leq\, \frac{1}{2\delta'}C_{\Omega}^{2}D_{\infty}^{2}\|\boldsymbol{\eta}_{E}^{n}\|^{2} + \frac{\delta'}{2}\left(\|\eta_{\phi}^{n}\| + \|(P_{h}^{k}-I)\phi(t_{n})\|\right)^{2} + \frac{1}{2\delta''}\|(P_{h}^{k}-I)\phi(t_{n})\|^{2} + \frac{\delta''}{2}\|\eta_{\phi}^{n}\|^{2}, \end{aligned}$$

which is equivalent to

$$\left(1 - \delta' - \frac{\delta''}{2}\right) \|\eta_{\phi}^{n}\|^{2} \leq \frac{1}{2\delta'} C_{\Omega}^{2} D_{\infty}^{2} \|\eta_{E}^{n}\|^{2} + \left(\delta' + \frac{1}{2\delta''}\right) \|(P_{h}^{k} - I)\phi(t_{n})\|^{2}$$

with $1 > \delta' + \delta''/2$, $\delta' > 0$, $\delta'' > 0$. With $\delta' \coloneqq 1/4$ and $\delta'' \coloneqq 1/2$, we obtain

$$\|\eta_{\phi}^{n}\|^{2} \leq 4C_{\Omega}^{2}D_{\infty}^{2}\|\boldsymbol{\eta}_{\boldsymbol{E}}^{n}\|^{2} + \frac{5}{2}\|(P_{h}^{k} - I)\phi(t_{n})\|^{2}.$$

$$(4.4)$$

Substituting (4.4) into (4.3) yields

$$\left(D_{\alpha} - \delta\left(\frac{1}{2} + 4C_{\Omega}^{2}D_{\infty}^{2}\right)\right) \|\boldsymbol{\eta}_{\boldsymbol{E}}^{n}\|^{2} \leq \frac{1}{2\delta}D_{\infty}^{2}\|(\boldsymbol{\Pi}_{h}^{k} - \boldsymbol{I})\boldsymbol{E}(t_{n})\|^{2} + \frac{7}{2}\delta\|(P_{h}^{k} - \boldsymbol{I})\phi(t_{n})\|^{2} + \frac{1}{\delta}\sum_{i\in\{+,-\}}\|\boldsymbol{\eta}_{c^{i}}^{n}\|^{2}$$
(4.5)

with the constraint $0 < \delta < D_{\alpha}/(1/2 + 4C_{\Omega}^2 D_{\infty}^2)$. Fixing δ , inserting the estimate (4.5) into (4.4), summing up the resulting equation with (4.5), and using (P5) ends the proof.

Proposition 4.3. Let $(\boldsymbol{u}, p, \boldsymbol{j}^+, c^+, \boldsymbol{j}^-, c^-, \boldsymbol{E}, \phi)$ and $(\boldsymbol{u}_h^n, p_h^n, \boldsymbol{j}_h^{+,n}, c_h^{+,n}, \boldsymbol{j}_h^{-,n}, c_h^{-,n}, \boldsymbol{E}_h^n, \phi_h^n)$ be solutions of Problem 2.2 and Problem 3.3, respectively. Then, if in addition the regularity requirements of (H7) and (H9) are satisfied, for $q \in \{1, 2\}, n \in \{q, \ldots, N\}$, and sufficiently small τ ,

$$\begin{aligned} \|\eta_{c^{\pm}}^{n}\|^{2} + \tau \sum_{m=q}^{n} \|\boldsymbol{\eta}_{j^{\pm}}^{m}\|^{2} &\lesssim \sum_{j=0}^{q-1} \|\eta_{c^{\pm}}^{j}\|^{2} + \tau^{2q} \|\partial_{t}^{q+1} c^{\pm}\|_{L^{2}(]0,t_{n}[\times\Omega)}^{2} + h^{2l_{3}} \tau \sum_{m=q}^{n} |\boldsymbol{j}^{\pm}(t_{m})|_{\boldsymbol{H}^{l_{3}}(\Omega)}^{2} \\ &+ h^{2l_{4}} \Big(\int_{0}^{t_{n}} |\partial_{s} c^{\pm}(s)|_{\boldsymbol{H}^{l_{4}}(\Omega)}^{2} \, \mathrm{d}s + \tau \sum_{m=q}^{n} |c^{\pm}(t_{m})|_{\boldsymbol{H}^{l_{4}}(\Omega)}^{2} \Big) + \tau \sum_{m=q}^{n} \Big(\|\boldsymbol{\eta}_{\boldsymbol{E}}^{m}\|^{2} + \|\boldsymbol{\eta}_{\boldsymbol{u}}^{m}\|^{2} + \|\boldsymbol{\eta}_{c^{\pm}}^{m}\|^{2} \Big). \end{aligned}$$
(4.6)

In the proof that follows we make use of the following version of discrete Gronwall lemma:

Lemma 4.4 (Discrete Gronwall). Let $(a_k)_{k \in \mathbb{N}}$, $(b_k)_{k \in \mathbb{N}}$ be nonnegative sequences of real numbers, (b_n) nondecreasing, and c be a (fixed) positive constant. If (a_n) satisfies

$$\forall n \in \mathbb{N}, \quad a_n \leq b_n + c \sum_{m=q}^{n-1} a_m, \quad then \quad \forall n \in \mathbb{N}, \quad a_n \leq (1+c)^n b_n.$$

Proof. (See [17], Lem. 2.4).

Note that for n = 1 the sum is zero by definition. We continue with the proof of Proposition 4.3. Some ideas of the proof stem from [29, 30].

