

Research Article

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On the well-posedness of a multiscale mathematical model for Lithium-ion batteries

<https://doi.org/10.1515/anona-2018-0041>

Received February 17, 2018; accepted February 19, 2018

Abstract: We consider the mathematical treatment of a system of nonlinear partial differential equations based on a model, proposed in 1972 by J. Newman, in which the coupling between the Lithium concentration, the phase potentials and temperature in the electrodes and the electrolyte of a Lithium battery cell is considered. After introducing some functional spaces well-adapted to our framework, we obtain some rigorous results showing the well-posedness of the system, first for some short time and then, by considering some hypothesis on the nonlinearities, globally in time. As far as we know, this is the first result in the literature proving existence in time of the full Newman model, which follows previous results by the third author in 2016 regarding a simplified case.

Keywords: Lithium-ion battery cell, multiscale mathematical model, Green operators, fixed point theory, Browder–Minty existence results, super and sub solutions

MSC 2010: 35M10, 35Q60, 35C15, 35B50, 35B60

1 Introduction

Let us suppose we have a mathematical system of differential equations involving, after a homogenization process (or other averaging methods), two different scales, that we may call macro and micro, for simplicity. A macro-scale domain is given by $x \in (0, L)$, where different processes may occur in three relevant subintervals: $(0, L_1)$, $(L_1, L_1 + \delta)$ and $(L_1 + \delta, L)$. At each point $x \in (0, L_1) \cup (L_1 + \delta, L)$ we consider that there is a micro-scale domain given by a sphere with radius $R(x) > 0$. Different processes are modeled in each scale with differential equations, which are coupled at different levels, including boundary conditions.

Let us considered, motivated by the modeling of charge transport in Lithium batteries (as we will show below) the following (relatively) abstract framework (which can be generalized to other cases).

Our system has five unknowns functions: $u(x, t)$, $v(x; r, t)$, $\varphi(x, t)$, $\phi(x, t)$ and $\theta(t)$ such that

- $u : (0, L) \times (0, t_{\text{end}}) \rightarrow \mathbb{R}$,
- $v : \Omega_\delta \times (0, t_{\text{end}}) \rightarrow \mathbb{R}$,
- $\varphi : (0, L) \times (0, t_{\text{end}}) \rightarrow \mathbb{R}$,

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- $\phi : (0, L_1) \cup (L_1 + \delta, L) \times (0, t_{\text{end}}) \rightarrow \mathbb{R}$,
- $\theta : (0, t_{\text{end}}) \rightarrow \mathbb{R}$,

where $t_{\text{end}} > 0$ and $\Omega_\delta = \{(x, r) : x \in (0, L_1) \cup (L_1 + \delta, L) \text{ and } r \in [0, R(x)]\}$. These functions satisfy the following system of macro-scale equations:

$$\left\{ \begin{array}{l} \varepsilon \frac{\partial u}{\partial t} - \mathcal{L}_1 u = F_1(x, u, v, \varphi, \phi, \theta) \quad \text{in } (0, L) \times (0, t_{\text{end}}) \\ \text{with suitable boundary and initial conditions, and, for each } t \in (0, t_{\text{end}}), \\ -\mathcal{L}_2 \varphi + \mathcal{L}_3 f(u) = F_3(x, u, v, \varphi, \phi, \theta) \quad \text{in } (0, L), \\ -\mathcal{L}_4 \phi = F_4(x, u, v, \varphi, \phi, \theta) \quad \text{in } (0, L_1) \cup (L_1 + \delta L) \\ \text{with suitable boundary conditions.} \end{array} \right. \quad (1.1)$$

This system is coupled with the following system of micro-scale diffusion equation: For almost each point $x \in (0, L_1) \cup (L_1 + \delta, L)$,

$$\left\{ \begin{array}{l} \frac{\partial v}{\partial t} - \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 D_2 \frac{\partial v}{\partial r} \right) = 0 \quad \text{in } (0, R(x)) \times (0, t_{\text{end}}), \\ \frac{\partial v}{\partial r}(x; 0, \cdot) = 0 \quad \text{in } (0, t_{\text{end}}), \\ -D_2 \frac{\partial v}{\partial r}(x; R(x), \cdot) = F_2(x, u, v, \varphi, \phi, \theta) \quad \text{in } (0, t_{\text{end}}), \\ v(\cdot, 0) = v_0 \quad \text{in } (0, L). \end{array} \right. \quad (1.2)$$

In the equations written above, \mathcal{L}_1 to \mathcal{L}_4 are second-order differential operators (which may also depend on x, u, v, φ, ϕ and θ), ε is a function depending on $x \in (0, L)$ and f, F_1, F_2, F_3 and F_4 are real-valued functions.

