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Sufficient conditions for the existence of solutions for a thermoelectrochemical problem

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Abstract. A mathematical model is introduced for thermoelectrochemical phenomena in an electrolysis cell, and its qualitative analysis is focused on existence of solutions. The model consists of a system of nonlinear parabolic PDEs in conservation form expressing conservation of energy, mass and charge. On the other hand, an integral form of Newton's law is used to describe heat exchange at the electrolyte/electrode interface, a nonlinear radiation condition is enforced on the heat flux at the wall and a nonlinear boundary condition is considered for the electrochemical flux in order to account for Butler–Volmer kinetics. The main objective is the nonconstant character of each parameter, that is, the coefficients are assumed to be dependent on the spatial variable and the temperature. Making recourse of known estimates of solutions for some auxiliary elliptic and parabolic problems, which are explicitly determined by the Gehring–Giaquinta–Modica theory, we find sufficient smallness conditions on the data to guarantee the existence of the original solutions via the Schauder fixed point argument. These conditions may provide useful information for numerical as well as real applications. We conclude with an example of application, namely the electrolysis of molten sodium chloride.

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1. Introduction

The conservative laws are universal in the description of the physicochemical phenomena. Their particular applications depend on the transport coefficients behavior. The introduction of the thermal effects into physicochemical devices are being addressed by applied mathematicians [27]. Quantitative description of the heat rate data is discussed in [4, 16]. The model parameters (such as the electrical mobilities u_i and the thermal conductivity k, among others) are assumed to be constant positive quantities whose values are specified to numerical simulations. Our first shortcoming is that these coefficients are commonly discontinuous.

In view of the above discussion, we develop a thermoelectrochemical model for an electrolyte domain. Our second shortcoming is that the physicochemical phenomena truly pass on the boundary of the domain. We mention [33] for a mathematical modeling of the interaction of electric, thermal, and diffusion processes in infinitely diluted solutions of electrolytes. The production of nuclear grade heavy water, including water electrolysis, distillation, and chemical exchange processes, provide a process matched to the feed supply [23, 31]. We refer the reader to [21] for a mathematical model of Li-ion batteries based exclusively on universally accepted principles of nonequilibrium thermodynamics and the assumption of the one-step intercalation reaction at the interface of electrolyte and active particles; and to [24, 32] for other attractive thermoelectrochemical approaches.

In thermoelectrochemical modeling, the force-flux relations are (see, at the steady-state, [8] and the references therein)

$$\begin{aligned} \mathbf{q} &= -\mathsf{K}\nabla\theta - R\theta^2\sum_{i=1}^{I} D_i'\nabla c_i - \Pi\sigma\nabla\phi; \\ \mathbf{J}_i &= -c_iS_i\nabla\theta - D_i\nabla c_i - u_ic_i\nabla\phi \quad (i=1,\dots,I); \\ \mathbf{j} &= -\alpha\sigma\nabla\theta - F\sum_{i=1}^{I} z_iD_i\nabla c_i - \sigma\nabla\phi. \end{aligned} \tag{1.1}$$

Here, $\mathbf{q}$, $\mathbf{J}_i$ and $\mathbf{j}$ are, respectively, the measurable heat flux (in $\mathrm{W}\cdot\mathrm{m}^{-2}$), the ionic flux of component i (in $\mathrm{mol}\cdot\mathrm{m}^{-2}\cdot\mathrm{s}^{-1}$), and the electric current density (in $\mathrm{C}\cdot\mathrm{m}^{-2}\cdot\mathrm{s}^{-1}$). The unknown functions are the temperature θ, the molar concentration vector $\mathbf{c}=(c_1,\dots,c_I)$, and the electric potential ϕ. Hereafter the subscript i stands for the correspondence to the ionic component i intervener in the reaction process. As the problem involves several symbols, we summarize their notation in the Appendix. In particular, K denotes the thermal conductivity tensor, reflecting anisotropic properties of the medium. Also the Peltier coefficient Π can be a tensor [3]. For this reason, we keep both α and Π as known functions, although the first Kelvin relation correlates Π with the Seebeck coefficient α. All transport coefficients can be either experimentally measured or calculated as dependent on temperature and spatial variable, while the Soret effect and the related Dufour effect include the concentration of the corresponding ionic component [17, 22].

Dealing with these issues, our main concerns are:

- from the physical point of view, to introduce thermal radiation on one part of the boundary, and to approach the Butler–Volmer equation on the other part of the boundary;
- from the mathematical point of view, to find sufficient explicit conditions for the existence of solutions, under minimal assumptions on the transport coefficients, as a consequence of the fixed point theory.

The key of an integrability exponent larger than n for the solution (say in n space dimensions) is the need of making severe restrictions on the corresponding leading coefficient function—as is carried out in the literature [10].

2. Statement of the problem and main theorem

Let $T > 0$ be an arbitrary (but preassigned) time, and let Ω represent an electrolysis cell, which consists (as in general) of two electrodes and an electrolyte. We abbreviate $Q_T = \Omega \times]0, T[$.

From the conservation of energy, the mass balance equations, and the conservation of electric charge, we derive, respectively, in Q_T

$$\rho c_\mathrm{p} \frac{\partial \theta}{\partial t} + \nabla \cdot \mathbf{q} = 0; \tag{2.1}$$

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i = 0; \tag{2.2}$$

$$\nabla \cdot \mathbf{j} = 0, \tag{2.3}$$

where the density ρ and the specific heat capacity c_p (at constant volume) are assumed to be (positive) constants. The absence of external forces, assumed in (2.1)–(2.3), is due to their occurrence at the surface of the electrodes.

The boundary $\partial\Omega$ is decomposed into four pairwise disjoint open subsets Γ_l, $l = \mathrm{a}, \mathrm{c}, \mathrm{w}, \mathrm{o}$, representing, respectively, the anode, the cathode, the wall, and the (remaining) outer surfaces such that (cf. Figure 1)

$$\partial\Omega = \overline{\Gamma}_\mathrm{a} \cup \overline{\Gamma}_\mathrm{c} \cup \overline{\Gamma}_\mathrm{w} \cup \overline{\Gamma}_\mathrm{o}.$$

For the sake of simplicity, we denote the electrode/electrolyte interface

$$\Gamma_\mathrm{e} = \Gamma_\mathrm{a} \cup \Gamma_\mathrm{c}$$

by simply Γ, and we set $\Sigma_T = \Gamma_\mathrm{w} \times]0, T[$. Hence further, for each $l = \mathrm{a}, \mathrm{c}, \mathrm{w}$, θ_l represents a given temperature at Γ_l, and $\mathbf{n}$ is the outward unit normal to the boundary $\partial\Omega$.

The parabolic-elliptic system (2.1)–(2.3) is accomplished by the following boundary conditions. For a.e. in $]0, T[$, we consider the heat balance described by the global Newton law of cooling

$$\int_{\Gamma_\mathrm{a}} \mathbf{q} \cdot \mathbf{n} \, \mathrm{ds} + \int_{\Gamma_\mathrm{c}} \mathbf{q} \cdot \mathbf{n} \, \mathrm{ds} = \int_{\Gamma_\mathrm{e}} h_\mathrm{C} (\theta - \theta_\mathrm{e}) \, \mathrm{ds}, \tag{2.4}$$

where

$$\theta_\mathrm{e} = \begin{cases} \theta_\mathrm{a} & \text{on } \Gamma_\mathrm{a}, \\ \theta_\mathrm{c} & \text{on } \Gamma_\mathrm{c}, \end{cases}$$

and h_C denotes the conductive heat transfer coefficient. By the constitutive law (1.1) of $\mathbf{q}$, the left-hand side of (2.4) says that the heat generated is divided into the irreversible reaction heat due to efficiency losses of the electrode reaction, and the reversible reaction heat mainly due to the entropy change of the electrode reaction which is called Peltier heat and changes sign with changing current direction (cf. [15]).

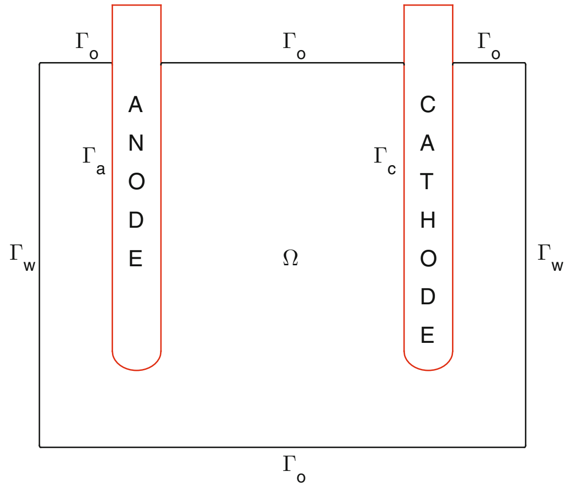

Figure 1. Schematic sagittal representation of an electrolytic cell (with corners being smoothed by circumferences).

A gas bubble behavior at a hydrogen-evolution electrode was reported by some researchers [5, 19, 30]. This hydrogen gas generated at the cathode causes turbulence of water or wastewater flow (see [6]). At each electrode/electrolyte interface ($l = \mathrm{a}, \mathrm{c}$), we consider

$$-Fz_i\mathbf{J}_i\cdot\mathbf{n}_l = g_{i,l}(\cdot,\theta,\phi).$$

Here, $g_{i,l}$ may represent the generalized Butler–Volmer kinetics that is composed by the involved charge and mass balances in the charge-transfer reaction under illumination [28], and the Butler–Volmer expression itself

$$J_l\left(\exp\left[\frac{\beta_i s_l F\eta}{R\theta}\right]-\exp\left[-\frac{(1-\beta_i)s_l F\eta}{R\theta}\right]\right), \tag{2.5}$$

where J_l represents the transfer (exchange) current density due to the electrode reaction, s_l is the stoichiometric coefficient of electrons in the anode/cathode ($l = \mathrm{a}, \mathrm{c}$), β_i is the transfer coefficient ($i = 1, \dots, I$), and $\eta = \phi - \phi_{\mathrm{eq}}$ denotes the surface overpotential.