Proof of Proposition 4.3. We abbreviate $c^{\pm}(t_n)$ by $c^{\pm,n}$ (and also analogously further quantities) keeping in mind that c^{\pm} is a function existing everywhere in J. Subtraction of (2.3c), (2.3d) from (3.3c), (3.3d) yields the following error equations for $n \in \{q, \ldots, N\}$:

$$-\left(\mathbf{D}^{-1}\boldsymbol{\eta}_{\boldsymbol{j}^{\pm}}^{n},\boldsymbol{v}_{h}\right)+\left(\boldsymbol{\nabla}\cdot\boldsymbol{v}_{h},\boldsymbol{\eta}_{c^{\pm}}^{n}\right)+\left(\mathbf{D}^{-1}\left(\left(\boldsymbol{u}_{h}^{n}\pm\boldsymbol{E}_{h}^{n}\right)\mathcal{M}(\boldsymbol{c}_{h}^{\pm,n})-\left(\boldsymbol{u}^{n}\pm\boldsymbol{E}^{n}\right)\boldsymbol{c}^{\pm,n}\right),\boldsymbol{v}_{h}\right)\ =\ 0,$$
$$\left(\overline{\partial}_{q}\boldsymbol{c}_{h}^{\pm,n}-\partial_{t}\boldsymbol{c}^{\pm,n},\boldsymbol{w}_{h}\right)+\left(\boldsymbol{\nabla}\cdot\boldsymbol{\eta}_{\boldsymbol{j}^{\pm}}^{n},\boldsymbol{w}_{h}\right)\ =\ \left(\boldsymbol{r}^{\pm}(t_{n},\boldsymbol{x},\boldsymbol{c}_{h}^{+,n},\boldsymbol{c}_{h}^{-,n})-\boldsymbol{r}^{\pm}(t_{n},\boldsymbol{x},\boldsymbol{c}^{+,n},\boldsymbol{c}^{-,n}),\boldsymbol{w}_{h}\right)$$

for all $\boldsymbol{v}_h \in \mathbb{RT}_k(\mathcal{T}_h)$ and for all $w_h \in \mathbb{P}_k(\mathcal{T}_h)$. We proceed analogously to the proof of (4.1) in order to eliminate the divergence terms by using the projector properties (P1), (P2), (P3) and choosing $\boldsymbol{v}_h = \boldsymbol{\Pi}_h^k \boldsymbol{\eta}_{j^{\pm}}^n \in \mathbb{RT}_k(\mathcal{T}_h)$ and $w_h = P_h^k \boldsymbol{\eta}_{c^{\pm}}^n \in \mathbb{P}_k(\mathcal{T}_h)$. The resulting equation reads

$$\left(\overline{\partial}_{q}c_{h}^{\pm,n} - \partial_{t}c^{\pm,n}, P_{h}^{k}\eta_{c^{\pm}}^{n}\right) + \left(\mathbf{D}^{-1}\boldsymbol{\eta}_{j^{\pm}}^{n}, \boldsymbol{\Pi}_{h}^{k}\boldsymbol{\eta}_{j^{\pm}}^{n}\right) = \left(\mathbf{D}^{-1}\left((\boldsymbol{u}_{h}^{n} \pm \boldsymbol{E}_{h}^{n})\mathcal{M}(c_{h}^{\pm,n}) - (\boldsymbol{u}^{n} \pm \boldsymbol{E}^{n})c^{\pm,n}\right), \boldsymbol{\Pi}_{h}^{k}\boldsymbol{\eta}_{j^{\pm}}^{n}\right) \\
+ \left(r^{\pm}(t_{n},\boldsymbol{x},c_{h}^{+,n},c_{h}^{-,n}) - r^{\pm}(t_{n},\boldsymbol{x},c^{+,n},c^{-,n}), P_{h}^{k}\boldsymbol{\eta}_{c^{\pm}}^{n}\right). \tag{4.7}$$

Following the idea of [3], we use the projector property (P2) and the fact that $\overline{\partial}_q$ commutes with P_h^k to decompose the first term as follows:

$$\begin{split} \left(\overline{\partial}_{q}c_{h}^{\pm,n} - \partial_{t}c^{\pm,n}, P_{h}^{k}\eta_{c^{\pm}}^{n}\right) &= \left(\overline{\partial}_{q}c_{h}^{\pm,n}, P_{h}^{k}\eta_{c^{\pm}}^{n}\right) - \left(\partial_{t}c^{\pm,n}, P_{h}^{k}\eta_{c^{\pm}}^{n}\right) \\ &= \left(\overline{\partial}_{q}\eta_{c^{\pm}}^{n}, P_{h}^{k}\eta_{c^{\pm}}^{n}\right) + \left(\overline{\partial}_{q}c^{\pm,n}, P_{h}^{k}\eta_{c^{\pm}}^{n}\right) - \left(\partial_{t}c^{\pm,n}, P_{h}^{k}\eta_{c^{\pm}}^{n}\right) \\ &= \left(\overline{\partial}_{q}P_{h}^{k}\eta_{c^{\pm}}^{n}, \eta_{c^{\pm}}^{n}\right) + \left((\overline{\partial}_{q} - \partial_{t})c^{\pm,n}, P_{h}^{k}\eta_{c^{\pm}}^{n}\right) \\ &= \left(\overline{\partial}_{q}\eta_{c^{\pm}}^{n}, \eta_{c^{\pm}}^{n}\right) - \left(\overline{\partial}_{q}(P_{h}^{k} - I)c^{\pm,n}, \eta_{c^{\pm}}^{n}\right) + \left((\overline{\partial}_{q} - \partial_{t})c^{\pm,n}, P_{h}^{k}\eta_{c^{\pm}}^{n}\right). \end{split}$$