Finally, we add the following initial value problem:

$$\left\{ \begin{array}{l} \theta'(t) = f(t, \theta(t); u, v, \varphi, \phi), \\ \theta(0) = \theta_0, \end{array} \right. \quad (1.3)$$

where the dependence of f on u, v, φ, ϕ may be global in space.

The question that arises is the following. Under which conditions can we prove existence and/or uniqueness of a local (in time) solution $(u, v, \varphi, \phi, \theta)$ of equations (1.1)–(1.3) and under which conditions is it global in time?

We study here a particular interesting case arising in the modeling of Lithium batteries. Lithium-ion batteries are currently used extensively for storing electricity in mobile devices, from phones to cars. Nevertheless, they are still many drawbacks for them, as their reduced charge capacity, the long time needed to charge them, thermal runaways, etc. Therefore, an intensive research is being done in order to improve these devices. A good mathematical model of the transport mechanisms within batteries is very important in that research in order to understand the physics involved in the processes and to allow quick numerical experiments. But this models need to be well understood from a mathematical point of view, so that conclusions extracted from them are more rigorous. The well-posedness of the mathematical models being used is, therefore, one of the key points to be considered. This is, indeed, the goal of this paper.

In [31] a full model for Lithium ion batteries was presented, based on the well-known J. Newman model (see [27]), and partial results for the well-posedness were given. In this paper, we intend to complete those well-posedness results and study the regularity of the solutions. Let us write the complete system as presented in [31] but using in the electrolyte the electric potential measured by a reference Lithium electrode (φ_e) instead of its real electric potential. This is done because in electrochemical applications the potential in an electrolyte is typically measured by inserting a reference electrode of a pure compound, typically a Lithium electrode (see [7, 33, 35]). Local existence means that we are able to prove existence of solutions if the final time t_{end} is “small enough”. In a special case, we will show that t_{end} can be taken as large as wanted, making the existence of solutions global in time.

A typical Lithium-ion battery cell has three regions: a porous negative electrode, a porous positive electrode and an electro-blocking separator. Furthermore, the cell contains an electrolyte, which is a con-

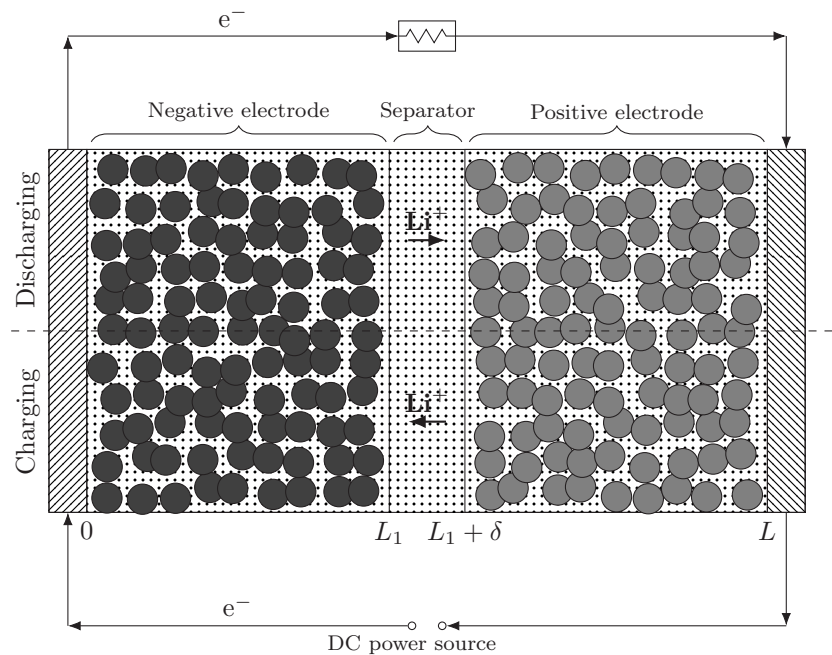


Figure 1: Schematic representation of a battery. Dark gray disks represent negative electrode particles, light gray disks represent positive electrode particles, the dotted region represents the presence of electrolyte. On both sides of the cell the lined region represents the current collectors.

centrated solution containing charged species that move along the cell in response to an electrochemical potential gradient.

