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This article 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 a 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 $L^\infty$ 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 copes without semi-discrete intermediate formulations and reveals convergence rates of optimal orders in time and space. Numerical simulations verify the theoretical results for lowest order finite element spaces in two dimensions.

Keywords  Stokes/Darcy–Nernst–Planck–Poisson system · mixed finite elements · backward difference formula · error analysis · porous media
MSC (2010)  65M12 · 65M15 · 65M60 · 65L06 · 76Rxx · 76Wxx

1 Mathematical Model

Let $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$ be a polygonally bounded convex domain with boundary $\partial \Omega$, let $\nu$ denote the outward unit normal, and let $J := ]0, T[$ be a time interval, where $T > 0$ denoting the end time. We consider the system

\[
\begin{align*}
\mathbf{u} &= -K \nabla p + KD^{-1}E(c^+ - c^-) \quad \text{in } J \times \Omega, \quad (1a) \\
\nabla \cdot \mathbf{u} &= 0 \quad \text{in } J \times \Omega, \quad (1b) \\
\mathbf{j}^+ &= -D \nabla c^\pm + uc^\pm \pm Ec^\pm \quad \text{in } J \times \Omega, \quad (1c) \\
\partial_t c^\pm + \nabla \cdot \mathbf{j}^\pm &= r^\pm(t, x, c^+, c^-) \quad \text{in } J \times \Omega, \quad (1d) \\
E &= -D \nabla \phi \quad \text{in } J \times \Omega, \quad (1e) \\
\nabla \cdot E &= c^+ - c^- + \sigma \quad \text{in } J \times \Omega, \quad (1f)
\end{align*}
\]
with \( c_{\pm,0} \) satisfying the boundary conditions (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 system (1) that we refer to as the *Darcy–Nernst–Planck–Poisson (DNPP)* system is a recent rigorous homogenization result of Ray et al. [28], obtained by the method of two-scale convergence. The homogenization was based on the well-known Stokes–Nernst–Planck–Poisson system, which describes the dynamics of dilute electrolytes and of dissolved charged particles within a porous medium at the pore scale [17, 19, 22]. The averaged physical quantities in (1) are the fluid velocity \( u \), 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 \( E \) and the electric potential \( \phi \). The stationary, constant coefficients \( D, K \) are effective tensors of second order, the closed-form expression of which is provided by averaging the solutions of so-called cell problems [12, Def. 1, 28, Def. 4.4]. Here, we consider these two coefficients given. The reaction rates \( r^\pm = r^\pm(t, x, c^+, c^-) \) depend on \( (t, x) \in J \times \Omega \) since potential source or sink terms are incorporated in this term.

### 2 Preliminaries

**Sobolev spaces.** We use the standard notation for Sobolev spaces [1, 11]. Let \( L^p(\Omega) \) denote the space of Lebesgue-measurable functions, which \( p \)th power is Lebesgue-integrable on \( \Omega \), i.e., for which the norm

\[
||v||_{L^p(\Omega)} := \left\{ \left( \int_\Omega |v(x)|^p \, dx \right)^{1/p}, \quad 1 \leq p < \infty \right\}
\]

is finite. 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. Let \( H^k(\Omega) \) be the set of \( k \)-times differentiable functions in \( L^2(\Omega) \) with weak derivatives in \( L^2(\Omega) \), equipped with the usual scalar product \( \langle \cdot, \cdot \rangle_{H^k(\Omega)} \), \( k \in \mathbb{N}_0 \) [cf. 33, Def. 1.3.2, 10, Thm. B.27]. Let the space \( H^{1/2}(\partial \Omega) \) contain those functions on the boundary \( \partial \Omega \) for which the norm

\[
||v||_{H^{1/2}(\partial \Omega)}^2 := \int_{\partial \Omega} |v(x)|^2 \, ds_x + \int_{\partial \Omega} \int_{\partial \Omega} \frac{|v(x) - v(y)|^2}{|x - y|^{d+1}} \, ds_x \, ds_y
\]

is finite, let \( H^{-1/2}(\partial \Omega) \) denote its dual space [cf. 1, Chap. 7, p. 208], 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 \( H^k(\Omega) := (H^k(\Omega))^d = H^k(\Omega; \mathbb{R}^d) \),
the space of vector-valued functions \( v = (v_1, \ldots, v_d)^T : \Omega \to \mathbb{R}^d \), which components are in \( H^k(\Omega) \) equipped with the norm and the scalar product

\[
\|v\|^2_{H^k(\Omega)} := \sum_{i=1}^d \|v_i\|^2_{H^k(\Omega)} \quad \text{and} \quad (v, w)_{H^k(\Omega)} := \sum_{i=1}^d (v_i, w_i)_{H^k(\Omega)},
\]

respectively. Furthermore, let \( H^{\text{div}}(\Omega) := \{v \in L^2(\Omega); \nabla \cdot v \in L^2(\Omega)\} \). With the scalar product \((v_1, v_2)_{H^{\text{div}}(\Omega)} = (v_1, v_2)_{L^2(\Omega)} + (\nabla \cdot v_1, \nabla \cdot v_2)_{L^2(\Omega)}\) and the induced norm \( \|\cdot\|_{H^{\text{div}}(\Omega)} = (\cdot, \cdot)_{H^{\text{div}}(\Omega)} \), the space \( H^{\text{div}}(\Omega) \) is a Hilbert space. In proofs, we occasionally suppress the subindex for \( V = L^2(\Omega) \) or \( L^2(\Omega) \) and 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 such that the norm

\[
\|v\|_{L^p(J; V)} := \left\{ \left(\int_J |v(t, \cdot)|_V^p \, dt\right)^{1/p}, \quad 1 \leq p < \infty \right\}
\]

is finite, which makes \( L^p(J; V) \) a Banach space. For the case of \( V = L^2(\Omega) \), we identify \( L^p(J \times \Omega) = L^p(J; V) \).

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 \( \gamma_\nu : H^{\text{div}}(\Omega) \ni v \mapsto v \cdot \nu_{|\partial \Omega} \in H^{-1/2}(\partial \Omega) \), which are both linear, continuous, and surjective. We also recall Green’s formula: let \( v \in H^{\text{div}}(\Omega) \), then \( v \cdot \nu_{|\partial \Omega} \in H^{-1/2}(\partial \Omega) \) and there holds

\[
\forall w \in H^1(\Omega), \quad (\nabla \cdot v, w)_{L^2(\Omega)} + (v, \nabla w)_{L^2(\Omega)} = (v \cdot \nu, w)_{H^{-1/2}(\partial \Omega), H^{1/2}(\partial \Omega)}.
\]

If, in addition, \( v \cdot \nu_{|\partial \Omega} \in L^2(\partial \Omega) \) the duality pairing in (3) can be identified by \( \int_{\partial \Omega} v \cdot w = (v \cdot \nu, w)_{L^2(\partial \Omega)} \). We define the following constrained ansatz spaces:

\[
H_0^{\text{div}}(\Omega) := \left\{ v \in H^{\text{div}}(\Omega); v \cdot \nu = a \text{ on } \partial \Omega \right\}, \quad H^1_0(\Omega) := \left\{ w \in H^1(\Omega); w = b \text{ on } \partial \Omega \right\},
\]

where \( a \in H^{-1/2}(\partial \Omega) \) and \( b \in H^{1/2}(\partial \Omega) \). The spaces \( H_0^{\text{div}}(\Omega) \) and \( H^1_0(\Omega) \) therefore consist of functions with vanishing normal trace and vanishing trace, respectively.

**Triangulation and discrete spaces.** Let \( \mathcal{T}_h \) be a regular family of decompositions [7, (H1), p. 131] into closed \( d \)-simplices \( T \) of characteristic size \( h \) (also called fineness or mesh size) such that \( \overline{\Omega} = \bigcup T \). For the treatment of curved domains in the context of finite element methods for second-order problems we refer to Ciarlet [7, Chap. VI].