Although the electroneutrality assumption says that

$$\mathbf{j} = \sum_{i=1}^{I} z_i F\mathbf{J}_i,$$

we consider

$$-\mathbf{j}\cdot\mathbf{n} = g \quad \text{on } \Gamma\times\,]0,T[, \tag{2.6}$$

with g being a prescribed surface electric current assumed to be tangent to the surface for all $t > 0$. We refer as an open problem for the nonlocal Dirichlet boundary condition for the electric potential, $\phi = j(I)$ [12], on the part of the boundary (Γ_{e}) where the device is connected to the circuit, with j being a nonlinear function and

$$I = \int_{\Gamma_{\mathrm{e}}} \sigma(\theta) \frac{\partial \phi}{\partial n}$$

denoting the total current, when the voltage drop across the electrical circuits is not prescribed but is coupled to the remainder circuit.

Let temperature fulfill the radiative condition over $\Gamma_{\mathrm{w}} \times]0, T[$

$$\mathbf{q} \cdot \mathbf{n} = h_{\mathrm{R}} \, |\theta|^{\ell-2} \, \theta - \gamma. \tag{2.7}$$

This general exponent $\ell \geq 2$ (see [7]) accounts for the radiation behavior of the heavy water electrolysis [11, 20], namely the Stefan–Boltzmann radiation law if $\ell = 5$ with h_{R} denoting the radiative heat transfer coefficient; i.e.,

$$h_{\mathrm{R}} = \sigma_{\mathrm{SB}} \, \epsilon \quad \text{and} \quad \gamma = \sigma_{\mathrm{SB}} \, \alpha \, \theta_{\mathrm{w}}^4.$$

The parameters, the emissivity ϵ and the absorptivity α, both depend on the spatial variable and the temperature function θ.

The following outflows are considered:

$$\mathbf{q} \cdot \mathbf{n} = 0 \qquad \text{on } \Gamma_{\mathrm{o}} \times]0, T[; \tag{2.8}$$

$$\mathbf{J}_i \cdot \mathbf{n} = \mathbf{j} \cdot \mathbf{n} = 0, \quad i = 1, \ldots, I, \quad \text{on } (\Gamma_{\mathrm{w}} \cup \Gamma_{\mathrm{o}}) \times]0, T[. \tag{2.9}$$

Finally, the following initial conditions for all x in Ω are assumed:

$$\theta(x, 0) = \theta_0(x), \quad c_i(x, 0) = c_i^0(x), \quad i = 1, \ldots, I. \tag{2.10}$$

In the framework of Sobolev and Lebesgue functional spaces, we use the following spaces of test functions:

$$V_{p,\ell}(Q_T) = \left\{ v \in L^p\big(0, T; W^{1,p}(\Omega)\big) : v|_{\Sigma_T} \in L^\ell(\Sigma_T) \right\};$$
$$V_p(\Omega) = \left\{ v \in W^{1,p}(\Omega) : \int_{\partial\Omega} v \, \mathrm{ds} = 0 \right\},$$

with their usual norms, $p, \ell > 1$.

In order to derive our variational problem, we note that every ionic mobility $u_i = z_i D_i F / (R\theta)$ satisfies the Nernst–Einstein relation $\sigma_i = F z_i u_i c_i$, with $\sigma_i = t_i \sigma$ representing ionic conductivity, and t_i is the transference number (or transport number) of species i.

Then our variational problem under study is as follows.

($\mathcal{P}$) Find the triple temperature-concentration-potential $(\theta, \mathbf{c}, \phi)$ that verifies the variational problem

$$\begin{aligned}
&\rho c_{\mathrm{p}}\int_0^T \langle \partial_t\theta, v\rangle \,\mathrm{dt} + \int_{Q_T} \big(\mathsf{K}(\cdot,\theta)\nabla\theta\big)\cdot\nabla v \,\mathrm{dx}\,\mathrm{dt}\\
&\quad + \int_{\Sigma_T} h_{\mathrm{R}}(\cdot,\theta)\,|\theta|^{\ell-2}\,\theta v \,\mathrm{ds}\,\mathrm{dt} + \int_0^T\int_\Gamma h_{\mathrm{C}}(\cdot,\theta)\theta v\,\mathrm{ds}\,\mathrm{dt}\\
&\quad = \int_0^T\int_\Gamma h_{\mathrm{C}}(\cdot,\theta)\theta_{\mathrm{e}} v\,\mathrm{ds}\,\mathrm{dt} + \int_{\Sigma_T}\gamma(\cdot,\theta)v\,\mathrm{ds}\,\mathrm{dt} \qquad (2.11)\\
&\qquad - \int_{Q_T}\left(R\theta^2\sum_{i=1}^I D_i'(\cdot,c_i,\theta)\nabla c_i + \Pi(\cdot,\theta)\,\sigma(\cdot,\theta)\nabla\phi\right)\cdot\nabla v\,\mathrm{dx}\,\mathrm{dt}\\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \forall v\in V_{p',\ell}(Q_T);
\end{aligned}$$

$$\begin{aligned}
&\int_0^T \big\langle\partial_t c_i, v\big\rangle\,\mathrm{dt} + \int_{Q_T} D_i(\cdot,\theta)\nabla c_i\cdot\nabla v\,\mathrm{dx}\,\mathrm{dt}\\
&\quad = \int_0^T\int_\Gamma g_i(\cdot,\theta,\phi)v\,\mathrm{ds}\,\mathrm{dt} \qquad (2.12)\\
&\qquad - \int_{Q_T}\left(c_iS_i(\cdot,c_i,\theta)\nabla\theta + \frac{t_i}{Fz_i}\sigma(\cdot,\theta)\nabla\phi\right)\cdot\nabla v\,\mathrm{dx}\,\mathrm{dt}\\
&\qquad\qquad\qquad \forall v\in L^{p'}\big(0,T;W^{1,p'}(\Omega)\big),\quad i=1,\dots,I;
\end{aligned}$$

$$\begin{aligned}
&\int_\Omega \sigma(\cdot,\theta)\nabla\phi\cdot\nabla v\,\mathrm{dx}\\
&\quad = -\int_\Omega\left(\alpha(\cdot,\theta)\,\sigma(\cdot,\theta)\nabla\theta + F\sum_{i=1}^I z_i\,D_i(\cdot,\theta)\nabla c_i\right)\cdot\nabla v\,\mathrm{dx} \qquad (2.13)\\
&\qquad + \int_\Gamma gv\,\mathrm{ds} \qquad \forall v\in V_{p'}(\Omega),\quad \text{a.e. in } [0,T[,
\end{aligned}$$

where p' accounts for the conjugate exponent of p: $p' = p/(p-1)$.

We assume the following.

(H1) The electrical conductivity, Peltier, Seebeck, Soret, Dufour, and diffusion coefficients $\sigma,\Pi,\alpha,S_i,D_i',D_i$ $(i=1,\dots,I)$ are Carathéodory functions, i.e., measurable with respect to $x\in\Omega$ and continuous with respect to other variables, such that

$$\exists\sigma_\#,\sigma^\# > 0: \qquad \sigma_\# \le \sigma(x,e)\le\sigma^\#; \tag{2.14}$$

$$\exists\Pi^\# > 0: \qquad |\Pi(x,e)\mathbf{a}| \le \Pi^\#|\mathbf{a}|; \tag{2.15}$$

$$\exists\alpha^\# > 0: \qquad |\alpha(x,e)| \le \alpha^\#; \tag{2.16}$$

$$\exists S_i^\# > 0: \qquad |dS_i(x,d,e)| \le S_i^\#; \tag{2.17}$$

$$\exists (D_i')^\# > 0: \qquad Re^2|D_i'(x,d,e)| \le (D_i')^\#; \tag{2.18}$$

$$\exists D_i^\# > 0: \qquad F|z_i|D_i(x,e) \le D_i^\#; \tag{2.19}$$

$$\exists (D_i)_\# > 0: \qquad D_i(x,e) \ge (D_i)_\#, \tag{2.20}$$

for a.e. $x\in\Omega$, for all $\mathbf{a}\in\mathbb{R}^n$, and for all $d,e\in\mathbb{R}$.

(H2) The thermal conductivity $\mathsf{K} : \Omega \times \mathbb{R} \to \mathbb{M}_{n\times n}$ is a Carathéodory tensor, where $\mathbb{M}_{n\times n}$ denotes the set of $n \times n$ matrices, such that

$$\exists k_\# > 0 : \quad K_{jl}(x,e)\xi_j\xi_l \geq k_\#|\xi|^2 \quad \text{for a.e. } x \in \Omega,\ \forall e \in \mathbb{R}, \tag{2.21}$$

for all $\xi \in \mathbb{R}^n$, under the summation convention over repeated indices: $\mathsf{A}\mathbf{a} \cdot \mathbf{b} = A_{jl}a_j b_l = \mathbf{b}^\top \mathsf{A}\mathbf{a}$; and

$$\exists k^\# > 0 : \quad |K_{jl}(x,e)| \leq k^\# \quad \text{for a.e. } x \in \Omega,\ \forall e \in \mathbb{R}, \tag{2.22}$$

for all $j, l \in \{1, \ldots, n\}$.