Let L be the length of a cell of a battery, let L_1 be the length of the negative electrode and let δ be the length of the separator. We assume the radius of an electrode particle to be $R_s(x)$, with

$$R_s(x) = \begin{cases} R_{s,-} & \text{if } x \in (0, L_1), \\ R_{s,+} & \text{if } x \in (L_1 + \delta, L). \end{cases} \quad (1.4)$$

A schematic representation of a cell is given in Figure 1.

The unknowns in the system of equations that we study are:

- the concentration of Lithium ions in the electrolyte $c_e = c_e(x, t)$ in every macroscopic point $x \in (0, L)$,
- the concentration of Lithium ions in the electrodes $c_s = c_s(r, t; x)$, which for every macroscopic point $x \in (0, L_1) \cup (L_1 + \delta, L)$ is defined in a microscopic ball of radius $R_s(x)$, with r indicating the distance to the center. We assume radial symmetry in the diffusion taking place in each particle. Therefore, we do not need to consider angular coordinates,
- the electric potential $\phi_s = \phi_s(x, t)$ in the electrodes,
- the electric potential measured by a reference Lithium electrode in the electrolyte, $\varphi_e = \varphi_e(x, t)$,
- the temperature $T(t)$ in the cell.

The system of equations is given by (1.5)–(1.9) below.

The transport of Lithium through the electrolyte can be modeled by the following macro-scale system of equations (conservation of Lithium in the electrolyte):

$$\begin{cases} \frac{\partial c_e}{\partial t} - \frac{\partial}{\partial x} \left(D_e \frac{\partial c_e}{\partial x} \right) = \alpha_e j^{\text{Li}} & \text{in } (0, L) \times (0, t_{\text{end}}), \\ \frac{\partial c_e}{\partial x}(0, t) = \frac{\partial c_e}{\partial x}(L, t) = 0, & t \in (0, t_{\text{end}}), \\ c_e(x, 0) = c_{e,0}(x), & x \in (0, L), \end{cases} \quad (1.5)$$

where $j^{\text{Li}} = j^{\text{Li}}(x, c_e(x, t), c_s(R_s(x), t; x), \varphi_e(x, t), \phi_s(x, t), T(t))$ is the reaction current resulting from intercalation on Li into solid electrode particles and represents the Lithium flux between the electrodes and the

electrolyte (which is a nonlinear function of all the variables, an expression that will be given later), $D_e > 0$ is a diffusion function, $\alpha_e > 0$ is constant and $c_{e,0}$ is a known initial state.

The transport of Lithium through the electrodes can be modeled, at almost every macroscopic point $x \in (0, L_1) \cup (L_1 + \delta, L)$, by the following micro-scale system of equations (conservation of Lithium in the electrodes), written in radial coordinates due to the radial symmetry:

$$\begin{cases} \frac{\partial c_s}{\partial t} - \frac{D_s}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_s}{\partial r} \right) = 0 & \text{in } (0, R_s(x)) \times (0, t_{\text{end}}), \\ \frac{\partial c_s}{\partial r}(0, t; x) = 0, & t \in (0, t_{\text{end}}), \\ -D_s \frac{\partial c_s}{\partial r}(R_s(x), t; x) = \alpha_s(x) j^{\text{Li}}, & t \in (0, t_{\text{end}}), \\ c_s(r, 0; x) = c_{s,0}(r; x), & r \in (0, R_s(x)), \end{cases} \quad (1.6)$$

where $D_s > 0$ is a diffusion coefficient and $\alpha_s > 0$, both with a constant value in $(0, L_1)$ and another constant in $(L_1 + \delta, L)$. Furthermore, $c_{s,0}$ is a radially symmetric initial state. Notice that problem (1.6) is written in spherical coordinates.