We denote by \( \mathcal{P}_k(T) \) the space of polynomials of degree at most \( k \) on a triangle \( T \in \mathcal{T}_h \) and define by \( \mathcal{RT}_k(T) := \mathcal{P}_k(T)^d \oplus \mathcal{P}_k(T) = \{v_h : T \to \mathbb{R}^d; v_h(x) = ax + b, a \in \mathcal{P}_k(T), b \in \mathcal{P}_k(T)^d\} \) the local Raviart–Thomas space of order \( k \) [21, 27, 31]. We define by \( \mathcal{P}_k(\mathcal{T}_h) := \{w_h : \Omega \to \mathbb{R}; \forall T \in \mathcal{T}_h, w_h|_T \in \mathcal{P}_k(T)\} \) the global polynomial spaces on the triangulation \( \mathcal{T}_h \). Clearly, \( \mathcal{P}_k(\mathcal{T}_h) \subset L^2(\Omega) \). The global Raviart–Thomas space of order \( k \) is defined by \( \mathcal{RT}_k(\mathcal{T}_h) := H^{\text{div}}(\Omega) \cap \bigcap_{T \in \mathcal{T}_h} \mathcal{RT}_k(T) \). The inclusion \( \mathcal{RT}_k(\mathcal{T}_h) \subset H^{\text{div}}(\Omega) \) 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 $P^k_h : H^{div}(\Omega) \cap \prod_{T \in T_h} H^1(T) \ni v \mapsto P^k_h v$ and $P^k : L^2(\Omega) \ni w \mapsto P^k w \in P_k(T_h)$ be the global interpolation operators due to Raviart and Thomas [4, 9]. The projectors fulfill the following well-known properties [9, Lem. 3.5, 27, Thm. 4, p. 310, 6, Lem. 3.7, p. 164, 4, Prop. 3.9, p. 132, 23, (3.5.24)]:

(P1) $\nabla \cdot P^k_h = P^k \nabla \cdot \text{ and } \nabla \cdot \mathbf{RT}_k(T_h) = P_k(T_h).$

(P2) For $w \in L^2(\Omega)$ given, $\forall w_h \in P_k(T_h), \left( P^k_h w , w_h \right)_{L^2(\Omega)} := (w, w_h)_{L^2(\Omega)}.$

(P3) For $v \in H^{div}(\Omega) \cap \prod_{T \in T_h} H^1(T)$ given, $\forall w_h \in P_k(T_h), \left( \nabla \cdot P^k_h v, w_h \right)_{L^2(\Omega)} = (\nabla \cdot v, w_h)_{L^2(\Omega)}.$

(P4) For $w \in L^2(\Omega)$ given, $\forall w_h \in \mathbf{RT}_k(T_h), \left( P^k_h w, \nabla \cdot w_h \right)_{L^2(\Omega)} = (w, \nabla \cdot w_h)_{L^2(\Omega)}.$

(P5) Given $w_h \in P_k(T_h)$, there exists $v_h \in \mathbf{RT}_k(T_h)$ such that $\nabla \cdot v_h = w_h$ and $\|w_h\|_{H^{div}(\Omega)} \leq C_\Omega \|w_h\|_{H^1(\Omega)}$ holds with a constant $C_\Omega$ depending only on $\Omega$.

(P6) For any $v \in H^1(\Omega)$ and $w \in H^1(\Omega)$, for $l \in \{1, \ldots, k + 1\},$

$$\| (P^k_h - I) v \|_{L^2(\Omega)} \leq h^l \| v \|_{H^l(\Omega)}, \quad \| (P^k_h - I) w \|_{L^2(\Omega)} \leq h^l \| w \|_{H^l(\Omega)}.$$

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

**Time discretization.** 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 $v_h^n \in P_k(T_h)$, the first and the second order backward difference quotient is defined by

$$\overline{\partial_1 v_h^n} := \frac{1}{\tau} (v_h^n - v_h^{n-1}), \quad \overline{\partial_2 v_h^n} := \frac{3}{2} \overline{\partial_1 v_h^n} - \frac{1}{2} \overline{\partial_1 v_h^{n-1}} = \frac{1}{\tau} (\frac{3}{2} v_h^n - 2 v_h^{n-1} + \frac{1}{2} v_h^{n-2}) (4)$$

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 $t_n \in J$:

$$\eta_v^n := v_h^n - v(t_n), \quad \eta_w^n := w_h^n - w(t_n)$$

for time and space continuous, vector-valued functions $v$ and corresponding fully discrete approximations $v_h^n \in \mathbf{RT}_k(T_h)$ and for time and space continuous, scalar-valued functions $w$ and corresponding fully discrete approximations $w_h^n \in P_k(T_h)$, respectively. In the analysis that follows, we make frequent use of the identities $\eta_v^n = P^k_h \eta_v^n + (P^k_h - I) v$ and $\eta_w^n = P^k_h \eta_w^n + (P^k_h - I) w$. 

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F. Frank · P. Knabner — Convergence analysis of a BDF2/MFE disc. of a DNPP system
Miscellaneous. 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. The following version of the discrete Gronwall lemma [13, Lem. 2.4] is required in the analysis: let \((a_k)_{k \in \mathbb{N}}, (b_k)_{k \in \mathbb{N}}\) be nonnegative sequences of real numbers, \((b_n)\) non-decreasing, and \(c\) be a (fixed) positive constant. If \((a_n)\) satisfies
\[
\forall n \in \mathbb{N}, \quad a_n \leq b_n + c \sum_{m=q}^{n-1} a_m, \quad \text{then} \quad \forall n \in \mathbb{N}, \quad a_n \leq (1 + c)^n b_n.
\]
Note that for \(n = 1\) the sum is zero by definition. The following identities are required for the BDF1 respectively BDF2 time discretization, to show a priori bounds for \(c^\pm\) [5]:
\[
2(a - b)a = a^2 - b^2 + (a - b)^2, \quad (5a)
\]
\[
2(3a - 4b + c)a = a^2 - b^2 + (2a - b)^2 - (2b - c)^2 + (a - 2b + c)^2. \quad (5b)
\]

3 Error Analysis

The hypotheses imposed on the data of system (1) are as follows:

**Hypotheses 1** (Hypotheses on the data).

(H1) The inverse of the coefficient \(D \in \mathbb{R}^{d \times d}\) is bounded and positive definite, i.e., there exist strictly positive constants \(D_\alpha, D_\infty,\) such that
\[
\forall \xi \in \mathbb{R}^d, \quad \forall \xi_1, \xi_2 \in \mathbb{R}^d, \quad \xi \cdot D^{-1} \xi \geq D_\alpha |\xi|^2, \quad \xi_1 \cdot D^{-1} \xi_2 \leq D_\infty |\xi_1| |\xi_2|.
\]

(H2) The hypothesis (H1) holds for the coefficient \(K\) with the constants \(K_\alpha, K_\infty.\)

(H3) The 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 \(c^{\pm,0}(x) \geq 0\) for a.e. \(x \in \Omega.\)

(H5) The coefficient \(\phi_D\) is bounded in \(H^1(J; H^{1/2}(\partial\Omega)).\)

(H6) The coefficient \(\sigma\) is bounded in \(L^\infty(J \times \Omega).\)

As (1) being a model obtained by periodic homogenization, the coefficients \(D\) and \(K\) have closed-form expressions and can be obtained by solving so-called cell problems [12, 28]. The symmetry and positive definiteness of these upscaled tensors as postulated in (H1) and (H2) is naturally satisfied [8, 15]. Note that the symmetry and positive definiteness of the matrices in hypotheses (H1) and (H2) imply the symmetry and positive definiteness of their inverses [e.g., 18, Thm. 4.135]. In the homogenization context, \(\sigma\) 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) by the inverse tensors and using the Green formula (3):