(H3) The boundary operator h_R is a Carathéodory function from $\Gamma_\mathrm{w} \times \mathbb{R}$ into $\mathbb{R}$ such that

$$\exists b_\#, b^\# > 0 : \quad b_\# \leq h_\mathrm{R}(x,e) \leq b^\# \quad \text{for a.e. } x \in \Gamma_\mathrm{w},\ \forall e \in \mathbb{R}. \tag{2.23}$$

(H4) The transference coefficient $t_i \in L^\infty(\Omega)$ is such that

$$\exists t_i^\# > 0 : \quad 0 \leq t_i(x) \leq F|z_i|t_i^\# \quad \text{for a.e. } x \in \Omega. \tag{2.24}$$

(H5) For some $\delta > 0$, $g \in L^{2+\delta}(\Gamma)$ such that $\int_\Gamma g \,\mathrm{ds} = 0$.

(H6) For some $\delta > 0$, $\theta_\mathrm{e} \in L^{2+\delta}(\Gamma \times]0,T[)$, and the boundary operators γ and h_C are Carathéodory functions from $\Gamma_\mathrm{w} \times]0,T[\times \mathbb{R}$ and $\Gamma \times]0,T[\times \mathbb{R}$, respectively, into $\mathbb{R}$, i.e., measurable with respect to (x,t) and continuous with respect to the real variable. Moreover, they satisfy

$$\exists \gamma_\mathrm{w} \in L^{2+\delta}(\Sigma_T) : \qquad |\gamma(x,t,e)| \leq \gamma_\mathrm{w}(x,t) \quad \text{for a.e. } x \in \Gamma_\mathrm{w}; \tag{2.25}$$

$$\exists h_\mathrm{C}^\# > 0 : \qquad 0 \leq h_\mathrm{C}(x,t,e) \leq h_\mathrm{C}^\# \quad \text{for a.e. } x \in \Gamma \tag{2.26}$$

for a.e. $t \in]0,T[$, and for all $e \in \mathbb{R}$.

(H7) For some $\delta > 0$, and for each $i = 1, \ldots, I$, the boundary operator

$$g_i = g_{i,\mathrm{a}}\chi_{\Gamma_\mathrm{a}} + g_{i,\mathrm{c}}\chi_{\Gamma_\mathrm{c}}$$

is a Carathéodory function from $\Gamma \times]0,T[\times \mathbb{R} \times \mathbb{R}$ into $\mathbb{R}$ and there exists $\gamma_i \in L^{2+\delta}(\Gamma \times]0,T[)$ such that

$$\exists g_i^\# \geq 0 : \quad |g_i(x,t,e,d)| \leq \gamma_i(x,t) + g_i^\#(|d| + |e|) \tag{2.27}$$

for a.e. $(x,t) \in \Gamma \times]0,T[$, and for all $e, d \in \mathbb{R}$.

(H8) For some $\delta > 0$, $\theta_0, c_i^0 \in L^{2+\delta}(\Omega)$, $i = 1, \ldots, I$.

For the sake of simplicity, we assume in (H5)–(H8) the same designation $\delta > 0$. Note that (2.27) is verified for a truncated version of the Butler–Volmer expression (2.5).

The main interest of the mathematical model under study (governing equations and boundary conditions) is strictly related to real-world applications (thermoelectrochemical phenomena in an electrolysis cell Ω). In this respect, the consideration of a number n of space dimensions greater than 3 is not really relevant. From the mathematical point of view, the broader dimensional range, if available, is more meaningful in fact. Therefore, we state our main result in the unified way.

Theorem 2.1. *Under hypotheses* (H1)–(H8), *there exists a solution*

$$(\theta, \mathbf{c}, \phi) \in V_{p,\ell}(Q_T) \times [L^p(0,T; W^{1,p}(\Omega))]^I \times V_p(\Omega),$$

for some $p > 2$, *to* (2.11)–(2.13) *with the initial condition* (2.10) *if provided by the smallness conditions* (5.11) *and* (5.12)–(5.13).

Remark 2.2. The existence of p is restricted to $[2, 2+\delta]$, where $\delta > 0$ is chosen smaller than $\min\{2/[n(\upsilon-1)], 1/(\varkappa-1)\}$ with $\upsilon, \varkappa > 1$ being well-determined constants by the Gehring–Giaquinta–Modica theory [1, 2, 14].

3. Strategy of the proof of Theorem 2.1

In this section we discuss the key of the proof, and we recall a known result for the solvability. The proof of Theorem 2.1 is based on the Schauder fixed point theorem [35]. We keep the concentration-temperature pair $(\mathbf{c}, \theta)$ in the closed convex set

$$\mathcal{K} = \Big\{ (\mathbf{v}, v) \in [L^p(0,T; W^{1,p}(\Omega))]^I \times V_{p,\ell}(Q_T) : \|\nabla v\|_{p,Q_T} + \|v\|_{\ell,\Sigma_T} \leq R, \\ \|\nabla v_i\|_{p,Q_T} + \|v_i\|_{p,Q_T} \leq R_i,\ i = 1, \ldots, I \Big\},$$

where $p, \ell \geq 2$, and we built the well-defined functional $\mathcal{T}$ such that

$$(\mathbf{c}, \theta) \in \mathcal{K} \mapsto \phi \in V_p(\Omega) \mapsto (\mathbf{\Psi}, \Theta), \tag{3.1}$$

where ϕ, $\mathbf{\Psi}$, and Θ are the unique functions given in Propositions 4.1, 4.2, and 4.3, respectively. Their proofs rely on existence results due to a weak reverse Hölder inequality for local solutions [1, 2, 14]. For the reader's convenience, we recall the parabolic existence result [2, 14].

Theorem 3.1. *Let* Ω *be a* C^1 *domain,* $T > 0$, *and let assumptions* (2.21)–(2.23) *be fulfilled. There exists* $\upsilon > 1$ *such that for any* $0 < \delta < 2/[n(\upsilon - 1)]$ *and* $p \in [2, 2+\delta]$ *if* $\mathbf{f} \in \mathbf{L}^{2+\delta}(Q_T)$, $f \in L^{2+\delta}(\Gamma \times]0,T[)$, $H \in L^{2+\delta}(\Sigma_T)$, *and* $u_0 \in L^{2+\delta}(\Omega)$, *then the variational problem*

$$\int_0^T \langle \partial_t u, v \rangle \,\mathrm{dt} + \int_{Q_T} (\mathsf{K}\nabla u) \cdot \nabla v \,\mathrm{dx}\,\mathrm{dt} + \int_{\Sigma_T} h_{\mathrm{R}}(u)|u|^{\ell-2} u v \,\mathrm{ds}\,\mathrm{dt} \\ = \int_{Q_T} \mathbf{f} \cdot \nabla v \,\mathrm{dx}\,\mathrm{dt} + \int_0^T \int_\Gamma f v \,\mathrm{ds}\,\mathrm{dt} + \int_{\Sigma_T} H v \,\mathrm{ds}\,\mathrm{dt} \quad \forall v \in V_{p',\ell}(Q_T) \tag{3.2}$$

has a solution u *in* $L^{p,\infty}(Q_T) \cap V_{p,\ell+p-2}(Q_T)$ *such that* $\partial_t u \in [V_{p',\ell}(Q_T)]'$, *and it verifies*

$$\operatorname*{ess\,sup}_{t \in [0,T]} \|u\|^p_{p,\Omega}(t) \leq \mathcal{H}(k_\#, b_\#, p) \exp[(p-1)T]; \tag{3.3}$$

$$\|u\|^{\ell+p-2}_{\ell+p-2,\Sigma_T} \leq (b_\#)^{-1} \mathcal{H}(k_\#, b_\#, p) \left(1 + (p-1)T \exp[(p-1)T]\right); \tag{3.4}$$

$$
\begin{aligned}
\|\nabla u\|_{p,Q_T} \leq \mathcal{C}(k_\#)^{-1} \\
& \times \Bigg[\sqrt{k_\# \mathcal{H}(k_\#, b_\#, 2)\,(1+T\exp[T])} \\
& + \sqrt{1+k_\#}\, \Big(\|\mathbf{f}\|_{p,Q_T} + K_{2n/(n+1)} \\
& \qquad \times \big[\|f\|_{p,\Gamma\times]0,T[} + \|H\|_{p,\Sigma_T} \big] \Big) \Bigg],
\end{aligned}
\tag{3.5}
$$

with

$$
\begin{aligned}
\mathcal{H}(k_\#, b_\#, p) = \|u_0\|^p_{p,\Omega} + \left(\frac{p-1}{k_\#}\right)^{p/2} \|\mathbf{f}\|^p_{p,Q_T} \\
& + \frac{p(\ell-1)}{(\ell+p-2)b_\#^{(p-1)/(\ell-1)}} \int_{\Sigma_T} |H|^{\frac{\ell+p-2}{\ell-1}}\, \mathrm{d}s\, \mathrm{d}t \\
& + (p-1)\left(\left(\frac{p^2}{2k_\#(p-1)} \right)^{1/(p-1)} + 1 \right) \\
& \times K^{2/(p-1)}_{2n/(n+1)} |\Omega|^{[(p-1)n]^{-1}} \|f\|^{p'}_{p',\Gamma\times\,]0,T[}.
\end{aligned}
$$

Here, $K_{2n/(n+1)}$ *stands for the continuity constant of the trace embedding*

$$W^{1,2n/(n+1)}(\Omega) \hookrightarrow L^2(\Gamma),$$

and $\mathcal{C}$ *is a positive constant depending only on* υ*,* p*,* n*, and* Ω*. In particular, if* $b_\# = 0$ *and* $f = 0$*, then* (3.3) *and* (3.5) *remain true by replacing* $\mathcal{H}(k_\#, b_\#, p)$ *by*

$$
\begin{aligned}
\mathcal{H}(k_\#, p) = \|u_0\|^p_{p,\Omega} + \left(\frac{p-1}{k_\#}\right)^{p/2} \|\mathbf{f}\|^p_{p,Q_T} \\
& + (p-1)\left(\left(\frac{p^2}{2k_\#(p-1)} \right)^{1/(p-1)} + 1 \right) \\
& \times K^{2/(p-1)}_{2n/(n+1)} |\Omega|^{[(p-1)n]^{-1}} \|H\|^{p'}_{p',\Sigma_T}.
\end{aligned}
\tag{3.6}
$$

Remark 3.2. By the Aubin–Lions theorem [25], we have that $u \in L^p(Q_T)$, and the initial condition $u(0) = u_0$ makes sense at least in $L^p(\Omega)$.