The electric potential in the electrodes, ϕ_s , and the electric potential measured by a reference Lithium electrode in the electrolyte, φ_e , can be modelled, for each $t \in (0, t_{\text{end}})$, by the following equations expressing the conservation of charge in the electrolyte:

$$\begin{cases} -\frac{\partial}{\partial x} \left(\kappa \frac{\partial \varphi_e}{\partial x} \right) + \alpha_{\varphi_e} T \frac{\partial}{\partial x} \left(\kappa \frac{\partial}{\partial x} (f_{\varphi_e}(c_e)) \right) = j^{\text{Li}} & \text{in } (0, L), \\ \frac{\partial \varphi_e}{\partial x}(0, t) = \frac{\partial \varphi_e}{\partial x}(L, t) = 0, \end{cases} \quad (1.7)$$

and the conservation of charge in the electrodes

$$\begin{cases} -\frac{\partial}{\partial x} \left(\sigma \frac{\partial \phi_s}{\partial x} \right) = -j^{\text{Li}} & \text{in } (0, L_1) \cup (L_1 + \delta, L), \\ \sigma(0) \frac{\partial \phi_s}{\partial x}(0, t) = \sigma(L) \frac{\partial \phi_s}{\partial x}(L, t) = -\frac{I(t)}{A}, \\ \frac{\partial \phi_s}{\partial x}(L_1, t) = \frac{\partial \phi_s}{\partial x}(L_1 + \delta, t) = 0, \end{cases} \quad (1.8)$$

where $\kappa = \kappa(c_e, T)$, given by a function $\kappa \in \mathcal{C}^2((0, +\infty)^2)$, $\kappa > 0$, and $\sigma \in L^\infty((0, L_1) \cup (L_1 + \delta, L))$ are conductivity coefficients (uniformly positive), $\alpha_{\varphi_e} \geq 0$ is a constant, $f_{\varphi_e} \in \mathcal{C}^2(0, +\infty)$, A is the cross-sectional area (also the correct collector area) and I , the input current, is a piecewise constant function defined for $t \in [0, t_{\text{end}}^I]$. Naturally, if the input current is defined up to a time t_{end}^I , then we can only expect to solve the system up to a time $t_{\text{end}} \leq t_{\text{end}}^I$.

Finally, we consider the temperature $T = T(t)$ inside the battery, which we consider spatially constant. Its time evolution is given by

$$\begin{cases} \frac{dT}{dt}(t) = -\alpha_T(T(t) - T_{\text{amb}}) + F_T(c_e(\cdot, t), c_s(R_s(\cdot), t; \cdot), \varphi_e(\cdot, t), \phi_s(\cdot, t), T(t)), & t \in (0, t_{\text{end}}), \\ T(0) = T_0, \end{cases} \quad (1.9)$$

where α_T is a positive constant, T_{amb} represents the ambient temperature, $T_0 \geq 0$ is an initial known temperature and F_T is a continuous functional that represents the effect of the other variables over T (an expression that will be given later). F_T may depend of the values at time t of functions c_e , c_s , φ_e and ϕ_s locally or globally in space (see (1.18)–(1.22)).

In [31], instead of equations (1.5), (1.7) and (1.8) the author considers the equations

$$\begin{cases} \varepsilon_e \frac{\partial c_e}{\partial t} - \frac{\partial}{\partial x} \left(D_e \varepsilon_e^p \frac{\partial c_e}{\partial x} \right) = \alpha_e j^{\text{Li}} & \text{in } (0, L) \times (0, t_{\text{end}}), \\ -\frac{\partial}{\partial x} \left(\varepsilon_e^p \kappa \frac{\partial \varphi_e}{\partial x} \right) + \alpha_{\varphi_e} T \frac{\partial}{\partial x} \left(\varepsilon_e^p \kappa \frac{\partial}{\partial x} (f_{\varphi_e}(c_e)) \right) = j^{\text{Li}} & \text{in } (0, L), \\ -\varepsilon_s \sigma \frac{\partial \phi_s}{\partial x^2} = -j^{\text{Li}} & \text{in } (0, L_1) \cup (L_1 + \delta, L). \end{cases}$$