With this decomposition, the combined error equation (4.7) becomes

$$\left(\overline{\partial}_{q}\eta_{c^{\pm}}^{n},\eta_{c^{\pm}}^{n}\right) + D_{\alpha}\|\boldsymbol{\eta}_{j^{\pm}}^{n}\|^{2} \leq \left(\overline{\partial}_{q}(P_{h}^{k}-I)c^{\pm,n},\eta_{c^{\pm}}^{n}\right) - \left((\overline{\partial}_{q}-\partial_{t})c^{\pm,n},P_{h}^{k}\eta_{c^{\pm}}^{n}\right) \\
+ \left(\mathbf{D}^{-1}\boldsymbol{\eta}_{j^{\pm}}^{n},(\boldsymbol{\Pi}_{h}^{k}-I)\boldsymbol{j}^{\pm,n}\right) + \left(\mathbf{D}^{-1}\left((\boldsymbol{u}_{h}^{n}\pm\boldsymbol{E}_{h}^{n})\mathcal{M}(c_{h}^{\pm,n}) - (\boldsymbol{u}^{n}\pm\boldsymbol{E}^{n})c^{\pm,n}\right),\boldsymbol{\Pi}_{h}^{k}\boldsymbol{\eta}_{j^{\pm}}^{n}\right) \\
+ \left(r^{\pm}(t_{n},\boldsymbol{x},c_{h}^{+,n},c_{h}^{-,n}) - r^{\pm}(t_{n},\boldsymbol{x},c^{+,n},c^{-,n}),P_{h}^{k}\eta_{c^{\pm}}^{n}\right),$$
(4.8)

where the ellipticity of \mathbf{D}^{-1} according to (H1) was used. Next up, consider the term $(\overline{\partial}_q \eta_{c^{\pm}}^n, \eta_{c^{\pm}}^n)$. The following identities are required [7]:

$$2(a-b)a = a^2 - b^2 + (a-b)^2, (4.9a)$$

$$2(3a - 4b + c)a = a^{2} - b^{2} + (2a - b)^{2} - (2b - c)^{2} + (a - 2b + c)^{2}.$$
(4.9b)

Using the definition of $\overline{\partial}_q$, we see that if we replace n by m, for the sum from q to n multiplied by $2q\tau$, there holds

$$2q\tau \sum_{m=q}^{n} \left(\overline{\partial}_{q} \eta_{c^{\pm}}^{m}, \eta_{c^{\pm}}^{m}\right) = 2\sum_{m=q}^{n} \left\{ \begin{pmatrix} \eta_{c^{\pm}}^{m} - \eta_{c^{\pm}}^{m-1}, \eta_{c^{\pm}}^{m} \end{pmatrix}, \begin{array}{l} q=1 \\ \left(3\eta_{c^{\pm}}^{m} - 4\eta_{c^{\pm}}^{m-1} + \eta_{c^{\pm}}^{m-2}, \eta_{c^{\pm}}^{m} \end{pmatrix}, \begin{array}{l} q=2 \\ \end{pmatrix} \right\}$$

$$\stackrel{(4.9)}{\geq} \|\eta_{c^{\pm}}^{n}\|^{2} - \left\{ \frac{\|\eta_{c^{\pm}}^{0}\|^{2}}{\|\eta_{c^{\pm}}^{1}\|^{2} + \|2\eta_{c^{\pm}}^{1} - \eta_{c^{\pm}}^{0}\|^{2}}, \begin{array}{l} q=1 \\ q=2 \\ \end{pmatrix} \right\}$$

Multiplication of (4.8) by $2q\tau$, replacing n by m, summing up from q to n, and using the latter result yields

$$\begin{aligned} \|\eta_{c^{\pm}}^{n}\|^{2} + 2D_{\alpha}q\tau \sum_{m=q}^{n} \|\eta_{j^{\pm}}^{m}\|^{2} &\leq \begin{cases} \|\eta_{c^{\pm}}^{n}\|^{2} + \|2\eta_{c^{\pm}}^{n} - \eta_{c^{\pm}}^{0}\|^{2}, \ q=2 \end{cases} + 2q\tau \sum_{m=q}^{n} \left(\overline{\partial}_{q}(P_{h}^{k} - I)c^{\pm,m}, \eta_{c^{\pm}}^{m}\right) \\ &- 2q\tau \sum_{m=q}^{n} \left((\overline{\partial}_{q} - \partial_{t})c^{\pm,m}, P_{h}^{k}\eta_{c^{\pm}}^{m}\right) + 2q\tau \sum_{m=q}^{n} \left(\mathbf{D}^{-1}\eta_{j^{\pm}}^{m}, (\boldsymbol{\Pi}_{h}^{k} - \boldsymbol{I})\boldsymbol{j}^{\pm,m}\right) \\ &+ 2q\tau \sum_{m=q}^{n} \left(\mathbf{D}^{-1}\left((\boldsymbol{u}_{h}^{m} \pm \boldsymbol{E}_{h}^{m})\mathcal{M}(c_{h}^{\pm,m}) - (\boldsymbol{u}^{m} \pm \boldsymbol{E}^{m})c^{\pm,m}\right), \ \boldsymbol{\Pi}_{h}^{k}\eta_{j^{\pm}}^{m}\right) \\ &+ 2q\tau \sum_{m=q}^{n} \left(r^{\pm}(t_{m}, \boldsymbol{x}, c_{h}^{+,m}, c_{h}^{-,m}) - r^{\pm}(t_{m}, \boldsymbol{x}, c^{+,m}, c^{-,m}), P_{h}^{k}\eta_{c^{\pm}}^{m}\right). \end{aligned}$$

We denote the terms on the right side of (4.10) by I to VI and estimate II to VI in terms of time truncation and projection errors. Consider a function $v \in L^2(J \times \Omega)$. By application of the fundamental theorem of calculus and of the Jensen inequality, we have for q = 1:

$$\tau \sum_{m=1}^{n} \|\overline{\partial}_{1}v^{m}\|^{2} = \tau \sum_{m=1}^{n} \left\| \frac{1}{\tau} \int_{t_{m-1}}^{t_{m}} \partial_{s}v(s) \,\mathrm{d}s \right\|^{2} \le \sum_{m=1}^{n} \int_{t_{m-1}}^{t_{m}} \|\partial_{s}v(s)\|^{2} \,\mathrm{d}s = \|\partial_{t}v\|_{L^{2}(]0,t_{n}[\times\Omega)}^{2}.$$