4. Existence of auxiliary solutions

Let us establish the existence of solutions according to Section 3. Fix

$$\delta \in]0, 2/[n(\upsilon-1)][,$$

with $\upsilon > 1$ being given from Theorem 3.1.

First, let us recall the existence of the required auxiliary potential solving a second order elliptic equation of divergence form with a discontinuous leading coefficient.

Proposition 4.1 (Auxiliary potential). *Let* $\delta > 0$, $t \in]0,T[$,

$$\theta(t), c_i(t) \in W^{1,2+\delta}(\Omega) \quad \textit{for every } i = 1,\dots,I,$$

let $g \in L^{2+\delta}(\partial\Omega)$ *verify that*

$$\int_{\partial\Omega} g \,\mathrm{ds} = 0,$$

and let (2.14), (2.16), *and* (2.19) *hold. Then there exists* $\varkappa > 1$ *such that the Neumann problem* (2.13) *is uniquely (up to constants) solvable in* $W^{1,p}(\Omega)$ *for any* $p \in [2, 2+\delta] \cap [2, 2+1/(\varkappa-1)[$. *Moreover, for each* $]0,T[$ *we have*

$$\sigma_\# \|\nabla\phi\|_{2,\Omega} \le K\|g\|_{2,\Gamma} + \sigma^\#\alpha^\#\|\nabla\theta\|_{2,\Omega} + \sum_{j=1}^{I} D_j^\# \|\nabla c_j\|_{2,\Omega}; \tag{4.1}$$

$$\begin{aligned} \|\nabla\phi\|_{p,\Omega} \le M_1\|\nabla\phi\|_{2,\Omega} + M_2(\sigma_\#)^{-1}\sqrt{2(1+\sigma_\#)}\,\|\mathcal{F}(\theta,\mathbf{c})\|_{p,\Omega} \\ + M_3(\sigma_\#)^{-1}\sqrt{2+2^{-1/n}\sigma_\#}\,\|g\|_{p,\Gamma}, \end{aligned} \tag{4.2}$$

where K *stands for a positive constant depending on* n *and* Ω,

$$\mathcal{F}(\theta,\mathbf{c}) = \sigma^\#\alpha^\#\,|\nabla\theta| + \sum_{j=1}^{I} D_j^\#\,|\nabla c_j|,$$

and M_1, M_2, *and* M_3 *are positive constants depending on* n, p, $\varkappa$, *and* Ω.

Proof. The existence of a weak unique solution satisfying (4.1) is classical (for details see, for instance, [9]). A similar proof of the regularity estimate (4.2) can be found in [1, 2]. □

The existence of the auxiliary concentration-temperature pair $(\mathbf{\Psi}, \Theta)$ is a consequence of Theorem 3.1 as follows.

Proposition 4.2 (Auxiliary concentration vector). *Let* $\theta \in L^p(0,T;W^{1,p}(\Omega))$ *and* $\phi \in V_p(\Omega)$ *be in accordance with Proposition* 4.1, *with*

$$p \in [2, 2+\delta] \cap [2, 2+1/(\varkappa-1)[.$$

Under assumptions (2.14), (2.17), (2.19), (2.20), (2.24), *and* (2.27), *there exists a function* $\mathbf{\Psi} \in [L^p(0,T;W^{1,p}(\Omega))]^I$ *which is the unique solution to the variational problem*

$$\begin{aligned} &\int_0^T \langle \partial_t \Psi_i, v\rangle \,\mathrm{dt} + \int_{Q_T} D_i(\theta)\nabla\Psi_i \cdot \nabla v \,\mathrm{dx}\,\mathrm{dt} \\ &\quad = \int_0^T \int_\Gamma g_i(\theta,\phi) v \,\mathrm{ds}\,\mathrm{dt} - \int_{Q_T} \left(c_i S_i(c_i,\theta)\nabla\theta + \frac{t_i}{F z_i}\,\sigma(\theta)\nabla\phi \right) \cdot \nabla v \,\mathrm{dx}\,\mathrm{dt} \end{aligned} \tag{4.3}$$

for each $i = 1,\dots,I$ *and for all* $v \in L^{p'}(0,T;W^{1,p'}(\Omega))$. *In particular,*

$$\partial_t \mathbf{\Psi} \in [L^p(0,T;[W^{1,p'}(\Omega)]')]^I \quad \textit{and} \quad \mathbf{\Psi} \in [C([0,T];L^2(\Omega))]^I.$$

Moreover, for every $i = 1, \ldots, I$, we have

$$\begin{aligned}
\|\Psi_i\|_{p,Q_T}^p &\le T\|\Psi_i\|_{\infty,p,Q_T}^p \\
&\le T\exp\big[(p-1)T\big] \\
&\quad \times \Bigg[\|c_{0,i}\|_{p,\Omega}^p + \left(\frac{p-1}{(D_i)_\#}\right)^{p/2} \\
&\qquad \times \Big(S_i^\# \|\nabla\theta\|_{p,Q_T} + t_i^\# \sigma^\# \|\nabla\phi\|_{p,Q_T}\Big)^p \\
&\qquad + \left(\left(\frac{p^2(p-1)^{p-2}}{2(D_i)_\#}\right)^{1/(p-1)} + p - 1\right) K_{\frac{2n}{n+1}}^{2p'/p} |\Omega|^{p'(pn)^{-1}} \\
&\qquad \times \bigg(\|\gamma_i\|_{p',\Gamma\times\,]0,T[} + g_i^\# K_{\frac{pn}{n+p-1}} |\Omega|^{1-1/p} \\
&\qquad\quad \times \big(\|\nabla\theta\|_{p,Q_T} + \|\theta\|_{p,Q_T} + P_p\|\nabla\phi\|_{p,Q_T}\big)\bigg)^{p'} \Bigg];
\end{aligned} \tag{4.4}$$

$$\begin{aligned}
\|\nabla\Psi_i\|_{p,Q_T} &\le \mathcal{C}(D_i)_\#^{-1} \Bigg[\sqrt{(D_i)_\#(1+T\exp[T])}\,\|c_{0,i}\|_{2,\Omega} + \mathcal{G}_i^\# \\
&\qquad + X_i\,\|\nabla\phi\|_{2,Q_T} + Y_i\,\|\nabla\phi\|_{p,Q_T} \\
&\qquad + \Big(S_i^\# \mathcal{Z}\big(|Q_T|^{1/2-1/p}, (D_i)_\#, 1\big) + \mathcal{Q}_i\Big) \\
&\qquad \times \big(\|\nabla\theta\|_{p,Q_T} + \|\theta\|_{p,Q_T}\big)\Bigg],
\end{aligned} \tag{4.5}$$

with

$$\begin{aligned}
\mathcal{G}_i^\# = K_{2n/(n+1)} \bigg(&\sqrt{(1+T\exp[T])(2+(D_i)_\#)\,|\Omega|^{1/n}}\,\|\gamma_i\|_{2,\Gamma\times\,]0,T[} \\
&+ \sqrt{1+(D_i)_\#}\,\|\gamma_i\|_{p,\Gamma\times\,]0,T[}\bigg);
\end{aligned} \tag{4.6}$$

$$X_i = \sqrt{1+T\exp[T]}\left(t_i^\#\sigma^\# + g_i^\#\sqrt{2+(D_i)_\#}|\Omega|^{\frac{1+1/n}{2}} K_{\frac{2n}{n+1}}^2 P_2\right); \tag{4.7}$$

$$Y_i = \sqrt{1+(D_i)_\#}\left(t_i^\#\sigma^\# + g_i^\# K_{\frac{2n}{n+1}} K_{\frac{pn}{n+p-1}} |\Omega|^{1-1/p} P_p\right); \tag{4.8}$$

$$\begin{aligned}
\mathcal{Q}_i = K_{2n/(n+1)} g_i^\# \bigg(&\sqrt{1+(D_i)_\#}\,K_{pn/(n+p-1)}|\Omega|^{1-1/p} \\
&+ \sqrt{(1+T\exp[T])(2+(D_i)_\#)|\Omega|^{1/n}} \\
&\times K_{2n/(n+1)}|\Omega|^{1-1/p}T^{1/2-1/p}\bigg);
\end{aligned} \tag{4.9}$$

$$\mathcal{Z}(a,d,e) = a\sqrt{1+T\exp[T]} + e\sqrt{1+d}, \quad a, d, e > 0, \tag{4.10}$$

and P_p stands for the Poincaré constant corresponding to the space exponent p.