where $\varepsilon_e > 0$ is constant in $(0, L_1)$, $(L_1, L_1 + \delta)$, $(L_1 + \delta, L)$ and ε_s in $(0, L_1)$, $(L_1 + \delta, L)$. This general case, which is not in divergence form for c_e and φ_e , introduces an extra level of difficulty we will not consider here. The same techniques we present in this paper apply to that case, but with the introduction of some additional technicalities (see, e.g., [4, 16] and the references therein). Here we have considered ε_e constant in $(0, L)$, and therefore we can remove it by assimilating ε_e^{p-1} in D_e , ε_e^{-1} in α_e and ε_e^p in κ .

We simplify the domain notation by introducing the following sets:

$$J_\delta = (0, L_1) \cup (L_1 + \delta, L),$$

$$D_\delta = \bigcup_{x \in J_\delta} \{x\} \times [0, R_s(x)].$$

In fact, we will consider R_s constant in both $(0, L_1)$ and $(L_1 + \delta, L)$ as in (1.4) (see Figure 2).

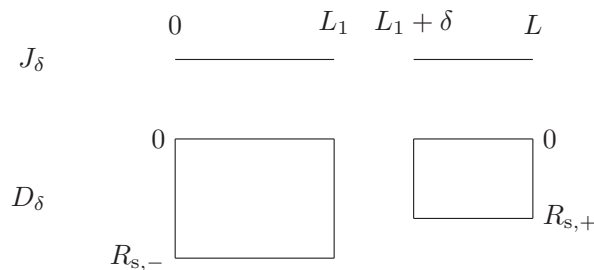


Figure 2: Domains J_δ (spatial domain of definition of c_e , φ_e , ϕ_s) and D_δ (spatial domain of definition of c_s). Notice that, since we are using a radial coordinate, every segment $\{x\} \times [0, R_s(x)]$ in D_δ represents a ball $\{x\} \times B_{R_s(x)}$ in $\{x\} \times \mathbb{R}^3$.

The analytical expression of j^{Li} is given as follows: for $(c_e, c_s, \varphi_e, \phi_s, T) \in \mathbb{R}^5$,

$$j^{\text{Li}}(x, c_e, c_s, \varphi_e, \phi_s, T) = \begin{cases} \bar{j}^{\text{Li}}(x, c_e, c_s, T, \eta(x, c_e, c_s, \varphi_e, \phi_s, T)), & x \in J_\delta, \\ 0, & \text{otherwise,} \end{cases} \quad (1.10)$$

$$\eta(x, c_e, c_s, \varphi_e, \phi_s, T) = \phi_s - \varphi_e - U(x, c_e, c_s, T), \quad x \in J_\delta, \quad (1.11)$$

where U is the open circuit potential and η the surface overpotential of the corresponding electrode reaction.

There is no common agreement on the structural assumptions of U . Some papers use a fitting function either polynomial [36] or exponential [6], whereas other authors propose an improved version with logarithmic behavior close to the limit cases [32, 35]. We will start working in a general framework, which contains as a particular important example the Butler–Volmer flux (see [27, 31, 35]), in which the functions are taken as

$$\bar{j}^{\text{Li}} = c_e^{\alpha_a} c_s^{\alpha_c} (c_{s,\max} - c_s)^{\alpha_a} h\left(x, \frac{1}{T} \eta\right), \quad (1.12)$$

$$h(x, \eta) = \delta_1(x) \exp(\alpha_a \eta) - \delta_2(x) \exp(-\alpha_c \eta), \quad (1.13)$$

$$f_{\varphi_e}(c_e) = \ln c_e, \quad (1.14)$$

$$\alpha_a \in (0, 1), \quad (1.15)$$

$$\alpha_c \in (0, 1), \quad (1.16)$$

where δ_1 , δ_2 are positive and constant in each electrode, $c_{s,\max}$ is a constant that represents the maximum value of c_s , and α_a and α_c (dimensionless constants) are anodic and cathodic coefficients, respectively, for an electrode reaction.