Recalling (3.1), we get for q = 2:

$$\tau \sum_{m=2}^{n} \|\overline{\partial}_{2}v^{m}\|^{2} \leq \sum_{m=2}^{n} \left(3\int_{t_{m-1}}^{t_{m}} \|\partial_{s}v(s)\|^{2} \,\mathrm{d}s + \int_{t_{m-2}}^{t_{m-1}} \|\partial_{s}v(s)\|^{2} \,\mathrm{d}s \right) \leq 4 \|\partial_{t}v\|_{L^{2}(]0,t_{n}[\times\Omega)}^{2},$$

i.e., $\tau \sum_{m=q}^{n} \|\overline{\partial}_{q} v^{m}\|^{2} \leq q^{2} \|\partial_{t} v\|_{L^{2}(]0,t_{n}[\times\Omega)}^{2}$. With this and the fact that P_{h}^{k} commutes with the time derivative we conclude

$$II \leq \delta_2 q \tau \sum_{m=q}^n \|\eta_{c^{\pm}}^m\|^2 + \frac{q^3}{\delta_2} \|(P_h^k - I) \,\partial_t c^{\pm}\|_{L^2(]0, t_n[\times \Omega)}^2.$$

For the third term we have

$$|III| \leq \delta_3 q \tau \sum_{m=q}^n \|P_h^k \eta_{c^{\pm}}^m\|^2 + \frac{q}{\delta_3} \tau \sum_{m=q}^n \|(\overline{\partial}_q - \partial_t) c^{\pm,m}\|^2.$$

By Taylor expansion around t_{m-q} , the truncation error on the right can be expressed by the truncation error of the corresponding integral remainder ([37], *cf.*, p. 169):

$$\begin{aligned} \tau \sum_{m=q}^{n} \|(\overline{\partial}_{q} - \partial_{t})c^{\pm,m}\|^{2} &= \tau \sum_{m=q}^{n} \left\| (\overline{\partial}_{q} - \partial_{t}) \frac{1}{q!} \int_{t_{m-q}}^{t} (t-s)^{q} \partial_{s}^{q+1} c^{\pm}(s) \, \mathrm{d}s \, \right\|_{t=t_{m}}^{2} \\ &\lesssim \frac{1}{\tau} \sum_{m=q}^{n} \sum_{j=m-q}^{m} \left\| \int_{t_{j-q}}^{t_{j}} (t_{j} - s)^{q} \partial_{s}^{q+1} c^{\pm}(s) \, \mathrm{d}s \right\|^{2} + \tau \sum_{m=q}^{n} \left\| \int_{t_{m-q}}^{t_{m}} q(t_{m} - s)^{q-1} \partial_{s}^{q+1} c^{\pm}(s) \, \mathrm{d}s \right\|^{2} \\ &\lesssim \tau^{2q-1} \sum_{m=q}^{n} \left\| \int_{t_{m-q}}^{t_{m}} \partial_{s}^{q+1} c^{\pm}(s) \, \mathrm{d}s \right\|^{2} \lesssim \tau^{2q} \|\partial_{t}^{q+1} c^{\pm}\|_{L^{2}(]0,t_{n}[\times\Omega)}^{2}, \end{aligned}$$

where we used the fact that $\|\overline{\partial}_q v^m\| \leq \frac{q}{\tau} \sum_{j=m-q}^m \|v^j\|$, the Leibniz integral rule, and the Jensen inequality. We eventually obtain

$$|III| \leq \delta_3 2q\tau \sum_{m=q}^n \|\eta_{c^{\pm}}^m\|^2 + \delta_3 2q\tau \sum_{m=q}^n \|(P_h^k - I)c^{\pm,m}\|^2 + \frac{q}{\delta_3}\tau^{2q} \|\partial_t^{q+1}c^{\pm}\|_{L^2(]0,t_n[\times\Omega)}^2$$

For the fourth term, we immediately get

$$IV \leq \delta_4 D_{\infty} q \tau \sum_{m=q}^n \|\boldsymbol{\eta}_{\boldsymbol{j}^{\pm}}^m\|^2 + \frac{q}{\delta_4} D_{\infty} \tau \sum_{m=q}^n \|(\boldsymbol{\Pi}_h^k - \boldsymbol{I}) \boldsymbol{j}^{\pm,m}\|^2$$

due to (H1). We continue estimating the term V. We derive the following estimate using (H1), the boundedness of u^m and E^m in $L^{\infty}(\Omega)$ due to (H8) and (H10), and Lemma 3.2:

$$\| \mathbf{D}^{-1} ((\boldsymbol{u}_{h}^{m} \pm \boldsymbol{E}_{h}^{m}) \mathcal{M}(c_{h}^{\pm,m}) - (\boldsymbol{u}^{m} \pm \boldsymbol{E}^{m}) c^{\pm,m}) \| \leq D_{\infty} (\| (\boldsymbol{\eta}_{\boldsymbol{u}}^{m} \pm \boldsymbol{\eta}_{\boldsymbol{E}}^{m}) \mathcal{M}(c_{h}^{\pm,m}) \| \\ + \| (\boldsymbol{u}^{m} \pm \boldsymbol{E}^{m}) (\mathcal{M}(c_{h}^{\pm,m}) - \mathcal{M}(c^{\pm,m})) \|) \leq D_{\infty} (M (\| \boldsymbol{\eta}_{\boldsymbol{u}}^{m} \| + \| \boldsymbol{\eta}_{\boldsymbol{E}}^{m} \|) + C_{5} \| \boldsymbol{\eta}_{c^{\pm}}^{m} \|)$$

with $C_5 := \| \boldsymbol{u}^m \pm \boldsymbol{E}^m \|_{\boldsymbol{L}^{\infty}(\Omega)}$. The above estimate yields the estimate for the fifth term:

$$V \le 2qD_{\infty} \tau \sum_{m=q}^{n} \left(\delta_{5} \left(\|\boldsymbol{\eta}_{\boldsymbol{j}^{\pm}}^{m}\|^{2} + \|(\boldsymbol{\Pi}_{h}^{k} - \boldsymbol{I})\boldsymbol{j}^{\pm,m}\|^{2} \right) + \frac{1}{\delta_{5}} \left(2M^{2} \left(\|\boldsymbol{\eta}_{\boldsymbol{u}}^{m}\|^{2} + \|\boldsymbol{\eta}_{\boldsymbol{E}}^{m}\|^{2} \right) + C_{5}^{2} \|\boldsymbol{\eta}_{c^{\pm}}^{m}\|^{2} \right) \right).$$