Proof. The existence of the required auxiliary concentration vector is a consequence of Theorem 3.1 and Remark 3.2. In particular, we have

$$\begin{aligned}\|\nabla\Psi_i\|_{p,Q_T} \leq \mathcal{C}(D_i)_\#^{-1}\Bigg[&\sqrt{(D_i)_\#(1+T\exp[T])}\,\|c_{0,i}\|_{2,\Omega} + H_i(\theta,\phi)\\ &+ t_i^\#\sigma^\#\left(\sqrt{1+T\exp[T]}\,\|\nabla\phi\|_{2,Q_T} + \sqrt{1+(D_i)_\#}\,\|\nabla\phi\|_{p,Q_T}\right)\\ &+ S_i^\#\left(\sqrt{1+T\exp[T]}\,\|\nabla\theta\|_{2,Q_T} + \sqrt{1+(D_i)_\#}\,\|\nabla\theta\|_{p,Q_T}\right)\Bigg],\end{aligned}$$

with

$$\begin{aligned}H_i(\theta,\phi) = \mathcal{G}_i^\# + K_{2n/(n+1)}g_i^\#\Bigg(&\sqrt{1+(D_i)_\#}\,\left(\|\theta\|_{p,\Gamma\times]0,T[} + \|\phi\|_{p,\Gamma\times]0,T[}\right)\\ &+ \sqrt{(1+T\exp[T])(2+(D_i)_\#)|\Omega|^{1/n}}\\ &\times\left(\|\theta\|_{2,\Gamma\times\,]0,T[} + \|\phi\|_{2,\Gamma\times\,]0,T[}\right)\Bigg).\end{aligned}$$

Then, (4.5) holds by taking the following inequalities into account:

$$\begin{aligned}\|v\|_{p,\Gamma} &\leq K_{pn/(n+p-1)}\,|\Omega|^{1-1/p}\big(\|\nabla v\|_{p,\Omega} + \|v\|_{p,\Omega}\big);\\ \|w\|_{p,\Gamma} &\leq K_{pn/(n+p-1)}\,|\Omega|^{1-1/p}P_p\|\nabla w\|_{p,\Omega}\end{aligned}$$

for all $v \in W^{1,p}(\Omega)$ and $w \in V_p(\Omega)$.

With analogous argument, we find (4.4). □

Proposition 4.3 (Auxiliary temperature). *Let*

$$\theta, c_i \in L^p(0,T;W^{1,p}(\Omega)), \quad i = 1,\ldots,I,$$

and $\phi \in V_p(\Omega)$ be in accordance with Proposition 4.1, where

$$p \in [2, 2+\delta] \cap [2, 2+1/(\varkappa-1)[,$$

and let assumptions (2.14), (2.15), (2.18), (2.21)–(2.23), (2.25), and (2.26) be fulfilled. Then, the variational problem

$$\begin{aligned}\rho c_{\mathrm{p}}\int_0^T \langle\partial_t\Theta, v\rangle\,\mathrm{dt} &+ \int_{Q_T}(\mathsf{K}(\theta)\nabla\Theta)\cdot\nabla v\,\mathrm{dx}\,\mathrm{dt}\\ &+ \int_{\Sigma_T} h_{\mathrm{R}}(\theta)|\Theta|^{\ell-2}\Theta v\,\mathrm{ds}\,\mathrm{dt} + \int_0^T\int_\Gamma h_{\mathrm{C}}(\theta)\Theta\,v\,\mathrm{ds}\,\mathrm{dt}\\ =& \int_0^T\int_\Gamma h_{\mathrm{C}}(\theta)\theta_{\mathrm{e}}v\,\mathrm{ds}\,\mathrm{dt} + \int_{\Sigma_T}\gamma(\theta)v\,\mathrm{ds}\,\mathrm{dt}\\ &- \int_{Q_T}\left(R\theta^2\sum_{j=1}^I D_j'(c_j,\theta)\nabla c_j + \sigma(\theta)\Pi(\theta)\nabla\phi\right)\cdot\nabla v\,\mathrm{dx}\,\mathrm{dt},\end{aligned} \tag{4.11}$$

for all $v \in V_{p',\ell}(Q_T)$*, is uniquely solvable in* $V_{p,\ell}(Q_T)$*. In particular,*

$$\partial_t\Theta \in L^p(0,T;[W^{1,p'}(\Omega)]') \quad \textit{and} \quad \Theta \in C([0,T];L^2(\Omega)).$$

Moreover, the following estimates hold:

$$\|\Theta\|_{\infty,p,Q_T} \leq \mathcal{H}_0^{1/p}\big(\|\nabla\phi\|_{p,Q_T}, \|\nabla\mathbf{c}\|_{p,Q_T}\big)\exp[(p-1)T/p]; \tag{4.12}$$

$$\|\Theta\|_{\ell+p-2,\Sigma_T}^{\ell+p-2} \leq \frac{1+(p-1)T\exp[(p-1)T]}{(\rho c_\mathrm{p})^{-1}b_\#}\,\mathcal{H}_0\big(\|\nabla\phi\|_{p,Q_T}, \|\nabla\mathbf{c}\|_{p,Q_T}\big); \tag{4.13}$$

$$\begin{aligned}\|\nabla\Theta\|_{p,\Omega} \leq{}& \mathcal{C}(k_\#)^{-1}\\ &\times\Bigg[\sqrt{\rho c_\mathrm{p} k_\#(1+T\exp[T])}\,\|\theta_0\|_{2,\Omega} + \mathcal{H}^\#\\ &\quad+\sigma^\#\,\Pi^\#\,\mathcal{Z}\big(\|\nabla\phi\|_{2,Q_T}, (\rho c_\mathrm{p})^{-1}k_\#, \|\nabla\phi\|_{p,Q_T}\big)\\ &\quad+\mathcal{Z}\Bigg(|Q_T|^{1/2-1/p}, (\rho c_\mathrm{p})^{-1}k_\#, \sum_{j=1}^{I}(D_j')^\#\,\|\nabla c_j\|_{p,Q_T}\Bigg)\Bigg],\end{aligned} \tag{4.14}$$

with $\gamma_\mathrm{e} := h_\mathrm{C}^\#|\theta_\mathrm{e}|$*,* $\mathcal{Z}$ *is given as in* (4.10)*, and*

$$\begin{aligned}\mathcal{H}_0(a,\mathbf{b}) ={}& \|\theta_0\|_{p,\Omega}^p + (\rho c_\mathrm{p})^{-p/2}\left(\frac{p-1}{k_\#}\right)^{p/2}\left(\sigma^\#\,\Pi^\#\,a + \sum_{j=1}^{I}(D_j')^\#\,b_j\right)^p\\ &+(\rho c_\mathrm{p})^{-1}\,\frac{p(\ell-1)}{(\ell+p-2)b_\#^{(p-1)/(\ell-1)}}\int_{\Sigma_T}|\gamma_\mathrm{w}|^{\frac{\ell+p-2}{\ell-1}}\,\mathrm{d}s\,\mathrm{d}t\\ &+(\rho c_\mathrm{p})^{-p'}\left(\left(\frac{p^2(p-1)^{p-2}}{2k_\#(\rho c_\mathrm{p})^{-1}}\right)^{\frac{1}{p-1}} + p - 1\right)\\ &\times K_{\frac{2n}{n+1}}^{2/(p-1)}\,|\Omega|^{\frac{1}{(p-1)n}}\,\|\gamma_\mathrm{e}\|_{p',\Gamma\times\,]0,T[}^{p'};\end{aligned}$$

$$\begin{aligned}\mathcal{H}^\# ={}& \sqrt{1+(\rho c_\mathrm{p})^{-1}k_\#}\,K_{2n/(n+1)}\big(\|\gamma_\mathrm{w}\|_{p,\Sigma_T} + \|\gamma_\mathrm{e}\|_{p,\Gamma\times\,]0,T[}\big)\\ &+\sqrt{k_\#(1+T\exp[T])}\\ &\times\Bigg(\sqrt{\frac{2(\ell-1)}{\ell(b_\#)^{1/(\ell-1)}}}\,\|\gamma_\mathrm{w}\|_{\ell',\Sigma_T}^{\ell'/2}\\ &\quad+\sqrt{2+k_\#}\,K_{2n/(n+1)}\,|\Omega|^{1/(2n)}\,\|\gamma_\mathrm{e}\|_{2,\Gamma\times\,]0,T[}\Bigg).\end{aligned}$$

Proof. The existence of the required auxiliary temperature is a consequence of Theorem 3.1 and Remark 3.2, by dividing (4.11) by $\rho c_\mathrm{p} > 0$. □

The continuous dependence is stated in the following proposition.

Proposition 4.4. *The mapping $\mathcal{T}$ is continuous and compact from $\mathcal{K}$ into*

$$[L^p(0,T;W^{1,p}(\Omega))]^I \times V_{p,\ell}(Q_T)$$

for the strong topology.

Proof. Let $\{(\mathbf{c}_m,\theta_m)\}_{m\in\mathbb{N}} \subset \mathcal{K}$ be a sequence such that $(\mathbf{c}_m,\theta_m) \to (\mathbf{c},\theta)$ in

$$[L^p(0,T;W^{1,p}(\Omega))]^I \times V_{p,\ell}(Q_T).$$

It is clear that $(\mathbf{c},\theta) \in \mathcal{K}$. We select a weakly converging subsequence with respect to the norms from estimates (4.1), (4.2), (4.5), and (4.14). That is, the corresponding solutions $(\phi_m, \mathbf{\Psi}_m, \Theta_m)$ in accordance with Propositions 4.1, 4.2, and 4.3 verify

$$\begin{aligned} \phi_m &\rightharpoonup \phi && \text{in } W^{1,p}(\Omega)/\mathbb{R}, \\ (\mathbf{\Psi}_m, \Theta_m) &\rightharpoonup (\mathbf{\Psi}, \Theta) && \text{in } [L^p(0,T;W^{1,p}(\Omega))]^{I+1}. \end{aligned}$$

Moreover, $\phi_m \rightharpoonup \phi$ in $V_p(\Omega)$. Under the compact embeddings

$$W^{1,p}(\Omega) \hookrightarrow\hookrightarrow L^p(\Omega) \quad \text{and} \quad W^{1,p}(\Omega) \hookrightarrow\hookrightarrow L^p(\partial\Omega)$$

the compactness Aubin–Lions theorem states that we may extract a sequence in the set of approximate concentration-temperature solutions, $(\mathbf{\Psi}_m, \Theta_m)$, which converges strongly in $L^p(Q_T)$ and $L^p(\Sigma_T)$. Thanks to (4.13), $\Theta_m \to \Theta$ in $L^\ell(\Sigma_T)$.