The function U was later proposed in [32] as

$$U = -\alpha(x)T \ln c_s + \beta(x)T \ln(c_{s,\max} - c_s) + \gamma(x)T \ln c_e + p(c_e, c_s, T), \quad (1.17)$$

where α, β, γ are positive functions in $L^\infty(J_\delta)$ and p is a smooth bounded function.

The following particular choice of F_T can be considered (see, e.g., [31]):

$$F_T = q_r + q_j + q_c + q_e, \quad (1.18)$$

$$q_r = A \int_0^L j^{\text{Li}} \eta \, dx, \quad (1.19)$$

$$q_j = A \int_{J_\delta} \sigma \left(\frac{\partial \phi_s}{\partial x} \right)^2 + A \int_0^L \left[\kappa \left(\frac{\partial \varphi_e}{\partial x} \right)^2 + \alpha_s T \kappa \left(\frac{\partial \ln c_e}{\partial x} \right) \left(\frac{\partial \varphi_e}{\partial x} \right) \right] dx, \quad (1.20)$$

$$q_c = \frac{R_f}{A} I(t)^2, \quad (1.21)$$

$$q_e = TA \int_{J_\delta} \left[j^{\text{Li}} \frac{\partial U}{\partial T} \left(\frac{c_s(R_s(x), t; x)}{c_{s,\max}} \right) \right] dx, \quad (1.22)$$

where \ln is the natural logarithm and R_f is the film resistance of the electrodes.

We point out that T has been assumed to be uniform across the whole cell. Nonetheless, a more complete model (specially one dealing with temperature blow-up) with a heat diffusion equation could be used. The study of blow-up in this type of equations has been largely studied (see, for example, [2, 12]).

By using this model, the voltage at time t of the cell can be estimated (see [31]) as

$$V(t) = \phi_s(L, t) - \phi_s(0, t) - \frac{R_f}{A} I. \quad (1.23)$$

The model, as written above, presents a number of difficulties: pseudo-two-dimensional (P2D) model, elliptic equations coupled with parabolic equations, discontinuities in space of some of the involved functions, the fact that j^{Li} is not smooth and not monotone, etc. As far as we know, there is no proof in the literature of the global existence of solution before this work.

In order to state the results, we will introduce the following definitions, which we introduce as a mathematical tool:

$$\begin{aligned} c_{s,B}(x, t) &= c_s(R_s(x), t; x), \\ \varphi_{e,\text{Li}}(x, t) &= \varphi_e(x, t) - \alpha_{\varphi_e} T(t) f_{\varphi_e}(c_e(x, t)). \end{aligned} \quad (1.24)$$

Notice that $c_{s,B}$ represents the only values of c_s that affect j^{Li} and $\varphi_{e,\text{Li}}$ is the solution of

$$\begin{cases} -\frac{\partial}{\partial x} \left(\kappa \frac{\partial \varphi_{e,\text{Li}}}{\partial x} \right) = j^{\text{Li}} & \text{in } (0, L), \\ \kappa \frac{\partial \varphi_{e,\text{Li}}}{\partial x} = 0 & \text{at } \{0, L\}, \end{cases} \quad (1.25)$$

which is a system simpler than (1.7).

First we will state four general results for a large class of functions j^{Li} , regarding the local in time existence of solutions of the general abstract problem and their maximal extension in time. Although the detailed expression of the assumptions are only given in the next section the reader can be aware now of the different nature of our mathematical results.

Theorem 1 (Well-posedness with general flux and nature of the possible blow-up). *Let Assumptions 2.1–2.3 and 2.5 hold. Then, if t_{end} is small enough, there exists a unique weak-mild solution by parts of (1.5)–(1.9) (in the sense of Definition 2.9 and satisfying Assumption 2.13). Moreover, there exists a unique maximal extension defined for $t \in [0, t_{\text{end}})$, where t_{end} is some constant $t_{\text{end}} \leq t_{\text{end}}^I$. If $t_{\text{end}} < t_{\text{end}}^I$, then one the following conditions holds as $t \nearrow t_{\text{end}}$:*

$$\begin{aligned} \min_{J_\delta \times [0, t]} c_{s,B} \rightarrow 0 \quad \text{or} \quad \max_{J_\delta \times [0, t]} c_{s,B} \rightarrow c_{s,\max} \quad \text{or} \quad \min_{[0, L] \times [0, t]} c_e \rightarrow 0 \quad \text{or} \quad \max_{[0, t] \times [0, L]} c_e \rightarrow +\infty \\ \text{or} \quad \min_{[0, t]} T \rightarrow 0 \quad \text{or} \quad \max_{[0, t]} T \rightarrow +\infty. \end{aligned} \quad (1.26)$$

We remark that without Assumption 2.13 existence for potentials φ_e , ϕ_s can only be established up to a constant (as expected).