Lastly, we estimate the sixth term VI. Due to (H3) the inequality

$$\|r^{\pm}(t_m, \boldsymbol{x}, c_h^{+,m}, c_h^{-,m}) - r^{\pm}(t_m, \boldsymbol{x}, c^{+,m}, c^{-,m})\| \leq r_{\mathrm{L}} \left\| \begin{pmatrix} c_h^{+,m} \\ c_h^{-,m} \end{pmatrix} - \begin{pmatrix} c^{+,m} \\ c^{-,m} \end{pmatrix} \right\| \leq r_{\mathrm{L}} \|\eta_{c^+}^m\| + r_{\mathrm{L}} \|\eta_{c^-}^m\|$$

holds, where $r_{\rm L}$ denotes the Lipschitz constant. Hence,

$$VI \leq \left(\frac{1}{\delta_6} + \delta_6\right) 2qr_{\rm L} \,\tau \sum_{m=q}^n \|\eta_{c^{\pm}}^m\|^2 + \delta_6 2qr_{\rm L} \,\tau \sum_{m=q}^n \|\eta_{c^{\mp}}^m\|^2 + \frac{1}{\delta_6} 2qr_{\rm L} \,\tau \sum_{m=q}^n \|(P_h^k - I)c^{\pm,m}\|^2.$$

With the estimates of II to VI, it follows from (4.10) that

$$\begin{split} \|\eta_{c^{\pm}}^{n}\|^{2} + 2q \Big(D_{\alpha} - \frac{\delta_{4}}{2} D_{\infty} - \delta_{5} D_{\infty} \Big) \tau \sum_{m=q}^{n} \|\eta_{j^{\pm}}^{m}\|^{2} &\leq \begin{cases} \|\eta_{c^{\pm}}^{0}\|^{2}, q=1\\ 2\|\eta_{c^{\pm}}^{0}\|^{2}, q=2 \end{cases} \\ &+ \frac{q^{3}}{\delta_{2}} \|(P_{h}^{k} - I) \partial_{t} c^{\pm}\|_{L^{2}(]0,t_{n}[\times\Omega)}^{2} + \frac{q}{\delta_{3}} \tau^{2q} \|\partial_{t}^{q+1} c^{\pm}\|_{L^{2}(]0,t_{n}[\times\Omega)}^{2} \\ &+ 2q \left(\frac{\delta_{2}}{2} + \delta_{3} + \frac{C_{5}^{2}}{\delta_{5}} D_{\infty} + \left(\delta_{6} + \frac{1}{\delta_{6}}\right) r_{L}\right) \tau \sum_{m=q}^{n} \|\eta_{c^{\pm}}^{m}\|^{2} \\ &+ 2q D_{\infty} \left(\frac{1}{2\delta_{4}} + \delta_{5}\right) \tau \sum_{m=q}^{n} \|(\Pi_{h}^{k} - I)j^{\pm,m}\|^{2} + 2q \left(\delta_{3} + \frac{r_{L}}{\delta_{6}}\right) \tau \sum_{m=q}^{n} \|(P_{h}^{k} - I)c^{\pm,m}\|^{2} \\ &+ \frac{4q}{\delta_{5}} D_{\infty} M^{2} \tau \sum_{m=q}^{n} \|\eta_{E}^{m}\|^{2} + \frac{4q}{\delta_{5}} D_{\infty} M^{2} \tau \sum_{m=q}^{n} \|\eta_{u}^{m}\|^{2} + \delta_{6} 2qr_{L} \tau \sum_{m=q}^{n} \|\eta_{c^{\mp}}^{m}\|^{2} \end{split}$$

with the constraint that $\delta_4, \delta_5 > 0$ have to be chosen small enough. The discretization error in c^{\pm} at time level t_n on the right side can be absorbed for sufficiently small τ . In doing so, application of the discrete Gronwall lemma yields

$$\begin{aligned} \|\eta_{c^{\pm}}^{n}\|^{2} + \tau \sum_{m=q}^{n} \|\eta_{j^{\pm}}^{m}\|^{2} &\lesssim \sum_{j=0}^{q-1} \|\eta_{c^{\pm}}^{j}\|^{2} + \tau^{2q} \|\partial_{t}^{q+1} c^{\pm}\|_{L^{2}(]0,t_{n}[\times\Omega)}^{2} + \|(P_{h}^{k} - I) \partial_{t} c^{\pm}\|_{L^{2}(]0,t_{n}[\times\Omega)}^{2} \\ &+ \tau \sum_{m=q}^{n} \|(\Pi_{h}^{k} - I)j^{\pm,m}\|^{2} + \tau \sum_{m=q}^{n} \|(P_{h}^{k} - I)c^{\pm,m}\|^{2} + \tau \sum_{m=q}^{n} \|\eta_{E}^{m}\|^{2} + \tau \sum_{m=q}^{n} \|\eta_{u}^{m}\|^{2} + \tau \sum_{m=q}^{n} \|\eta_{c^{\pm}}^{m}\|^{2}. \end{aligned}$$

Conclude by accounting for the initial conditions (1.1j) and by using the projection error estimates of (P5).

Proposition 4.5. Let $(\boldsymbol{u}, p, \boldsymbol{j}^+, c^+, \boldsymbol{j}^-, c^-, \boldsymbol{E}, \phi)$ and $(\boldsymbol{u}_h^n, p_h^n, \boldsymbol{j}_h^{+,n}, c_h^{+,n}, \boldsymbol{j}_h^{-,n}, c_h^{-,n}, \boldsymbol{E}_h^n, \phi_h^n)$ be solutions of Problem 2.2 and Problem 3.3, respectively. Then, if in addition the regularity requirements of (H7), (H8), and (H10) are satisfied, for $n \in \{q, \ldots, N\}$,

$$\|\boldsymbol{\eta}_{\boldsymbol{u}}^{n}\|^{2} + \|\boldsymbol{\eta}_{p}^{n}\|^{2} \lesssim h^{2l_{1}} |\boldsymbol{u}(t_{n})|_{\boldsymbol{H}^{l_{1}}(\Omega)}^{2} + h^{2l_{2}} |p(t_{n})|_{H^{l_{2}}(\Omega)}^{2} + h^{2l_{5}} |\boldsymbol{E}(t_{n})|_{\boldsymbol{H}^{l_{5}}(\Omega)}^{2} + h^{2l_{6}} |\phi(t_{n})|_{H^{l_{6}}(\Omega)}^{2} + \sum_{i \in \{+,-\}} \|\boldsymbol{\eta}_{c^{i}}^{n}\|^{2}.$$