The above limits ensure that the weak limit $(\Phi, \mathbf{\Psi}, \Theta)$ verifies

$$(\Phi, \mathbf{\Psi}, \Theta) = \mathcal{T}(\mathbf{c}, \theta).$$

Next we prove the strong convergence of ϕ_m to ϕ. Since the weak limit ϕ verifies (2.13), we write

$$\begin{aligned} &\int_\Omega \sigma(\theta_m)\nabla(\phi_m - \phi)\cdot\nabla v \,\mathrm{dx} \\ &\qquad = \int_\Omega (\sigma(\theta) - \sigma(\theta_m))\nabla\phi\cdot\nabla v\,\mathrm{dx} \\ &\qquad\quad + \int_\Omega \big(\alpha(\theta)\sigma(\theta)\nabla\theta - \alpha(\theta_m)\sigma(\theta_m)\nabla\theta_m\big)\cdot\nabla v\,\mathrm{dx} \\ &\qquad\quad + F\sum_{i=1}^I z_i \int_\Omega \big(D_i(\theta)\nabla c_i - D_i(\theta_m)\nabla(c_i)_m\big)\cdot\nabla v\,\mathrm{dx}. \end{aligned}$$

Thus, we may estimate $\nabla(\phi_m - \phi)$ in $L^p(\Omega)$ such that

$$\|\nabla(\phi_m - \phi)\|_{p,\Omega} \to 0 \quad \text{as } m \to \infty.$$

Finally, the strong convergence for the concentration-temperature pair is obtained via the identities

$$\begin{aligned}
&\int_0^T \left\langle \partial_t \left((\Psi_i)_m - \Psi_i\right), v\right\rangle \mathrm{dt} + \int_{Q_T} D_i(\theta_m)\nabla\left((\Psi_i)_m - \Psi_i\right)\cdot\nabla v \,\mathrm{dx}\,\mathrm{dt} \\
&\quad = \int_{Q_T} \left(D_i(\theta) - D_i(\theta_m)\right)\nabla\Psi_i\cdot\nabla v\,\mathrm{dx}\,\mathrm{dt} \\
&\qquad + \int_{Q_T}\Big(c_i S_i(c_i,\theta)\nabla\theta - (c_i)_m S_i((c_i)_m,\theta_m)\nabla\theta_m\Big)\cdot\nabla v\,\mathrm{dx}\,\mathrm{dt} \\
&\qquad + \int_{Q_T}\frac{t_i}{Fz_i}\big(\sigma(\theta)\nabla\phi - \sigma(\theta_m)\nabla\phi_m\big)\cdot\nabla v\,\mathrm{dx}\,\mathrm{dt} \\
&\qquad + \int_0^T\int_\Gamma \big(g_i(\theta_m,\phi_m) - g_i(\theta,\phi)\big)v\,\mathrm{ds}\,\mathrm{dt} \quad \forall v\in L^{p'}(0,T;W^{1,p'}(\Omega));
\end{aligned}$$

$$\begin{aligned}
&\rho c_\mathrm{p}\int_0^T \left\langle \partial_t\left(\Theta_m - \Theta\right), v\right\rangle \mathrm{dt} + \int_{Q_T}(\mathsf{K}(\theta_m)\nabla(\Theta_m - \Theta))\cdot\nabla v\,\mathrm{dx}\,\mathrm{dt} \\
&\quad = \int_{Q_T}((\mathsf{K}(\theta) - \mathsf{K}(\theta_m))\nabla\Theta)\cdot\nabla v\,\mathrm{dx}\,\mathrm{dt} \\
&\qquad + \int_{\Sigma_T}\Big(h_\mathrm{R}(\theta)|\Theta|^{\ell-2}\Theta - h_\mathrm{R}(\theta_m)|\Theta_m|^{\ell-2}\Theta_m + \gamma(\theta_m) - \gamma(\theta)\Big)v\,\mathrm{ds}\,\mathrm{dt} \\
&\qquad + \int_0^T\int_\Gamma\Big(h_\mathrm{C}(\theta)\Theta - h_\mathrm{C}(\theta_m)\Theta_m + \left(h_\mathrm{C}(\theta_m) - h_\mathrm{C}(\theta)\right)\theta_\mathrm{e}\Big)v\,\mathrm{ds}\,\mathrm{dt} \\
&\qquad + R\int_{Q_T}\sum_{j=1}^I\Big(\theta^2 D_j'(c_j,\theta)\nabla c_j - \theta_m^2 D_j'((c_j)_m,\theta_m)\nabla(c_j)_m\Big)\cdot\nabla v\,\mathrm{dx}\,\mathrm{dt} \\
&\qquad + \int_{Q_T}\Big(\sigma(\theta)\Pi(\theta)\nabla\phi - \sigma(\theta_m)\Pi(\theta_m)\nabla\phi_m\Big)\cdot\nabla v\,\mathrm{dx}\,\mathrm{dt} \quad \forall v\in V_{p',\ell}(Q_T).
\end{aligned}$$

Indeed, the estimates (4.5) and (4.14) applied to the differences

$$(\Psi_i)_m - \Psi_i \quad \text{and} \quad \Theta_m - \Theta,$$

respectively, yield their convergence to zero by the Lebesgue dominated convergence theorem. □

5. Proof of Theorem 2.1

The functional $\mathcal{T}$ (cf. (3.1)) is well defined from $\mathcal{K}$ into

$$[L^p(0,T;W^{1,p}(\Omega))]^I \times V_{p,\ell}(Q_T)$$

by Propositions 4.1, 4.2, and 4.3. Its continuity is ensured by Proposition 4.4. In order to apply the Schauder fixed point theorem, it remains to prove that $\mathcal{T}$

maps $\mathcal{K}$ into itself. To this aim, let $(\mathbf{c},\theta)\in\mathcal{K}$ be arbitrary in order to show that $\mathcal{T}(\mathbf{c},\theta)\in\mathcal{K}$. First, we rewrite (4.1)–(4.2) as

$$\|\nabla\phi\|_{p,Q_T}\le B^{\#}+A^{\#}\Bigl(\sigma^{\#}\alpha^{\#}R+\sum_{j=1}^{I}D_j^{\#}R_j\Bigr), \tag{5.1}$$

with

$$A^{\#}=(\sigma_{\#})^{-1}\left(M_1|\Omega|^{1/2-1/p}+M_2\sqrt{2(1+\sigma_{\#})}\right); \tag{5.2}$$

$$B^{\#}=(\sigma_{\#})^{-1}T^{1/p}\left(M_1K\|g\|_{2,\Gamma}+M_3\sqrt{2+2^{-1/n}\sigma_{\#}}\,\|g\|_{p,\Gamma}\right). \tag{5.3}$$

Secondly, we assume that

$$K_{2n/(n+1)}^{2/p}|\Omega|^{(pn)^{-1}}\Bigl[\|\gamma_i\|_{p',\Sigma_T}+g_i^{\#}K_{pn/(n+p-1)}|\Omega|^{1-1/p}\\ \times\Bigl(B^{\#}+\left(1+P_pA^{\#}\sigma^{\#}\alpha^{\#}\right)R+P_pA^{\#}\sum_{j=1}^{I}D_j^{\#}R_j\Bigr)\Bigr]>1,$$

otherwise an easier argument can be applied. Thus, we insert (5.1) into (4.4)–(4.5) resulting in

$$\begin{aligned}\|\Psi_i\|_{p,Q_T}&+\|\nabla\Psi_i\|_{p,Q_T}\\ &\le\mathcal{A}_i^0R+\mathcal{A}_i\sum_{j=1}^{I}(D_j')^{\#}R_j+\left(T\exp\left[(p-1)T\right]\right)^{1/p}\\ &\quad\times\Biggl[\|c_{0,i}\|_{p,\Omega}+Q_i^{\#}\,\|\gamma_i\|_{p',\Sigma_T}\\ &\qquad+\left(\sqrt{\frac{p-1}{(D_i)_{\#}}}\,t_i^{\#}\sigma^{\#}+g_i^{\#}K_{pn/(n+p-1)}|\Omega|^{1-1/p}P_p\right)B^{\#}\Biggr]\\ &\quad+\mathcal{C}(D_i)_{\#}^{-1}\Bigl[\sqrt{(D_i)_{\#}(1+T\exp[T])}\,\|c_{0,i}\|_{2,\Omega}+\mathcal{G}_i^{\#}+Y_iB^{\#}\\ &\qquad+X_i(\sigma_{\#})^{-1}T^{1/2}K\|g\|_{2,\Gamma}\Bigr],\end{aligned} \tag{5.4}$$

with

$$\begin{aligned}\mathcal{A}_i^0&=\left(T\exp\left[(p-1)T\right]\right)^{1/p}\\ &\quad\times\Biggl[\sqrt{\frac{p-1}{(D_i)_{\#}}}\left(S_i^{\#}+A^{\#}t_i^{\#}(\sigma^{\#})^2\alpha^{\#}\right)\\ &\qquad+g_i^{\#}Q_i^{\#}K_{pn/(n+p-1)}|\Omega|^{1-1/p}\left(1+P_pA^{\#}\sigma^{\#}\alpha^{\#}\right)\Biggr]\end{aligned}$$

$$+\,\mathcal{C}(D_i)_{\#}^{-1}\Big[S_i^{\#}\mathcal{Z}\big(|Q_T|^{1/2-1/p},(D_i)_{\#},1\big)+\mathcal{Q}_i + \big(X_i(\sigma_{\#})^{-1}\,|Q_T|^{1/2-1/p}+Y_iA^{\#}\big)\sigma^{\#}\alpha^{\#}\Big]; \tag{5.5}$$

$$\mathcal{A}_i=\mathcal{C}(D_i)_{\#}^{-1}\left(X_i(\sigma_{\#})^{-1}|Q_T|^{1/2-1/p}+Y_iA^{\#}\right) + A^{\#}\left(T\exp\left[(p-1)T\right]\right)^{1/p} \times\left(\sqrt{\frac{p-1}{(D_i)_{\#}}}\,t_i^{\#}\sigma^{\#}+g_i^{\#}Q_i^{\#}K_{\frac{pn}{n+p-1}}|\,\Omega|^{1-1/p}P_p\right); \tag{5.6}$$

$$Q_i^{\#}=\left(\left(\frac{p^2(p-1)^{p-2}}{2(D_i)_{\#}}\right)^{1/(p-1)}+p-1\right)^{1/p}K_{2n/(n+1)}^{2/p}|\Omega|^{(pn)^{-1}}, \tag{5.7}$$

where $\mathcal{G}_i^{\#}$, X_i, Y_i, $\mathcal{Q}_i$, $\mathcal{Z}$ and $A^{\#}$, $B^{\#}$ are given at (4.6)–(4.10), and (5.2)–(5.3), respectively.