In the particular case of j^{Li} being the Butler–Volmer flux, given by (1.10)–(1.17), under some physically reasonable hypothesis on the parameters (see Assumptions 2.19, 2.20, 2.21, 2.24 below), we will prove a general existence result, and characterize the nature of possible blow-up. It states that, under reasonable extra conditions, the non-physical obstructions for well-posedness $c_{s,B} \rightarrow 0$, $c_{s,\max}$ or $c_e \rightarrow 0, +\infty$ that appear in Theorem 1, are not the cause of the blow-up behavior of local solutions.

Theorem 2 (Well-posedness for the Butler–Volmer flux and nature of the possible blow-up). *Let us suppose that Assumptions 2.1, 2.2, 2.5, 2.19, 2.20, 2.21 and 2.24 hold. Then, if t_{end} is small enough, there exists a unique weak-mild solution by parts of (1.5)–(1.9) (in the sense of Definition 2.9 and satisfying Assumption 2.13). This solution admits a unique maximal extension in time with $t_{\text{end}} \leq t_{\text{end}}^I$. Moreover, if $t_{\text{end}} < t_{\text{end}}^I$ then, as $t \nearrow t_{\text{end}}$ either*

$$\max_{J_\delta \times [0, t]} |\phi_s - \varphi_{e, \text{Li}}| \rightarrow +\infty \quad \text{or} \quad \min_{[0, t]} T \rightarrow 0 \quad \text{or} \quad \max_{[0, t]} T \rightarrow +\infty. \quad (1.27)$$

Furthermore,

$$0 < c_s < c_{s,\max} \quad \text{and} \quad c_e > 0 \quad \text{for all } 0 \leq t < t_{\text{end}}.$$

In the last part of this paper (see Section 2.6), we give an *ad hoc* modification of the system for which we can state a global existence theorem by removing, in two steps, the impediments to global existence of solutions given by (1.27). Actually, since the blow-up conditions (1.27) do not correspond to the physical intuition, it is likely that the solutions do not, in fact, develop this kind of behavior.

In a first stage we will find a bound for the flux with respect to $\phi_s - \varphi_{e, \text{Li}}$, and show:

Theorem 3 (Blow up behavior when j^{Li} is bounded with respect to $\phi_s - \varphi_{e, \text{Li}}$). *Let Assumptions 2.1, 2.2, 2.5, 2.19, 2.20, 2.24 and 2.27 hold. Then, if t_{end} is small enough, there exists a unique weak-mild solution by parts of (1.5)–(1.9) (in the sense of Definition 2.9 and satisfying Assumption 2.13). This solution admits a unique maximal extension in time with $t_{\text{end}} \leq t_{\text{end}}^I$. If $t_{\text{end}} < t_{\text{end}}^I$, then as $t \rightarrow t_{\text{end}}$ either*

$$\min_{[0, t]} T \rightarrow 0 \quad \text{or} \quad \max_{[0, t]} T \rightarrow +\infty. \quad (1.28)$$

Finally, by assuming some additional conditions (see Assumptions 2.27 and 2.29), we will obtain a bound for the temperature T and prove what can be considered a first global existence result in the literature for this system:

Theorem 4 (Global existence in a modified case). *Let Assumptions 2.1, 2.2, 2.5, 2.19, 2.20, 2.24, 2.27 and 2.29 hold. Then there exists a unique weak-mild solution by parts of (1.5)–(1.9), defined for $t \in [0, t_{\text{end}}^I]$ (in the sense of Definition 2.8 and satisfying Assumption 2.13).*