$$(4.11)$$

Proof. The proof can be accomplished analogously to that of Proposition 4.2 with minor modifications. We suppress the time index n and the argument for the evaluation at t_n in this proof. Due to (2.3a), (2.3b), (3.3a), (3.3b), the error equations read

$$-\left(\mathbf{K}^{-1}\boldsymbol{\eta}_{\boldsymbol{u}},\,\boldsymbol{v}_{h}\right)+\left(\boldsymbol{\nabla}\cdot\boldsymbol{v}_{h},\,\boldsymbol{\eta}_{p}\right)\ =\ -\left(\mathbf{D}^{-1}\left(\boldsymbol{E}_{h}\mathcal{M}(\boldsymbol{c}_{h}^{+}-\boldsymbol{c}_{h}^{-})-\boldsymbol{E}(\boldsymbol{c}^{+}-\boldsymbol{c}^{-})\right),\,\boldsymbol{v}_{h}\right),\tag{4.12a}$$

$$(\boldsymbol{\nabla} \cdot \boldsymbol{\eta}_{\boldsymbol{u}}, w_h) = 0 \tag{4.12b}$$

for all $v_h \in \mathbb{RT}_k(\mathcal{T}_h)$ and for all $w_h \in \mathbb{P}_k(\mathcal{T}_h)$. The arising force term in (4.12a) requires a special treatment. Recalling the chosen cut-off level M for the cut-off operator \mathcal{M} (cf. Proposition 3.3), Lemma 3.2, and (H10), we see that

$$\|\boldsymbol{E}_{h}\mathcal{M}(c_{h}^{+}-c_{h}^{-})-\boldsymbol{E}(c^{+}-c^{-})\| \leq M \|\boldsymbol{\eta}_{\boldsymbol{E}}\| + \|\boldsymbol{E}\|_{\boldsymbol{L}^{\infty}(\Omega)} \sum_{i \in \{+,-\}} \|\boldsymbol{\eta}_{c^{i}}\|.$$
(4.13)

The choice of $w_h = P_h^k \eta_p \in \mathbb{P}_k(\mathcal{T}_h)$ in (4.12b) and the use of the projector property (P3) yields

$$\left(\boldsymbol{\nabla}\cdot\boldsymbol{\Pi}_{h}^{k}\boldsymbol{\eta}_{\boldsymbol{u}}, P_{h}^{k}\boldsymbol{\eta}_{p}\right) = 0.$$

$$(4.14)$$

Choosing the test function $v_h = \Pi_h^k \eta_u \in \mathbb{RT}_k(\mathcal{T}_h)$ in (4.12a), using (P1), (P2), and (4.14), we obtain

$$\left(\mathbf{K}^{-1}\boldsymbol{\eta}_{\boldsymbol{u}},\,\boldsymbol{\Pi}_{h}^{k}\boldsymbol{\eta}_{\boldsymbol{u}}\right) = \left(\mathbf{D}^{-1}\left(\boldsymbol{E}_{h}\mathcal{M}(\boldsymbol{c}_{h}^{+}-\boldsymbol{c}_{h}^{-})-\boldsymbol{E}(\boldsymbol{c}^{+}-\boldsymbol{c}^{-})\right),\,\boldsymbol{\Pi}_{h}^{k}\boldsymbol{\eta}_{\boldsymbol{u}}\right).$$

With (H1), (H2), (4.13), we arrive at the estimate

$$K_{\alpha} \|\boldsymbol{\eta}_{\boldsymbol{u}}\|^{2} \leq K_{\infty} \|\boldsymbol{\eta}_{\boldsymbol{u}}\| \|(\boldsymbol{\Pi}_{h}^{k} - \boldsymbol{I})\boldsymbol{u}\| + D_{\infty} \Big(M \|\boldsymbol{\eta}_{\boldsymbol{E}}\| + \|\boldsymbol{E}\|_{\boldsymbol{L}^{\infty}(\Omega)} \sum_{i \in \{+, -\}} \|\boldsymbol{\eta}_{c^{i}}\| \Big) \Big(\|\boldsymbol{\eta}_{\boldsymbol{u}}\| + \|(\boldsymbol{\Pi}_{h}^{k} - \boldsymbol{I})\boldsymbol{u}\| \Big).$$

Equation (4.1) and the projection error estimates of (P5) yield

$$\|\boldsymbol{\eta}_{\boldsymbol{u}}^{n}\|^{2} \lesssim h^{2l_{1}} |\boldsymbol{u}(t_{n})|^{2}_{\boldsymbol{H}^{l_{1}}(\Omega)} + h^{2l_{5}} |\boldsymbol{E}(t_{n})|^{2}_{\boldsymbol{H}^{l_{5}}(\Omega)} + h^{2l_{6}} |\phi(t_{n})|^{2}_{\boldsymbol{H}^{l_{6}}(\Omega)} + \sum_{i \in \{+,-\}} \|\boldsymbol{\eta}_{c^{i}}^{n}\|^{2}.$$

With a similar treatment of the additional force term, the error estimate for $\|\eta_p^n\|$ is obtained analogously to the second part of the proof of Proposition 4.2.