Next, on the one hand, we insert (4.1) into (4.13) resulting in

$$\begin{aligned}\|\Theta\|_{\ell,\Sigma_T}^{\ell}\leq{}&\frac{1+T\exp\left[T\right]}{b_{\#}}\\&\times\Bigg(\rho c_{\mathrm{p}}\|\theta_0\|_{2,\Omega}^2+\frac{2(\ell-1)}{\ell(b_{\#})^{1/(\ell-1)}}\,\|\gamma_{\mathrm{w}}\|_{\ell',\Sigma_T}^{\ell'}\\&+\left(\frac{2}{k_{\#}}+\frac{1}{\rho c_{\mathrm{p}}}\right)K_{2n/(n+1)}^2\,|\Omega|^{n^{-1}}\,\|\gamma_{\mathrm{e}}\|_{2,\Gamma\times\,]0,T[}^2+\frac{1}{k_{\#}}\\&\times\left[\frac{\Pi^{\#}\sigma^{\#}}{\sigma_{\#}}\sqrt{T}\,K\|g\|_{2,\Gamma}+|Q_T|^{1/2-1/p}\right.\\&\left.\times\left(\frac{\Pi^{\#}\alpha^{\#}(\sigma^{\#})^2}{\sigma_{\#}}\,R+\left(1+\frac{\Pi^{\#}\sigma^{\#}}{\sigma_{\#}}\right)\sum_{j=1}^{I}(D_j')^{\#}R_j\right)\right]^2\Bigg).\end{aligned}$$

Since $\ell\geq 2$, we assume that

$$\frac{\Pi^{\#}\sigma^{\#}}{\sigma_{\#}}\left(\sqrt{T}K\|g\|_{2,\Gamma}+|Q_T|^{1/2-1/p}\alpha^{\#}\sigma^{\#}R\right) + |Q_T|^{1/2-1/p}\left(1+\frac{\Pi^{\#}\sigma^{\#}}{\sigma_{\#}}\right)\sum_{j=1}^{I}(D_j')^{\#}R_j>1,$$

otherwise this term is upper bounded by one, and an easier argument can be applied. Thus, using the above inequalities, and inserting (5.1) into (4.14), we find

$$\begin{aligned}
&\|\Theta\|_{\ell,\Sigma_T}+\|\nabla\Theta\|_{p,\Omega}\\
&\quad\le \mathcal{B}_0R+\mathcal{B}\sum_{j=1}^{I}(D'_j)^{\#}R_j+\left(\frac{1+T\exp[T]}{b_{\#}}\right)^{1/\ell}\\
&\qquad\times\Bigg[\bigg(\rho c_{\mathrm{p}}\|\theta_0\|^2_{2,\Omega}+\frac{2(\ell-1)}{\ell(b_{\#})^{1/(\ell-1)}}\,\|\gamma_{\mathrm{w}}\|^{\ell'}_{\ell',\Sigma_T}\\
&\qquad\qquad+\left(\frac{2}{k_{\#}}+\frac{1}{\rho c_{\mathrm{p}}}\right)K^2_{2n/(n+1)}|\Omega|^{n^{-1}}\|\gamma_{\mathrm{e}}\|^2_{2,\Gamma\times\,]0,T[}\bigg)^{1/\ell}\\
&\qquad\qquad+\frac{\Pi^{\#}\sigma^{\#}}{(k_{\#})^{1/\ell}\sigma_{\#}}\,T^{1-1/p}K\|g\|_{2,\Gamma}\Bigg]+\mathcal{C}(k_{\#})^{-1}\\
&\qquad\times\bigg[\sqrt{\rho c_{\mathrm{p}}k_{\#}(1+T\exp[T])}\,\|\theta_0\|_{2,\Omega}+\mathcal{H}^{\#}\\
&\qquad\qquad+\Pi^{\#}\sigma^{\#}\mathcal{Z}\Big(T^{1/2}K\|g\|_{2,\Gamma}(\sigma_{\#})^{-1},(\rho c_{\mathrm{p}})^{-1}k_{\#},B^{\#}\Big)\bigg],
\end{aligned}\tag{5.8}$$

where

$$\begin{aligned}
\mathcal{B}_0=&\ \frac{\Pi^{\#}\alpha^{\#}(\sigma^{\#})^2}{\sigma_{\#}}\\
&\times\Bigg(\frac{\mathcal{C}\sqrt{1+(\rho c_{\mathrm{p}})^{-1}k_{\#}}}{k_{\#}}\,\sigma_{\#}A^{\#}\\
&\quad+\left[\frac{\mathcal{C}\sqrt{1+T\exp[T]}}{k_{\#}}+\left(\frac{1+T\exp[T]}{b_{\#}k_{\#}}\right)^{1/\ell}\right]|Q_T|^{1/2-1/p}\Bigg);
\end{aligned}\tag{5.9}$$

$$\begin{aligned}
\mathcal{B}=&\ \frac{\mathcal{C}\sqrt{1+(\rho c_{\mathrm{p}})^{-1}k_{\#}}}{k_{\#}}\left(1+\Pi^{\#}\sigma^{\#}A^{\#}\right)\\
&+\left[\frac{\mathcal{C}\sqrt{1+T\exp[T]}}{k_{\#}}+\left(\frac{1+T\exp[T]}{b_{\#}k_{\#}}\right)^{1/\ell}\right]\\
&\times\left(1+\frac{\Pi^{\#}\sigma^{\#}}{\sigma_{\#}}\right)|Q_T|^{1/2-1/p}.
\end{aligned}\tag{5.10}$$

We seek $(R,R_1,\dots,R_I)$ such that $(\mathbf{\Psi},\Theta)\in\mathcal{K}$. According to (5.8), we define the continuous function

$$\mathcal{P}(r)=(1-\mathcal{B}_0)\,r-\mathcal{P}(0),$$

where

$$\mathcal{P}(0)=C+\mathcal{B}\sum_{j=1}^{I}(D'_j)^{\#}R_j>0,$$

with the constant $C>0$ being independent of $R,R_1,\dots,R_I$.

For our purposes in finding the explicit smallness conditions on the data, we choose $R = \mathcal{P}(0)/(1-\mathcal{B}_0)$ as its positive root, considering the first smallness condition

$$\mathcal{B}_0 < 1. \tag{5.11}$$

With this choice, we may define in a recurrence manner the following linear functions, in accordance with (5.4),

$$\begin{aligned}
\mathcal{P}_1(r) &= -\mathcal{P}_1(0) + \left(1 - \mathcal{B}_1 (D'_1)^{\#}\right) r;\\
\mathcal{P}_2(r) &= -\mathcal{P}_2(0) + \left(1 - \mathcal{B}_2 (D'_2)^{\#} \left(1 - \frac{\mathcal{B}_1}{1-\mathcal{B}_1(D'_1)^{\#}}\right)\right) r;\\
\mathcal{P}_3(r) &= -\mathcal{P}_3(0) + \left(1 - \mathcal{B}_3 (D'_3)^{\#}\right.\\
&\qquad \left. \times \left(1 - \frac{\mathcal{B}_1}{1-\mathcal{B}_1(D'_1)^{\#}} - \frac{\mathcal{B}_2}{1-\mathcal{B}_2(D'_2)^{\#}\left(1-\frac{\mathcal{B}_1}{1-\mathcal{B}_1(D'_1)^{\#}}\right)}\right)\right) r,
\end{aligned}$$

where

$$\mathcal{B}_i := \frac{\mathcal{A}_i^0 \mathcal{B}}{1-\mathcal{B}_0} + \mathcal{A}_i,$$

and where $\mathcal{B}_0$, $\mathcal{B}$, $\mathcal{A}_i^0$, and $\mathcal{A}_i$ are given by (5.9), (5.10), (5.5), and (5.6), respectively. All functions admit positive roots (we call them $R_1, \dots, R_I$) since $\mathcal{P}_i(0) > 0$ for $i = 1, \dots, I$, and the smallness conditions $\mathcal{P}'_i(r) > 0$, i.e.,

$$\mathcal{B}_1 (D'_1)^{\#} < 1; \tag{5.12}$$

$$\mathcal{B}_i (D'_i)^{\#} \left(1 - \sum_{j=1}^{i-1} \frac{\mathcal{B}_j}{\mathcal{P}'_j(r)}\right) < 1, \quad i = 2, \dots, I, \tag{5.13}$$

hold. For the reader's convenience, we rewrite the above smallness conditions to the first two ionic components:

$$\mathcal{B}_1 := \frac{\mathcal{A}_1^0 \mathcal{B}}{1-\mathcal{B}_0} + \mathcal{A}_1 < \left((D'_1)^{\#}\right)^{-1};$$

$$\mathcal{B}_2 := \frac{\mathcal{A}_2^0 \mathcal{B}}{1-\mathcal{B}_0} + \mathcal{A}_2 < \left((D'_2)^{\#}\right)^{-1} \frac{1-\mathcal{B}_1(D'_1)^{\#}}{1-\mathcal{B}_1\left(1+(D'_1)^{\#}\right)}.$$