**Problem 1** (Mixed weak continuous DNPP problem). Let $D$, $K$, $r^+$, $c^\pm$, $\phi_0$, $\sigma$ be given and let (H1)–(H6) hold. Seek $(u, p, j^+, j^-, c^+, c^-, E, \phi)$ with $u \in L^2(J; H_0^{\text{inv}}(\Omega))$, $p \in L^2(J; L^2(\Omega)/\mathbb{R})$, $j^\pm \in L^2(J; H^{\text{inv}}(\Omega))$, $c^\pm \in L^\infty(J \times \Omega) \cap H^1(J; L^2(\Omega))$, $E \in L^\infty(J; H^{\text{inv}}(\Omega))$, $\phi \in L^\infty(J; L^2(\Omega))$ such that for a.e. $t \in J$, $\forall \theta \in H^{\text{inv}}(\Omega)$, $w \in L^2(\Omega)$

\[
-\left(K^{-1} u(t), \theta\right) + (\nabla \cdot v, p(t)) = -\left(D^{-1} E(t) (c^+(t) - c^-(t)), \theta\right),
\]

\[
(\nabla \cdot u(t), w) = 0,
\]

\[
-D^{-1} j^+(t), v) + (\nabla \cdot v, c^+(t)) + \left(D^{-1} u(t) \pm E(t) c^+(t), \theta\right) = 0,
\]

\[
(\partial_t c^+(t), w) + (\nabla \cdot j^+(t), w) = (r^+(t, x, c^+(t), c^-(t)), w),
\]

\[
-D^{-1} E(t), v) + (\nabla \cdot v, \phi(t)) = (v \cdot v, \phi_0(t))_{H^{-1/2}(\partial \Omega), H^{1/2}(\partial \Omega)},
\]

\[
(\nabla \cdot E(t), w) = (c^+(t) - c^-(t) + \sigma(t), w)
\]

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

We call the solution of Prob. 1 the true solution in contrast to the solution of the below defined discrete problem, which we call the discrete solution. Components of the solution vector $(u, p, j^+, j^-, c^+, c^-, E, \phi)$ are referred to as partial solutions.

In the formulation of the fully discrete counterpart of Prob. 1, we make use of the following cut-off operator [3, 29, 30]:

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

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

(i) $\forall w \in L^p(\Omega)$, $\|M(w)\|_{L^\infty(\Omega)} \leq M$.

(ii) Let $w \in L^\infty(\Omega)$. If $M$ satisfies $\|w\|_{L^p(\Omega)} \leq M$, then $M(w) = w$.

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

**Proof**: The properties (i) and (ii) are obvious. Property (iii) follows from the pointwise Lipschitz continuity $|M(v)(x) - M(w)(x)| \leq |v(x) - w(x)|$ 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 $\Omega$ for $1 \leq p < \infty$. A sketch of the proof of the pointwise property (iii), i.e., for $p = \infty$, is given in Sun et al. [30].

The cut-off operator $M$ is a crucial tool in the error analysis that follows. However, the associated numerical scheme is not defined properly yet as long as no explicit expression for the cut-off level $M$ is given that does not depend on the true solution itself. Especially, it has
to be ensured that $M$ is chosen sufficiently large such that the property (ii) of Lem. 1 holds for the partial true solutions $c^\pm(t)$. This means, in particular, that an $L^\infty$ a priori estimate is necessary providing an $L^\infty$ bound depending only on the data. To this end, we show that solutions of Prob. 1 also solve Prob. 2 in order to allow the exploitation of the estimate (iii) of Thm. 1 yielding the demanded explicit bound. The so obtained validity of Thm. 1 yields furthermore the existence and uniqueness of solutions of Prob. 1 and also the nonnegativity of concentrations.

Before we continue with discretization of Prob. 1, which is based on the mixed formulation of system (1), we cite an existence result of Herz et al. [14] that yields an explicit bound for $\sum_{i\in\{+,-\}}\|c^\pm\|_{L^\infty(J,\Omega)}$. The weak problem under investigation of Herz et al. [14] derives from the non-mixed formulation of $(1c), (1d), (1e)\) and reads as follows:

**Problem 2** (Non-mixed weak continuous DNPP problem). Let $D, K, r^\pm, c^{\pm,0}, \phi_D, \sigma$ be given and let (H1)-(H6) hold. Seek $(u, p, c^+, c^-, \phi)$ with $u \in L^2(J; H^{1}_{\text{div}}(\Omega)), \ p \in L^2(J; L^2(\Omega)/\mathbb{R}), \ c^\pm \in L^\infty(J \times \Omega) \cap L^2(J; H^1(\Omega)) \cap \mathcal{H}^0(J; H^{-1}(\Omega), \phi \in L^\infty(J; H^1(\Omega) \cap H^1_{\phi_0}(\Omega))$ such that for a. e. $t \in J, \forall u \in H^1_0(\Omega), \forall w \in L^2(\Omega), \forall z \in H^1_0(\Omega)$,

$$-
\left(\mathbf{K}^{-1}u(t), v\right) + \left(\nabla \cdot v, p(t)\right) = ((c^+(t) - c^-(t)) \nabla \phi, v), \quad (7a)
$$

$$\left(\nabla \cdot u(t), w\right) = 0, \quad (7b)
$$

$$\left< \partial_t c^\pm(t), z \right>_{H^{-1}(\Omega), H^1(\Omega)} + \left< D \nabla c^\pm(t), \nabla z \right> - \left< u(t) c^\pm(t), \nabla z \right> = \left< r^\pm(t, x, c^+(t), c^-(t)), z \right>, \quad (7c)
$$

$$\left(\nabla \cdot D \nabla \phi(t), w\right) = (c^+(t) - c^-(t) + \sigma(t), w) \quad (7d)
$$

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

We summarize the most important results of Herz et al. [14] in the following theorem:

**Theorem 1** (Well-posedness, nonnegativity, and explicit bound). Let $(u, p, c^+, c^-, \phi)$ be the solution of Prob. 2 and let (H1)-(H6) hold. Then the following statements hold:

(i) The solution $(u, p, c^+, c^-, \phi)$ uniquely exists.

(ii) The partial solutions $c^\pm$ are nonnegative, i. e.,

$$c^\pm(t, x) \geq 0 \quad \text{for a. e. } (t, x) \in J \times \Omega.
$$

(iii) The following estimate holds for arbitrary end time $T \in \mathbb{R}_+ := [0, \infty[$:

$$\sum_{i\in\{+,-\}} \|c^i\|_{L^\infty(J,\Omega)} \leq C(c^{\pm,0}, \sigma, \Omega, T), \quad (8)
$$

with $C(c^{\pm,0}, \sigma, \Omega, T) > 0$ depending only on $\|c^{\pm,0}\|_{L^\infty(\Omega)}$ on $\|\sigma\|_{L^\infty(J,\Omega)}$, on coefficients of the Sobolev embedding theorem, and on the end time $T$.
Proof. See Herz et al. [14, Thms. 3.4, 3.10, 3.11 and Remarks 2.2, 3.7]. Item (iii) can be deduced as follows: from [14, Thm. 3.5] we have
\[ \sum_{i \in \{+,-\}} \|c^i(t)\|_{L^2(J \times \Omega)} \leq C_M \sum_{i \in \{+,-\}} \|c^i\|_{L^2(J \times \Omega)} + 4 \sum_{i \in \{+,-\}} \|c^{i0}\|_{L^\infty(\Omega)} \]
with a constant $C_M > 0$ 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 [14, Remark 3.6]
\[ \frac{d}{dt} \sum_{i \in \{+,-\}} \|c^i(t)\|_{L^2(\Omega)} + \sum_{i \in \{+,-\}} \|\nabla c^i(t)\|_{L^2(\Omega)} \leq 2 \frac{2}{D_a} \|\sigma\|_{L^\infty(J \times \Omega)} \sum_{i \in \{+,-\}} \|c^i(t)\|_{L^2(\Omega)} \]
yields
\[ \forall t \in J, \quad \sum_{i \in \{+,-\}} \|c^i(t)\|_{L^2(\Omega)} \leq \exp \left( \frac{2T}{D_a} \right) \sum_{i \in \{+,-\}} \|c^{i0}\|_{L^2(\Omega)}, \]
which, inserted in the first equation, closes the proof. \qed

Proposition 1 (Solution of Prob. 1 solves Prob. 2). Let $(u, p, j^+, j^-, c^+, c^-, E, \phi)$ be a solution of Prob. 1. Then the partial solution $(u, p, c^+, c^-, \phi)$ is a solution of Prob. 2. In particular, $c^+ \in L^2(J; H^1_0(\Omega))$ and $\phi \in L^\infty(J; H^2(\Omega) \cap H^1_0(\Omega))$ holds.