Theorem 4.6 (A priori error estimate). Let $(\boldsymbol{u}, p, \boldsymbol{j}^+, c^+, \boldsymbol{j}^-, c^-, \boldsymbol{E}, \phi)$ and $(\boldsymbol{u}_h^n, p_h^n, \boldsymbol{j}_h^{+,n}, c_h^{+,n}, \boldsymbol{j}_h^{-,n}, c_h^{-,n}, \boldsymbol{E}_h^n, \phi_h^n)$ be solutions of Problem 2.2 and Problem 3.3, respectively. Then, if in addition the regularity requirements of (H7)–(H10) are satisfied, for $q \in \{1, 2\}$ and sufficiently small τ ,

$$\max_{m \in \{q,...,N\}} \|\boldsymbol{\eta}_{\boldsymbol{u}}^{m}\|^{2} + \max_{m \in \{q,...,N\}} \|\boldsymbol{\eta}_{p}^{m}\|^{2} + \sum_{i \in \{+,-\}} \tau \sum_{m=q}^{N} \|\boldsymbol{\eta}_{j^{i}}^{m}\|^{2} + \sum_{i \in \{+,-\}} \max_{m \in \{q,...,N\}} \|\boldsymbol{\eta}_{c^{i}}^{m}\|^{2} + \max_{m \in \{q,...,N\}} \|\boldsymbol{\eta}_{p}^{m}\|^{2} \lesssim \sum_{i \in \{+,-\}} \sum_{j=0}^{q-1} \|\boldsymbol{\eta}_{c^{i}}^{j}\|^{2} + \tau^{2q} + \sum_{i \in \{1,...,6\}} h^{2l_{i}}.$$

Proof. We sum up (4.6) for both signs, eliminate the discretization errors of c^{\pm} on the right-hand side as performed at the end of the proof of Proposition 4.3 to obtain

$$\sum_{i \in \{+,-\}} \|\eta_{c^{i}}^{n}\|^{2} + \sum_{i \in \{+,-\}} \tau \sum_{m=q}^{n} \|\eta_{j^{i}}^{m}\|^{2} \lesssim \sum_{i \in \{+,-\}} \sum_{j=0}^{q-1} \|\eta_{c^{i}}^{j}\|^{2} + \tau^{2q} \sum_{i \in \{+,-\}} \|\partial_{t}^{q+1}c^{i}\|_{L^{2}(]0,t_{n}[\times\Omega)}^{2} + h^{2l_{3}} \sum_{i \in \{+,-\}} \tau \sum_{m=q}^{n} |j^{i}(t_{m})|_{H^{l_{3}}(\Omega)}^{2} + h^{2l_{4}} \sum_{i \in \{+,-\}} \left(\int_{0}^{t_{n}} |\partial_{s}c^{i}(s)|_{H^{l_{4}}(\Omega)}^{2} \, \mathrm{d}s + \tau \sum_{m=q}^{n} |c^{i}(t_{m})|_{H^{l_{4}}(\Omega)}^{2} \right) \\ + \sum_{i \in \{+,-\}} \tau \sum_{m=q}^{n} \left(\|\eta_{E}^{m}\|^{2} + \|\eta_{u}^{m}\|^{2} \right). \quad (4.15)$$

Substitution of $\sum_{i \in \{+,-\}} \|\eta_{c^i}^n\|^2$ from (4.15) into (4.1), (4.11) and summation yields

$$\begin{aligned} \|\boldsymbol{\eta}_{\boldsymbol{u}}^{n}\|^{2} + \|\boldsymbol{\eta}_{p}^{n}\|^{2} + \|\boldsymbol{\eta}_{\phi}^{n}\|^{2} &\lesssim \sum_{i \in \{+,-\}} \sum_{j=0}^{q-1} \|\boldsymbol{\eta}_{c^{i}}^{j}\|^{2} + \tau^{2q} \sum_{i \in \{+,-\}} \|\boldsymbol{\partial}_{t}^{q+1}c^{i}\|_{L^{2}(]0,t_{n}[\times\Omega)}^{2} + h^{2l_{1}} |\boldsymbol{u}(t_{n})|_{\boldsymbol{H}^{l_{1}}(\Omega)}^{2} \\ &+ h^{2l_{2}} |\boldsymbol{p}(t_{n})|_{\boldsymbol{H}^{l_{2}}(\Omega)}^{2} + h^{2l_{3}} \sum_{i \in \{+,-\}} \tau \sum_{m=q}^{n} |\boldsymbol{j}^{i}(t_{m})|_{\boldsymbol{H}^{l_{3}}(\Omega)}^{2} \\ &+ h^{2l_{4}} \sum_{i \in \{+,-\}} \left(\int_{0}^{t_{n}} |\boldsymbol{\partial}_{s}c^{i}(s)|_{\boldsymbol{H}^{l_{4}}(\Omega)}^{2} \, \mathrm{d}s + \tau \sum_{m=q}^{n} |c^{i}(t_{m})|_{\boldsymbol{H}^{l_{4}}(\Omega)}^{2} \right) \\ &+ h^{2l_{5}} |\boldsymbol{E}(t_{n})|_{\boldsymbol{H}^{l_{5}}(\Omega)}^{2} + h^{2l_{6}} |\boldsymbol{\phi}(t_{n})|_{\boldsymbol{H}^{l_{6}}(\Omega)}^{2} + \tau \sum_{m=q}^{n} \|\boldsymbol{\eta}_{u}^{m}\|^{2} + \tau \sum_{m=q}^{n} \|\boldsymbol{\eta}_{E}^{m}\|^{2}. \end{aligned}$$

$$(4.16)$$

Adding (4.15) to (4.16) and eliminating the discretization errors of u and E on the right-hand side bounds the discretization errors in terms of the solution. We conclude by bounding the right-hand side by the respective maximum on J (admissible due to (H8)–(H10)) yielding a right-hand side that is independent of n such that the estimate holds for every $n \in \{q, \ldots, N\}$.

Loosely speaking, Theorem 4.6 states that if Raviart–Thomas elements of kth order and BDFq are used then the $L^2(\Omega)$ discretization error of each of the eight partial solutions is of order $O(\tau^q + h^{k+1})$ when the regularity requirements are met.

5. Numerical results

The numerical scheme of Section 3 for the lowest-order Raviart–Thomas elements was implemented using the software platform / programming language MATLAB [38]. This section compares numerically estimated orders of convergence with the respective ones revealed by the presented analysis for the case of BDF1 and BDF2, and lowest Raviart–Thomas elements, *i.e.*, q = 1, 2, k = 0. The cut-off operator used to define Problem 3.3 is an analytical tool. The implementation uses an iterative operator splitting approach analogously to [16, Alg. 1]. Implementation details are found in [15].