6. Electrolysis of molten sodium chloride (NaCl)

Many metals can be extracted in pure forms by electrolytic method: the alkali metals, and aluminum, as well as nonmetals: oxygen, hydrogen, and chlorine gas. We exemplify the electrolytic cell (cf. Figure 1) for NaCl, with

$$\rho = 1500\,\mathrm{kg\cdot m^{-3}} \quad \text{and} \quad c_{\mathrm{p}} = 1197.8\,\mathrm{J\cdot kg^{-1}\cdot K^{-1}}.$$

As in the industrial extraction of the sodium metal by Downs process, we consider a cylindrical container (with dimensions of 13 cm in diameter, and of 13 cm in height) with stainless steel walls ($\ell = 5$, the emissivity $0.2 \le \epsilon \le 0.5$, and the absorptivity is assumed to obey the Kirchhoff law), and with copper/nickel electrodes ($550 < h_{\mathrm{C}} \leq 1820\,\mathrm{W}\cdot\mathrm{m}^{-2}\cdot\mathrm{K}^{-1}$, see [34]). Thus, we suppose $|\Omega| = 1.5\times 10^{-3}\mathrm{m}^3$, which corresponds to

$$c_i^0 = 2.5667\times 10^4\ \mathrm{mol}\cdot\mathrm{m}^{-3}\quad (i = \mathrm{Na}^+, \mathrm{Cl}^-).$$

The sodium chloride conducts electricity when it is melted (high melting point 1073.15 K). At temperature range 1080–1250 K (805–980°C), we have the following available data:

$$\begin{aligned}
k^{\#} &= 0.6\ \mathrm{W}\cdot\mathrm{m}^{-1}\cdot\mathrm{K}^{-1}, \quad k_{\#} = 0.5\ \mathrm{W}\cdot\mathrm{m}^{-1}\cdot\mathrm{K}^{-1} \quad \text{(see [13])},\\
\sigma_{\#} &= 359.7\ \mathrm{S}\cdot\mathrm{m}^{-1}, \qquad \sigma^{\#} = 398.0\ \mathrm{S}\cdot\mathrm{m}^{-1},\\
(D_{\mathrm{Na}^+})_{\#} &= 7.7\times 10^{-9}\ \mathrm{m}^2\cdot\mathrm{s}^{-1},\\
(D_{\mathrm{Cl}^-})_{\#} &= 6.3\times 10^{-9}\ \mathrm{m}^2\cdot\mathrm{s}^{-1},\\
D^{\#}_{\mathrm{Na}^+} &= 12\times 10^{-9} F|z_{\mathrm{Na}^+}|\ \mathrm{m}^2\cdot\mathrm{s}^{-1}\cdot\mathrm{C}\cdot\mathrm{mol}^{-1},\\
D^{\#}_{\mathrm{Cl}^-} &= 9.5\times 10^{-9} F|z_{\mathrm{Cl}^-}|\ \mathrm{m}^2\cdot\mathrm{s}^{-1}\cdot\mathrm{C}\cdot\mathrm{mol}^{-1} \quad \text{(see [18, pp. 49–63])}.
\end{aligned}$$

The Seebeck coefficient has values in the range $10^{-5} - 10^{-4}\,\mathrm{V}\cdot\mathrm{K}^{-1}$ (see [26]). The parameters, $\Pi^{\#}$ and $(D_i')^{\#}$ ($i = \mathrm{Na}^+$, Cl^-), are according to the first Kelvin relation and the Onsager reciprocal relationship, respectively.

Under constant initial conditions, the upper bound in (2.24) can be given by

$$t_i^{\#} = F|z_i|D_i^{\#}c_i^0/(R\theta_0\sigma_{\#}).$$

The Soret coefficient (S/D) is of order 10^{-3}–$10^{-2}\,\mathrm{K}^{-1}$ in liquids and electrolytes [29], which implies that

$$S^{\#}_{\mathrm{Na}^+} = 1.2\times 10^{-12} c^0_{\mathrm{Na}^+} \quad \text{and} \quad S^{\#}_{\mathrm{Cl}^-} = 9.5\times 10^{-11} c^0_{\mathrm{Cl}^-}.$$

The electrolysis separates the molten ionic compound into its elements. The chemical half-reactions (and the standard state potentials) are

- in the cathode (−): $2\,\mathrm{Na}^+ + 2\,e^- \longrightarrow 2\,\mathrm{Na}$ ($E^0_{\mathrm{redution}} = -2.71\,\mathrm{V}$);
- in the anode (+): $2\,\mathrm{Cl}^- \longrightarrow \mathrm{Cl}_2(g) + 2\,e^-$ ($E^0_{\mathrm{oxidation}} = -1.36\,\mathrm{V}$).

Thus, the balanced chemical equation for the nonspontaneous overall reaction is

$$2\,\mathrm{NaCl} \longrightarrow 2\,\mathrm{Na} + \mathrm{Cl}_2(g) \qquad (E^0_{\mathrm{cell}} = -4.07\,\mathrm{V}).$$

The stoichiometric coefficients of electrons in the anode and cathode are, respectively, $s_{\mathrm{a}} = s_{\mathrm{c}} = 2$. Assuming symmetric electron transfer, the transfer coefficients are $\beta_i = 0.5$ ($i = \mathrm{Na}^+$, Cl^-). Then, the Butler–Volmer equation is

$$g_{i,l} = 2J_l \sinh\left[F\eta/(R\theta)\right].$$

The production of metallic sodium at the cathode and chloride gas at the anode may operate at $10^4\,\mathrm{A}\cdot\mathrm{m}^{-2}$, and at potential of 7 V, with the cathodic current being balanced by the anodic current.

Therefore, for some $T > 0$ the smallness conditions (5.11)–(5.13) hold under the above data, and

$$\mathcal{B}_0 = 0.0027\Big(2\mathcal{C}\Big(M_1 + 26.8589M_2 + \sqrt{1+T\exp[T]}\Big) + 44.643\,(1+T\exp\,[T])^{1/5}\Big);$$

$$\mathcal{B} = 48.9(1+T\exp[T])^{1/5} + \mathcal{C}\left[2\sqrt{1+T\exp[T]}+2\right];$$

$$\begin{aligned}\mathcal{A}^0_{Na^+} &= (T\exp[(p-1)T])^{1/p}\,[0.0351 + 0.0032M_1 + 0.0868M_2] \\ &\quad + \mathcal{C}\left[400\sqrt{1+T\exp[T]} + 436.8 + 36.8M_1 + 989.4M_2\right];\end{aligned}$$

$$\begin{aligned}\mathcal{A}_{Na^+} &= \mathcal{C}(1322.2 + 1322.2M_1 + 35513M_2) \\ &\quad + (0.1160M_1 + 3.1163M_2)(T\exp[(p-1)T])^{1/p};\end{aligned}$$

$$\left((D'_{Na^+})^{\#}\right)^{-1} = 6.9281\times 10^5.$$

Since the values of parameters for Cl^- are of the same order of those for Na^+, then $\mathcal{A}^0_{Cl^-}$ and $\mathcal{A}_{Cl^-}$ have similar expressions. Further optimization work should be done to precise the above universal constants. Their quantitative form is being a matter of study of ongoing work.

Appendix

TABLE 1. Universal constants

F	Faraday constant	$9.6485\times 10^4\,\mathrm{C}\cdot\mathrm{mol}^{-1}$
R	Gas constant	$8.314\,\mathrm{J}\cdot\mathrm{mol}^{-1}\cdot\mathrm{K}^{-1}$
σ_{SB}	Stefan–Boltzmann constant (for blackbodies)	$5.67\times 10^{-8}\,\mathrm{W}\cdot\mathrm{m}^{-2}\cdot\mathrm{K}^{-4}$

Nomenclature list

c	molar concentration	$\mathrm{mol}\cdot\mathrm{m}^{-3}$
c_{p}	specific heat capacity	$\mathrm{J}\cdot\mathrm{kg}^{-1}\cdot\mathrm{K}^{-1}$
D	diffusion coefficient	$\mathrm{m}^2\cdot\mathrm{s}^{-1}$
D'	Dufour coefficient	$\mathrm{m}^2\cdot\mathrm{s}^{-1}\cdot\mathrm{K}^{-1}$
h	heat transfer coefficient	$\mathrm{W}\cdot\mathrm{m}^{-2}\cdot\mathrm{K}^{-1}$
k	thermal conductivity	$\mathrm{W}\cdot\mathrm{m}^{-1}\cdot\mathrm{K}^{-1}$
S	Soret coefficient (thermal diffusion)	$\mathrm{m}^2\cdot\mathrm{s}^{-1}\cdot\mathrm{K}^{-1}$
t	transference number	(dimensionless)
u	mobility	$\mathrm{m}^2\cdot\mathrm{V}^{-1}\cdot\mathrm{s}^{-1}$

z	valence	(dimensionless)
α	Seebeck coefficient	$\mathrm{V}\cdot\mathrm{K}^{-1}$
ϕ	electric potential	V
Π	Peltier coefficient	V
ρ	density	$\mathrm{kg}\cdot\mathrm{m}^{-3}$
σ	electrical conductivity	$\mathrm{S}\cdot\mathrm{m}^{-1}$
θ	absolute temperature	K

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