Proof. We denote by $\mathcal{D}(\Omega)$ the space of infinitely differentiable functions with compact support on $\Omega$, and by $\mathcal{D}'(\Omega)$ the space of distributions [cf. 10, Sec. B.2].

Testing (6e) with $v \in \mathcal{D}(\Omega)^d \subset H^{\text{div}}(\Omega)$ yields
\[ \forall v \in \mathcal{D}(\Omega)^d, \quad \left( D^{-1}E(t), v \right) = \left( \phi(t), \nabla \cdot v \right) = -\left( \nabla \phi(t), v \right)_{\mathcal{D}'(\Omega)^d, \mathcal{D}(\Omega)^d}, \quad (9) \]
which is the defining equation for $\nabla \phi(t)$, i.e., $\nabla \phi(t)$ in the distributional sense is a function: $\forall t \in J, -\nabla \phi(t) = D^{-1}E(t)$. Since $\|D^{-1}E\|_{L^\infty(J; L^2(\Omega))} < \infty$ due to \{(H1), (H9)\} and $L^2(\Omega) \supset H^{\text{div}}(\Omega)$, it follows that $\nabla \phi \in L^\infty(J; L^2(\Omega))$. 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. 10, Thm. B.14, 33, Cor. 1.1.1], the variational equation
\[ \forall v \in L^2(\Omega), \quad \left( D^{-1}E(t), v \right) = -\left( \nabla \phi(t), v \right) \quad (10) \]
holds. Next, we show that $\phi(t) = \phi_D(t)$ for a.e. $t \in J$, which was demanded implicitly in Prob. 2 by the constrained ansatz space $H_{\text{div}}^1(\Omega)$ and explicitly in Prob. 1 by a boundary integral: using the fact that (10) also holds for $v \in H^{\text{div}}(\Omega) \subset L^2(\Omega)$ and application of Green’s formula yields
\[ \forall v \in H^{\text{div}}(\Omega), \quad \left( v \cdot v, \phi(t) \right)_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)} \overset{(3)}{=} \left( \phi(t), \nabla \cdot v \right) + \left( \nabla \phi(t), v \right) \overset{(10)}{=} \left( \phi(t), \nabla \cdot v \right) - \left( D^{-1}E(t), v \right) \overset{(6e)}{=} \left( v \cdot v, \phi_D(t) \right)_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)}. \]
In order to prove that $\phi(t)$ is also in $H^2(\Omega)$, we test (6f) with $w \in \mathcal{D}(\Omega) \subset L^2(\Omega)$:

$$\forall w \in \mathcal{D}(\Omega), \quad (c^+ - c^-(t) + \sigma(t), w) \overset{(6f)}{=} (\nabla \cdot E(t), w) = -(E(t), \nabla w) \overset{(10)}{=} (D\nabla \phi(t), \nabla w) = -(\nabla \cdot D\nabla \phi(t), w)_{L^2(\Omega) \times L^2(\Omega)},$$

which shows that the distributional divergence of $D\nabla \phi(t)$ is a function. Because $c^\pm$ and $\sigma$ are element of $L^\infty(J; L^2(\Omega)) \supset L^\infty(J \times \Omega)$ from assumption and due to (H6), respectively, we conclude—taking the previous considerations into account—that $\phi \in L^\infty(H^2(\Omega) \cap H^1_\partial(\Omega))$.

Thus $\phi(t)$ is a partial solution of (7d) for a.e. $t \in J$.

With (10) and the fact that $c^\pm \in L^\infty(J \times \Omega)$, the mixed variational subsystems \{(7a), (7b)\} and \{(6a), (6b)\} coincide. Hence, $(u(t), p(t)) \in H^\text{div}_0(\Omega) \times L^2(\Omega)/\mathbb{R}$ is also a partial solution of \{(7a), (7b)\}.

It remains to show that $c^\pm(t)$ are partial solutions of (7c). We test (6c) with $v \in \mathcal{D}(\Omega)^d \subset H^\text{div}_0(\Omega)$:

$$\forall v \in \mathcal{D}(\Omega)^d, \quad \left( D^{-1}(\tilde{J}^\pm(t) - (u(t) \pm E(t))c^\pm(t)), v \right) \overset{(6c)}{=} (c^\pm(t), \nabla \cdot v) = -(\nabla c^\pm(t), v)_{L^2(\Omega) \times L^2(\Omega)^d}, \quad (11)$$

eq \nabla c^\pm(t), v \in L^2(\Omega)$$

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. $t \in J$, since the left-hand side of the first scalar product is finite due to (H1) and $c^\pm(t) \in L^\infty(\Omega)$ for a.e. $t \in J$. In particular, (11) also holds in the $L^2(\Omega)$ sense. With this result, $c^\pm \in L^2(J; H^1(\Omega))$ is easily shown:

$$\|c^\pm\|^2_{L^2(J; H^1(\Omega))} \overset{(11)}{=} \|c^\pm\|^2_{L^2(J \times \Omega)} + \int J \|D^{-1}(\tilde{J}^\pm - (u \pm E)c^\pm)(s)\|^2_{L^2(\Omega)} \, ds$$
\leq \|c^\pm\|^2_{L^2(J \times \Omega)} + 2 \|D^{-1}c^\pm\|^2_{L^2(\Omega)} + \|u \pm E\|^2_{L^2(J \times \Omega)} \|c^\pm(t)\|^2_{L^\infty(J \times \Omega)} < \infty.$$

Eqn. (6c) also holds for $v \in \mathcal{D}(\Omega)^d \subset H^\text{div}_0(\Omega)$. We test (6c) with $v = D^T \nabla w$, where $w \in \mathcal{D}(\Omega)$, use (H1), and apply Green’s formula to the first and the second term:

$$\forall w \in \mathcal{D}(\Omega), \quad (\nabla \cdot \tilde{J}^\pm(t), w) = (D\nabla c^\pm(t), \nabla w) - ((u(t) \pm E(t))c^\pm(t), \nabla w). \quad (12)$$

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 (12) into (6d):

$$\forall w \in \mathcal{D}(\Omega), \quad (\partial_t c^\pm(t), w) + (D\nabla c^\pm(t), \nabla w) - ((u(t) \pm E(t))c^\pm(t), \nabla w)$$
\quad = \langle r^\pm(t, x, c^\pm(t), c^\pm(t)), w \rangle \quad (13)$$

for a.e. $t \in J$. Since $\mathcal{D}(\Omega) \subset H^1_\partial(\Omega)$ dense with respect to $\| \cdot \|_{H^1(\Omega)}$ [11, Sec. 5.2.2], (13) also holds for $w \in H^1_\partial(\Omega)$. Using that $E(t) = -D\nabla \phi(t)$ holds in $L^2(\Omega)$ for a.e. $t \in J$, as shown above, and noting that

$$\forall w \in H^1_\partial(\Omega), \quad (\partial_t c^\pm(t), w) = \langle \partial_t c^\pm(t), w \rangle_{H^{-1}(\Omega) \times H^1_\partial(\Omega)}$$

since $\partial_t c^\pm(t) \in L^2(\Omega)$ by the definition of Prob. 1 and $(H^1_\partial(\Omega), L^2(\Omega), H^{-1}(\Omega))$ is a Gelfand triple, it follows that the partial solutions $c^\pm(t)$ of Prob. 1 solve the non-mixed variational equation (7c) of Prob. 2. \hfill \square
From Prop. 1 it follows immediately the following corollary:

**Corollary 1.** Thm. 1 holds true for the solution \((u, p, j^+, c^+, j^-, c^-, E, \phi)\) of Prob. 1.

We continue with the formulation of the fully discrete problem. Recall (4)—the definition of the backward difference quotient. We assume that the (stationary) upscaling coefficients, namely \(D, K\), and \(\sigma\) and the data \(\phi_D\) are sufficiently precisely precomputed such that a discretization error in these coefficients is negligible. Owing to Cor. 1, the use of the cut-off operator \(M\) according to Def. 1 is now admissible for the definition of the **fully discrete weak problem**:

**Problem 3** (Mixed weak discrete DNPP problem). Let \(q \in \{1, 2\}\) and let \(D, K, r^+, \phi_D, \sigma, c_h^{+,0}, c_h^{+,q-1}\) be given. For \(n \in \{q, \ldots, N\}\), seek \((u_h^n, p_h^n, j_h^{+,n}, c_h^{+,n}, j_h^{-,n}, c_h^{-,n}, E_h^n, \phi_h^n) \in (RT_k(\mathcal{T}_h) \times P_k(\mathcal{T}_h))^4\) such that \(\forall v_h \in RT_k(\mathcal{T}_h), w_h \in P_k(\mathcal{T}_h),\)

\[
- (K^{-1} u_h^n, v_h) + (\nabla \cdot v_h, p_h^n) = - (D^{-1} E_h^n M (c_h^{+,n} - c_h^{-,n}), v_h), \tag{14a}
\]

\[
(\nabla \cdot u_h^n, w_h) = 0 , \tag{14b}
\]

\[
- (D^{-1} j_h^{+,n}, v_h) + (\nabla \cdot v_h, c_h^{+,n}) + (D^{-1} (u_h^n \pm E_h^n) M (c_h^{+,n}), v_h) = 0 , \tag{14c}
\]

\[
(\tilde{\partial}_c c_h^{+,n}, w_h) + (\nabla \cdot j_h^{+,n}, w_h) = \left( r^+(n, x, c_h^{+,n}, c_h^{-,n}), w_h \right) , \tag{14d}
\]

\[
- (D^{-1} E_h^n, v_h) + (\nabla \cdot v_h, \phi_h^n) = (v_h \cdot \nu, \phi_{\partial D}^n)_{L^2(\partial \Omega)} , \tag{14e}
\]

\[
(\nabla \cdot E_h^n, w_h) = \left( c_h^{+,n} - c_h^{-,n} + \sigma^n, w_h \right) , \tag{14f}
\]

where the cut-off level \(M\) for the cut-off operator \(M\) is set equal to the right-hand side of (8).

The cutting off of the terms in (14a), (14c) 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 \(L^\infty\) a priori estimates for \(u\) or \(E\).

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

**Hypotheses 2** (Hypotheses on the true solution).

Let \(l_1, \ldots, l_6 \in \{1, \ldots, k + 1\}\) be fixed integers \((k\) and \(q\) as in Prob. 3).

\[
(H7) \quad \text{For the partial true solution } (u, p) \text{ it holds that } u \in L^2(J; L^\infty(\Omega)) \cap H^1(J; H^1(\Omega)), p \in H^1(J; H^2(\Omega)).
\]

\[
(H8) \quad \text{For the partial true solutions } (j^+, c^+) \text{ it holds that } j^+ \in H^1(J; H^1(\Omega)), c^+ \in H^{p+1}(J; L^2(\Omega)) \cap H^1(J; H^2(\Omega)).
\]

\[
(H9) \quad \text{For the partial true solution } (E, \phi) \text{ it holds that } E \in L^2(J; L^\infty(\Omega)) \cap H^1(J; H^5(\Omega)), \phi \in H^1(J; H^6(\Omega)).
\]

**Proposition 2.** Let \((E, \phi, c^+, c^-)\) and \((E_h^n, \phi_h^n, c_h^{+,n}, c_h^{-,n})\) be partial solutions of Prob. 1 and Prob. 3, respectively. Then, if in addition the regularity requirements of (H9) are satisfied, for \(n \in \{q, \ldots, N\}\),

\[
\|u_h^n\|_{L^2(\Omega)}^2 + \|\phi_h^n\|_{L^2(\Omega)}^2 \leq \sum_{i \in \{+, -\}} h^{2l_i} |E(t_n)|_{H^3(\Omega)}^2 + h^{2l_i} |\phi(t_n)|_{H^3(\Omega)}^2 + \sum_{i \in \{+, -\}} \|\eta_{E_i}^n\|_{L^2(\Omega)}^2 . \tag{15}
\]
Proof. Subtraction of \((6e), (6f)\) from \((14e), (14f)\) yields the error equations
\[
\begin{align*}
(D^{-1} \eta^n_E, v_h) &= (\nabla \cdot v_h, \eta^n_h) \quad (P_4), \\
(\nabla \cdot \eta^n_E, w_h) &= (\eta^n_h, w_h) - (\eta^n_c, w_h) \quad (P_3),
\end{align*}
\]
for all \(v_h \in RT_k(T_h)\) and for all \(w_h \in P_k(T_h)\). The choice of \(v_h = H^k_n \eta^n_E \in RT_k(T_h)\) and \(w_h = P^k_n \eta^n_h \in P_k(T_h)\), subtraction of the resulting equations, and (H1) yields
\[
D_o ||\eta^n_E||^2 \leq \left(D^{-1} \eta^n_E, (P^k_n - I)E(t_o)\right) + \left(\eta^n_h -(P^k_n - I)\phi(t_o), \eta^n_c - \eta^n_c\right) \leq \frac{\delta}{2} ||\eta^n_E||^2 \\
+ \frac{1}{2\delta} D^2 ||(P^k_n - I)E(t_o)||^2 + \delta ||\eta^n_h||^2 + \delta ||(P^k_n - I)\phi(t_o)||^2 + \frac{1}{\delta} \sum_{i \in \{+,-\}} ||\eta^n_i||^2 
\tag{17}
\]
with \(0 < \delta < 2D_o\). Having the estimate (17) for \(||\eta^n_E||\) at hand, an estimate for \(||\eta^n_h||\) needs to be derived: according to (P5), we may choose \(v_h \in RT_k(T_h)\) in (16a) such that \(\nabla \cdot v_h = P^k_n \eta^n_h \in P_k(T_h)\):
\[
(P^k_n \eta^n_h, \eta^n_h) = (\nabla \cdot v_h, \eta^n_h) \quad (P_5).
\]
With (H1) and \(|v_h| \leq \|v_h\|_{H^{2v}(\Omega)} \leq C_{\Omega} ||P^k_n \eta^n_h||\) it follows
\[
(2 - 2\delta')||\eta^n_h||^2 \leq \left(\frac{1}{\delta'} + 2\right)\left(C_{\Omega}^2 D_o^2 ||\eta^n_E||^2 + \|P^k_n - I\|\phi(t_o)||^2\right) 
\tag{18}
\]
with \(0 < \delta' < 1\). Setting \(\delta' := 1/2\) and substituting \(||\eta^n_h||^2\) from (18) into (17) yields
\[
\left(D_o - \delta(1 + 4C_{\Omega}^2 D_o^2)\right)||\eta^n_E||^2 \leq \frac{1}{2\delta} D_o^2 ||(P^k_n - I)E(t_o)||^2 + \delta ||(P^k_n - I)\phi(t_o)||^2 + \frac{1}{\delta} \sum_{i \in \{+,-\}} ||\eta^n_i||^2 
\tag{19}
\]
with the constraint \(0 < \delta < D_o/(1/2 + 4C_{\Omega}^2 D_o^2)\). Fixing \(\delta\), inserting the estimate (19) into (18), summing up the resulting equation with (19), and using (P6) ends the proof. \(\square\)