Consider the time-space cylinder $J \times \Omega :=]0, T[\times]0, 1[^2$ with T := 0.1. In order to be able to use the method of manufactured solutions, we consider system (1.1) with $c^{\pm} = c_{\rm D}^{\pm}$ instead of (1.1h). We choose **D** and **K** equal to the unit matrix and

$$r^{+} \coloneqq -e^{-t} \sinh x \sin y \left(xe^{-2t} - e^{-t} \cos x \cosh y \right) - e^{-t} \cosh x \cos y \left(ye^{-2t} + e^{-t} \sin x \sinh y \right) - c^{+},$$

$$r^{-} \coloneqq -e^{-t} \cosh x \cos y \left(xe^{-2t} + e^{-t} \cos x \cosh y \right) + e^{-t} \sinh x \sin y \left(ye^{-2t} - e^{-t} \sin x \sinh y \right) - c^{-},$$

where $(x, y)^{\mathrm{T}} = \boldsymbol{x} \in \Omega$. We prescribe a solution by

$$u := \exp(-2t) (y, x)^{\mathrm{T}}, \quad p := \exp(-2t) \sin(x) \cosh(y), \quad \phi := \mathrm{e}^{-t} \cos(x) \sinh(y), \\ c^+ := \mathrm{e}^{-t} \sinh(x) \cos(y), \quad c^- := \mathrm{e}^{-t} \cosh(x) \sin(y)$$

and fluxes j^{\pm} , E such that (1.1c) and (1.1e) hold. In order to obtain a unique pressure p, we additionally demand that $\int_{\Omega} p_h^n = \int_{\Omega} p(t_n)$ is satisfied for each time level. The equations (1.1b) and (1.1d) hold by definition and (1.1a), (1.1f) are balanced by additional source/sink functions on the right-hand sides. The initial and boundary data are determined by the manufactured solution.

We start a refinement sequence with a time step size of $\tau = T = 0.1$ using a triangulation with h = 1/2, while halving τ and dividing h by four in each refinement level, since the $L^2(\Omega)$ discretization error of each

i	$\ {m \eta}_u\ $	$\ \eta_p\ $	$\ \boldsymbol{\eta}_{\boldsymbol{j}^+}\ $	$\ \eta_{c^+}\ $	$\ {oldsymbol \eta}_{j^-} \ $	$\ \eta_{c^-}\ $	$\ {m \eta}_E\ $	$\ \eta_{\phi}\ $
0	$3.34E{-1}$	$1.82E{-1}$	$3.83E{-1}$	2.43E-1	$7.50E{-1}$	2.01E-1	$3.36E{-1}$	2.43E-1
1	1.04E-1	4.63E-2	1.11E-1	6.25E-2	$1.86E{-1}$	5.04E-2	8.69E-2	6.25E-2
2	2.22E-2	1.14E-2	2.82E-2	1.57E-2	4.93E-2	1.26E-2	2.27E-2	1.56E-2
3	5.30E-3	2.84E - 3	7.07E-3	3.91E - 3	1.24E-2	3.14E-3	5.70E - 3	3.91E - 3
4	1.31E-3	7.11E-4	1.78E-3	9.79E-4	$3.10E{-3}$	7.88E-4	1.42E-3	9.78E-4
0-1	1.69	1.97	1.78	1.96	2.01	1.99	1.95	1.96
1 - 2	2.22	2.02	1.98	2.00	1.91	2.00	1.94	2.00
2 - 3	2.07	2.00	2.00	2.00	2.00	2.00	1.99	2.00
3-4	2.02	2.00	1.99	2.00	2.00	2.00	2.00	2.00

TABLE 1. Discretization errors at end time T = 0.1 measured in $L^2(\Omega)$ (top list) and corresponding reduction ratios (bottom list). For the *i*th refinement level we have $h = (1/2)(1/4)^i$, $\tau = T(1/2)^i$.

of the partial solutions $\boldsymbol{u}, p, \boldsymbol{j}^{\pm}, c^{\pm}, \boldsymbol{E}, \phi$ is expected to be of order $O(\tau^2 + h)$. Hence, this convergence order is considered confirmed if we observe an overall quadratic decrease of errors. We successively compute the $L^2(\Omega)$ discretization errors at the end time T for the partial solutions. For the first step, BDF1, *i.e.* the implicit Euler method, is used. As predicted by Theorem 4.6, we obtain a reduction factor of two, which means that we have a linear order of convergence in space and a second order of convergence in time in each partial unknown, cf. Table 1. This would also hold true if the chosen setting was dominated by the spatial error for all evaluated time points. However, this is not the case here: using BDF1, the reduction factor drops to of one for the overall discretization error.

6. CONCLUSION

This paper focuses on the *a priori* error analysis of a mixed finite element scheme for the DNPP system, which is a homogenized version of a nonlinear Stokes–Nernst–Planck–Poisson-type system. The latter describes the dynamics of dilute electrolytes and of dissolved charged particles at a small scale. The interest in the homogenized versions is to obtain an equivalent system valid on a larger scale that can be used to extrapolate from macroscopic to microscopic processes or vice versa. The discrete model uses Raviart–Thomas elements of fixed order in space and up to second order backward difference time-stepping formula (BDF2).

A mixed weak formulation of the DNPP system is presented and it is proven that its solution satisfies another weak formulation whose well-posedness has already been established. Essential boundedness of the concentrations are shown thereby allowing the usage of a cut-off operator, which is used to define the discrete scheme. The main result is the *a priori* error estimate stating that the discretization error is second order in time for BDF2 and first order in time for BDF1, and optimal in space.

To validate this result, a numerical experiment is presented using lowest order Raviart–Thomas elements and BDF2, which is initialized with one BDF1 step. The computed orders of convergence match with the *a priori* result: second order in time and first order in space is obtained.

The mixed approach of the DNPP system is attractive for practical simulations, as, on the one hand, it ensures local mass conservation (in particular of the solutes' concentrations, which are the quantities of interest). On the other hand, every subproblem can be discretized using the same pair of mixed finite element space.

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