Proposition 3. Let \((u, p, j^+, c^+, j^-, c^-, E, \phi)\) and \((u_h^n, p_h^n, j^+_h^n, c^+_h^n, j^-_h^n, c^-_h^n, E_h^n, \phi_h^n)\) be solutions of Prob. 1 and Prob. 3, respectively. Then, if in addition the regularity requirements of (H8) are satisfied, for \(q \in \{1, 2\}, n \in \{q, \ldots, N\}\), and sufficiently small \(\tau\),
\[
\begin{align*}
||\eta^n_c||^2_{L^2(\Omega)} + \tau \sum_{m=q}^n ||\eta_h^n||^2_{L^2(\Omega)} & \leq \sum_{j=0}^{q-1} ||\eta^n_j||^2_{L^2(\Omega)} + \tau^2 ||| \varphi^{j+1} c^+ |||_{L^2(\Omega)}^2 + \tau^2 \sum_{m=q}^n ||\varphi^{j}(t_m)||^2_{H^1(\Omega)} \\
+ \tau^2 \int_0^{t_n} ||\varphi^{j}(s)||^2_{H^1(\Omega)} ds + \tau \sum_{m=q}^n ||\varphi^{j}(t_m)||^2_{H^1(\Omega)} + \tau \sum_{m=q}^n \left(||\eta_h^n||^2_{L^2(\Omega)} + ||\eta_h^n||^2_{L^2(\Omega)} + ||\eta_h^n||^2_{L^2(\Omega)}\right).
\end{align*}
\tag{20}
\]
Proof. Some ideas of the proof stem from [24–26]. 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 \(|(6c), (6d)| \) from \(|(14c), (14d)| \) yields the following error equations for \( n \in \{q, \ldots, N\} \):

\[
-(D^{-1} \eta_j^-, v_h) + (\nabla \cdot v_h, \eta_c^+) + \left( D^{-1}(u_h^n \pm E_h^n) \mathcal{M}(c_h^{\pm n}) - (u^n \pm E^n) c^{\pm n}, v_h \right) = 0,
\]

\[
(\partial_q c_h^{\pm, n} - \partial_t c_h^{\pm, n}, w_h) + (\nabla \cdot \eta_j^+, w_h) = \left( r^\pm(t_n, x, c_h^{+ n}, c_h^{- n}) - r^\pm(t_n, x, c^{+ n}, c^{- n}), w_h \right)
\]

for all \( v_h \in RT_h(T_h) \) and for all \( w_h \in \mathcal{P}_h(T_h) \). We proceed analogously to the proof of (15) in order to eliminate the divergence terms by using the projector properties \(|(P3), (P4)| \) and choosing \( v_h = \Pi_h^t \eta_j^+ \in RT_h(T_h) \) and \( w_h = P_h^t \eta_c^+ \in \mathcal{P}_h(T_h) \). The resulting equation reads

\[
(\partial_q c_h^{\pm, n} - \partial_t c_h^{\pm, n}, P_h^t \eta_c^+) + (D^{-1} \eta_j^-, \Pi_h^t \eta_j^+) = \left( D^{-1}(u_h^n \pm E_h^n) \mathcal{M}(c_h^{\pm n}) - (u^n \pm E^n) c^{\pm n}, \Pi_h^t \eta_j^+ \right)
\]

\[
+ \left( r^\pm(t_n, x, c_h^{+ n}, c_h^{- n}) - r^\pm(t_n, x, c^{+ n}, c^{- n}), P_h^t \eta_c^+ \right). \tag{21}
\]

Following the idea of Arbogast et al. [2], we use the projector property \((P2)\) and the fact that \( \partial_q \) commutes with \( P_h^t \) to decompose the first term as follows:

\[
(\partial_q c_h^{\pm, n} - \partial_t c_h^{\pm, n}, P_h^t \eta_c^+) = (\partial_q \eta_c^+, \eta_c^+) - (\partial_q (P_h^t - I) c^{\pm, n}, \eta_c^+) + (\partial_q - \partial_t) c^{\pm, n}, P_h^t \eta_c^+).
\]

With this decomposition the combined error equation (21) becomes

\[
(\partial_q \eta_c^+, \eta_c^+) + D_q ||\eta_c^+||^2 \leq (\partial_q (P_h^t - I) c^{\pm, n}, \eta_c^+) - (\partial_q - \partial_t) c^{\pm, n}, P_h^t \eta_c^+ \]

\[
+ (D^{-1} \eta_j^-, (\Pi_h^t - I) j^+, \Pi_h^t \eta_j^+) + (D^{-1}((u_h^n \pm E_h^n) \mathcal{M}(c_h^{\pm n}) - (u^n \pm E^n) c^{\pm n}), \Pi_h^t \eta_j^+)
\]

\[
+ \left( r^\pm(t_n, x, c_h^{+ n}, c_h^{- n}) - r^\pm(t_n, x, c^{+ n}, c^{- n}), P_h^t \eta_c^+ \right). \tag{22}
\]

where the ellipticity of \( D^{-1} \) according to \((H1)\) was used. Next up, consider the term \((\partial_q \eta_c^+, \eta_c^+)\). Using the definition of \( \partial_q \), we see that if we replace \( n \) by \( m \), for the sum from \( q \) to \( n \) multiplied by \( 2q\tau \), there holds

\[
2q\tau \sum_{m=q}^{n} \left( \nabla \nabla \eta_c^m - \eta_c^{m-1} - \eta_c^{m-1}, \eta_c^m \right) = \sum_{m=q}^{n} \left( \begin{array}{c}
(3\eta_c^m - 4\eta_c^{m-1} + \eta_c^{m-2}, \eta_c^m), \\
(\eta_c^m)^2 - \left( \frac{\|\eta_c^m\|^2}{\|\eta_c^m\|^2 + \|\eta_c^n - \eta_c^0\|^2} \right), \\
(\frac{\|\eta_c^m\|^2}{\|\eta_c^m\|^2 + \|\eta_c^n - \eta_c^0\|^2})
\end{array} \right). \tag{5}
\]

Multiplication of (22) by \( 2q\tau \), replacing \( n \) by \( m \), summing up from \( q \) to \( n \), and using the latter result yields

\[
\|\eta_c^m\|^2 + 2D_q q\tau \sum_{m=q}^{n} ||\eta_j^m||^2
\]
truncation and projection errors. Consider a function fundamental theorem of calculus and of the Jensen inequality, we have for

\[ I \]

We denote the terms on the right side of (23) by \( I \) to \( VI \) and estimate \( II \) to \( VI \) in terms of time truncation and projection errors. Consider a function \( \nu \in L^2(J \times \Omega) \). By application of the fundamental theorem of calculus and of the Jensen inequality, we have for \( q = 1 \):

\[
\tau \sum_{m=1}^{n} |\bar{\partial} v^m|^2 = \sum_{m=1}^{n} \left( \frac{1}{\tau} \int_{t_{m-1}}^{t_m} |\bar{\partial} v(s)|^2 \, ds \right)^2 \leq \sum_{m=1}^{n} \int_{t_{m-1}}^{t_m} |\bar{\partial} v(s)|^2 \, ds = |\bar{\partial} v|^2_{L^2[0, t_n \times \Omega]}.
\]

Recalling (4), we get for \( q = 2 \):

\[
\tau \sum_{m=2}^{n} |\bar{\partial}^2 v^m|^2 \leq \sum_{m=2}^{n} \left( \frac{3}{\tau} \int_{t_{m-1}}^{t_m} |\bar{\partial} v(s)|^2 \, ds \right)^2 \leq 4 |\bar{\partial} v|^2_{L^2[0, t_n \times \Omega]}.
\]

With this and the fact that \( P_h^k \) commutes with the time derivative we conclude

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

For the third term we have

\[
|III| \leq \delta_3 q \tau \sum_{m=q}^{n} |P_h^k c_x^m|^2 + \frac{q}{\delta_3} \tau \sum_{m=q}^{n} |(\bar{\partial} - \partial_t) c_x^m|^2.
\]

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 [cf. 32, p. 169]:

\[
\tau \sum_{m=q}^{n} |(\bar{\partial} - \partial_t) c_x^m|^2 = \tau \sum_{m=q}^{n} \left| \int_{t_{m-q}}^{t_m} [(t - s)q^{(\sigma + 1)}] \partial_t^{\sigma+1} c_x^s \, ds \right|^2 \leq \frac{1}{\tau} \sum_{m=q}^{n} \sum_{j=m-q}^{m} \left| \int_{t_{j-q}}^{t_j} [(t_j - s)q^{\sigma + 1}] \partial_t^{\sigma+1} c_x^s \, ds \right|^2 + \tau \sum_{m=q}^{n} \left| \int_{t_{m-q}}^{t_m} q(t_m - s)q^{\sigma+1} \partial_t^{\sigma+1} c_x^s \, ds \right|^2 \leq \tau^{2q-1} \sum_{m=q}^{n} \left| \int_{t_{m-q}}^{t_m} \partial_t^{\sigma+1} c_x^s \, ds \right|^2 \leq \tau^{2q} |\partial_t^{\sigma+1} c_x^m|^2_{L^2[0, t_n \times \Omega]},
\]
where we used the fact that \( ||\partial_t q^m|| \leq \frac{q}{\tau} \sum_{j=m-q}^m ||v^j|| \), the Leibniz integral rule, and the Jensen inequality. We eventually obtain

\[
|\text{III}| \leq \delta_3 2q\tau \sum_{m=q}^n ||\eta_{c,m}^n||^2 + \delta_3 2q\tau \sum_{m=q}^n ||(P_h^k - I)c^{+=,m}||^2 + \frac{1}{\delta_3} C_3 \tau^{2q}\|\partial_t^{q+1}c^+\|^2_{L^2(\Omega)}
\]

with a constant \( C_3 > 0 \) depending only on \( q \). For the fourth term, we immediately get

\[
|\text{IV}| \leq \delta_4 D_\infty q\tau \sum_{m=q}^n ||\eta_{f,m}^n||^2 + \frac{q}{\delta_4} D_\infty \tau \sum_{m=q}^n ||(\mathbf{I}_h^k - I)j^{+,m}||^2
\]

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 (H7) and (H9), and Lem. 1:

\[
\left\| \mathbf{D}^{-1}(u_h^m \pm E_h^m)\mathcal{M}(c_h^{+,m}) - (u^m \pm E^m)c^{+,m} \right\| \leq D_\infty \left\| (\eta_{u}^m \pm \eta_{E}^m)\mathcal{M}(c_h^{+,m}) \right\| + \left\| (u^m \pm E^m)\left( \mathcal{M}(c_h^{+,m}) - \mathcal{M}(c^{+,m}) \right) \right\| \leq D_\infty \left( M(||\eta_{u}^m|| + ||\eta_{E}^m||) + C_5 ||\eta_{c}^m|| \right)
\]

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

\[
V \leq 2qD_\infty \tau \sum_{m=q}^n \left( \delta_5 \left( ||\eta_{f,m}^n||^2 + ||(\mathbf{I}_h^k - I)j^{+,m}||^2 \right) + \frac{1}{\delta_5} \left( M^2(||\eta_{f,m}^n||^2 + ||\eta_{E}^m||^2) + C_5^2 ||\eta_{c}^m||^2 \right) \right).
\]

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

\[
||r^+(t_m, x, c_h^{+,m}, c_h^{-,m}) - r^+(t_m, x, c^{+,m}, c^{-,m})|| \leq r_L \left\| \left( c_h^{+,m} - (c^{+,m}) \right) \right\| \leq r_L \eta_{c}^m + r_L \eta_{c}^m
\]

holds, where \( r_L \) denotes the Lipschitz constant. Hence,

\[
VI \leq \left( \frac{1}{\delta_6} + \delta_6 \right) 2qr_L \tau \sum_{m=q}^n ||\eta_{c}^m||^2 + \delta_6 2qr_L \tau \sum_{m=q}^n ||\eta_{c}^m||^2 + \frac{1}{\delta_6} 2qr_L \tau \sum_{m=q}^n ||(P_h^k - I)c^{+,m}||^2.
\]

With the estimates of II to VI, it follows from (23) that

\[
||\eta_{c}^n||^2 + 2q \left( D_\infty - \frac{\delta_4}{2} D_\infty - \delta_3 D_\infty \right) \tau \sum_{m=q}^n ||\eta_{c}^m||^2 \leq \left\{ \begin{array}{ll} \frac{1}{2} ||\eta_{c}^0||^2, & \text{q=1} \\ \frac{q^2}{2} ||\eta_{c}^0||^2 + 5 ||\eta_{c}^1||^2, & \text{q=2} \end{array} \right. \]

\[
+ \frac{q^3}{\delta_2} \|\partial_t c^+\|^2_{L^2(\Omega \times \mathbb{R}^d)} + C_3 \tau^{2q} \|\partial_t^{q+1}c^+\|^2_{L^2(\Omega \times \mathbb{R}^d)} + 2q \left( \frac{\delta_2}{2} + \delta_3 + \frac{C_3^2}{\delta_5} D_\infty + \left( \delta_6 + \frac{1}{\delta_6} \right) r_L \right) \tau \sum_{m=q}^n ||\eta_{c}^m||^2 + 2q D_\infty \left( \frac{1}{2} \frac{\delta_4}{2} + \delta_5 \right) \tau \sum_{m=q}^n ||(\mathbf{I}_h^k - I)j^{+,m}||^2 + 2q \left( \delta_3 + \frac{r_L}{\delta_6} \right) \tau \sum_{m=q}^n ||(P_h^k - I)c^{+,m}||^2
\]
The choice of $w$ is $\eta^+_n = P^k_n \eta_p$ in (25b) and the use of the projector property (P3) yields

$$\left( \nabla \cdot \Pi^k_n \eta_n, P^k_n \eta_p \right) = 0 .$$

Choosing the test function $v_h = \Pi^k_h \eta_n \in \mathcal{RT}_h(T_h)$ in (25a), using (P4) and (27), we obtain

$$\left( \mathbf{K}^{-1} \eta_n, \Pi^k_h \eta_n \right) = \left( \mathbf{D}^{-1}(E_h \mathcal{M}(c^+_h - c^-_h) - E(c^+ - c^-)), \Pi^k_h \eta_n \right) .$$

Conclude by accounting for the initial conditions (1j) and by using the projection error estimates of (P6).

**Proposition 4.** Let $(u, p, j^+, c^+, j^-, c^-, E, \phi)$ and $(u^n_k, p^n_k, j^n_k, c^n_k, j^n_k, c^n_k, E^n_k, \phi^n_k)$ be solutions of Prob. 1 and Prob. 3, respectively. Then, if in addition the regularity requirements of (H7) and (H9) are satisfied, for $n \in \{1, \ldots, N\}$,

$$\left\| \eta^+_n \right\|^2_{L^2(\Omega)} + \left\| \eta^-_n \right\|^2_{L^2(\Omega)} \leq h^{2j} \left| u(t_n) \right|^2_{H^1(\Omega)} + h^{2j} \left| p(t_n) \right|^2_{H^1(\Omega)} + h^{2j} \left| E(t_n) \right|^2_{H^1(\Omega)}$$

$$+ h^{2j} \left| \phi(t_n) \right|^2_{H^1(\Omega)} + \sum_{i \in \{+,-\}} \left\| \eta^i_n \right\|^2_{L^2(\Omega)} .$$

**Proof.** The proof can be accomplished analogously to that of Prop. 2 with minor modifications. We suppress the time index $n$ and the argument for the evaluation at $t_n$ in this proof. Due to \{(6a), (6b), (14a), (14b)\}, the error equations read

$$- \left( \mathbf{K}^{-1} \eta_n, v_h \right) + \left( \nabla \cdot v_h, \eta_n \right) = - \left( \mathbf{D}^{-1}(E_h \mathcal{M}(c^+_h - c^-_h) - E(c^+ - c^-)), v_h \right) ,$$

$$\left( \nabla \cdot \eta_n, w_h \right) = 0$$

for all $v_h \in \mathcal{RT}_h(T_h)$ and for all $w_h \in \mathcal{P}_k(T_h)$. The arising force term in (25a) requires a special treatment. Recalling the chosen cut-off level $M$ for the cut-off operator $\mathcal{M}$ (cf. Prop. 3), Lem. 1, and (H9), we see that

$$\left\| \mathcal{M}(c^+_h - c^-_h) - E(c^+ - c^-) \right\| \leq M \left\| \eta_n \right\| + \left\| E \right\|_{L^\infty(\Omega)} \sum_{i \in \{+,-\}} \left\| \eta^i_n \right\| .$$

The choice of $w_h = P^k_n \eta_p \in \mathcal{P}_k(T_h)$ in (25b) and the use of the projector property (P3) yields

$$\left( \nabla \cdot \Pi^k_n \eta_n, P^k_n \eta_p \right) = 0 .$$
With (H1), (H2), (26), we arrive at the estimate
\[
K_u \| \eta_u \|^2 \leq K_{\infty} \| \eta_u \| \| (I_h^2 - I) u \| + D_{\infty} (M \| \eta_E \| + \| E \|_{L^\infty(O)} \sum_{i \in \{+, -\}} \| \eta_{e_i} \|) \left( \| \eta_u \| + \| (I_h^k - I) u \| \right).
\]

Eqn. (15) and the projection error estimates of (P6) yield
\[
\| \eta_u^0 \| \leq h^{2\lambda} |u(t_n)|^2_{H^1(O)} + h^{2\lambda} |E(t_n)|^2_{H^1(O)} + h^{2\lambda} |\phi(t_n)|^2_{H^6(O)} + \sum_{i \in \{+, -\}} \| \eta_{e_i}^0 \|^2_{L^2(O)}.
\]

With a similar treatment of the additional force term, the error estimate for \( \| \eta_E^0 \| \) is obtained analogously to the second part of the proof of Prop. 2.

**Theorem 2** (A priori error estimate). Let \((u, p, j^+, j^-)\), \((c, \phi, e, \phi)\) and \((u_n, p_n, j_n, e_n, \phi)\) be solutions of Prob. 1 and Prob. 3, respectively. Then, in addition the regularity requirements of (H7)–(H9) are satisfied, for \( q \in \{1, 2, 0\} \) and sufficiently small \( \tau \),

\[
\max_{m \in \{q, \ldots, N\}} \| \eta_u^m \|^2_{L^2(O)} + \max_{m \in \{q, \ldots, N\}} \| \eta_E^m \|^2_{L^2(O)} + \sum_{i \in \{+, -\}} \sum_{m = q}^N \| \eta_{e_i}^m \|^2_{L^2(O)} + \sum_{i \in \{+, -\}} \max_{m \in \{q, \ldots, N\}} \| \eta_{e_i}^m \|^2_{L^2(O)} \leq \sum_{i \in \{+, -\}} \sum_{j = 0}^{q-1} \| \eta_i^j \|^2_{L^2(O)} + \tau^{2q} + \sum_{i \in \{1, \ldots, 6\}} h^{2\lambda}.
\]

**Proof.** We sum up (20) for both signs, eliminate the discretization errors of \( c^+ \) on the right-hand side as performed at the end of the proof of Prop. 3, and call the resulting inequality (28). Substitution of \( \sum_{i \in \{+, -\}} \| \eta_{e_i}^m \|^2_{L^2(O)} \) from (28) into \((15), (24)) and summation yields

\[
\| \eta_u^m \|^2 + \| \eta_E^m \|^2 + \| \eta_{e_i}^m \|^2 \leq \sum_{i \in \{+, -\}} \sum_{j = 0}^{q-1} \| \eta_i^j \|^2 + \tau^{2q} \sum_{i \in \{+, -\}} \| \partial_t^{q+1} \partial_i^m \|^2_{L^2([0, \tau] \times \Omega)} + h^{2\lambda} |u(t_n)|^2_{H^1(O)}
\]

\[
+ h^{2\lambda} |p(t_n)|^2_{H^2(O)} + h^{2\lambda} \sum_{i \in \{+, -\}} \sum_{m = q}^n \| \partial_j \partial_i^m \|^2_{H^2(O)} + h^{2\lambda} \sum_{i \in \{+, -\}} \left( \int_0^{t_n} \| \partial_j \partial_i^m \|^2_{H^2(O)} \right) + \tau \sum_{m = q}^n \| c_i^m \|^2_{L^2(O)}
\]

\[
+ h^{2\lambda} |E(t_n)|^2_{H^6(O)} + h^{2\lambda} |\phi(t_n)|^2_{H^6(O)} + \tau \sum_{m = q}^n \| \eta_{e_i}^m \|^2 + \tau \sum_{m = q}^n \| \eta_{e_i}^m \|^2. \tag{29}
\]

Adding (28) to (29) and eliminating the discretization errors of \( u \) and \( E \) on the right-hand side bounds the discretization errors in terms of the true solution. We conclude by bounding the right-hand side by the respective maximum on \( J \) (admissible due to (H7)–(H9)) and obtaining a right-hand side that is independent of \( n \) such that the estimate holds for every \( n \in \{q, \ldots, N\} \).

**4 Numerical Results**

The numerical scheme of Sec. 3 for the lowest-order Raviart–Thomas elements was implemented using the software platform/programming language Matlab [16, 20]. This section
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 $k$th refinement level we have $h = (1/4)^k$, $\tau = T(1/2)^k$.

<table>
<thead>
<tr>
<th>$k$</th>
<th>$\eta_u$</th>
<th>$\eta_p$</th>
<th>$\eta_{j^+}$</th>
<th>$\eta_{c^+}$</th>
<th>$\eta_{j^-}$</th>
<th>$\eta_{c^-}$</th>
<th>$\eta_E$</th>
<th>$\eta_\phi$</th>
</tr>
</thead>
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<tr>
<td>0</td>
<td>3.34E–1</td>
<td>1.82E–1</td>
<td>3.83E–1</td>
<td>2.43E–1</td>
<td>7.50E–1</td>
<td>2.01E–1</td>
<td>3.36E–1</td>
<td>2.01E–1</td>
</tr>
<tr>
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<td>1.04E–1</td>
<td>4.63E–2</td>
<td>1.11E–1</td>
<td>6.25E–2</td>
<td>1.86E–1</td>
<td>5.04E–2</td>
<td>1.86E–1</td>
<td>5.04E–2</td>
</tr>
<tr>
<td>2</td>
<td>2.22E–2</td>
<td>1.14E–2</td>
<td>2.82E–2</td>
<td>1.57E–2</td>
<td>4.93E–2</td>
<td>1.26E–2</td>
<td>2.27E–2</td>
<td>1.26E–2</td>
</tr>
<tr>
<td>3</td>
<td>5.30E–3</td>
<td>2.84E–3</td>
<td>7.07E–3</td>
<td>3.91E–3</td>
<td>1.24E–2</td>
<td>3.14E–2</td>
<td>5.70E–3</td>
<td>5.70E–3</td>
</tr>
</tbody>
</table>

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 2.00 1.91 2.00 1.94
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

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