2 Mathematical framework

2.1 Regularity assumptions of the nonlinear terms and initial data

Our most general formulation in this paper concerns the case of considering the following regularity conditions on the data:

Assumption 2.1. Let us assume the data:

$$c_{e,0} \in H^1(0, L), \quad c_{e,0} > 0, \quad c_{s,0} \in \mathcal{C}(\overline{D_\delta}), \quad 0 < c_{s,0} < c_{s,\max}, \\ T_0 > 0, \quad I \in \mathcal{C}_{\text{part}}([0, t_{\text{end}}^I]), \quad 0 < t_{\text{end}} \leq t_{\text{end}}^I < +\infty,$$

where $\mathcal{C}_{\text{part}}$ denotes the set of piecewise continuous functions

$$\mathcal{C}_{\text{part}}([a, b]) = \{f : [a, b] \rightarrow \mathbb{R} : \text{there exist } a = t_0 < t_1 < \dots < t_N = b \text{ such that } f \in \mathcal{C}([t_{i-1}, t_i])\}. \quad (2.1)$$

Notice that this implies that the lateral limits $f(t_i^\pm)$ exist, but need not coincide.

Assumption 2.2. We have $D_e \in L^\infty(0, L)$, $\kappa \in \mathcal{C}^2((0, +\infty)^2)$, $\sigma \in L^\infty(J_\delta)$, $D_e \geq D_{e,0} > 0$, $\kappa \geq \kappa_0 > 0$, $\sigma \geq \sigma_0 > 0$ and $f_{\varphi_e} \in \mathcal{C}^2((0, +\infty))$.

The key ingredient of our approach is to choose some suitable convex subsets of some appropriate functional spaces. The choice of spaces well adapted to the system is a delicate matter, and errors or loose approaches to this might result in incorrect results (for an explanation of this philosophy see, e.g., [9]). Let us define the following open convex sets where we expect to find the solutions:

$$\begin{aligned} X &= H^1(0, L) \times \mathcal{C}(\overline{J_\delta}) \times \mathbb{R}, \\ K_X &= \{(c_e, c_{s,B}, T) \in X : c_e > 0, 0 < c_{s,B} < c_{s,\max}, T > 0\}, \\ Y &= L^\infty(0, L) \times \mathcal{C}(\overline{J_\delta}) \times \mathbb{R}, \\ Z &= H^1(0, L) \times \mathcal{C}(\overline{J_\delta}) \times H^1(0, L) \times H^1(J_\delta) \times \mathbb{R}, \\ K_Z &= \{(c_e, c_{s,B}, \varphi_e, \phi_s, T) \in Z : (c_e, c_{s,B}, T) \in K_X\}, \end{aligned}$$

where $H^1(a, b)$ is the usual Sobolev space over the interval (a, b) (see, e.g., [10, 30]). It is important to point out that $H^1(a, b) \hookrightarrow \mathcal{C}([a, b])$. Finally, we define

$$X_\phi = \left\{ (u, v) \in H^1(0, L) \times H^1(J_\delta) : \int_0^L u(x) dx = 0 \right\},$$

the natural space in which we will look for the pair (φ_e, ϕ_s) .

Instead of narrowly focusing on (1.12)–(1.16), we shall state an assumption (sufficient to prove Theorem 1) satisfied by a broader family of functions:

Assumption 2.3. For the flux function we assume

$$\bar{j}^{\text{Li}} \in \mathcal{C}^2(J_\delta \times (0, +\infty) \times (0, c_{s,\max}) \times (0, +\infty) \times \mathbb{R}), \quad (2.2)$$

$$U \in \mathcal{C}^2(J_\delta \times (0, +\infty) \times (0, c_{s,\max}) \times (0, +\infty)) \quad (2.3)$$

such that

$$\frac{\partial \bar{j}^{\text{Li}}}{\partial \eta}(x, c_e, c_s, T, \eta) > 0 \quad (2.4)$$

for all $(x, c_e, c_s, T, \eta) \in J_\delta \times (0, +\infty) \times (0, c_{s,\max}) \times (0, +\infty) \times \mathbb{R}$.

Remark 2.4. In particular, it follows from Assumption 2.3 (in particular due to (2.2) and (2.4) applying the Mean Value Theorem) that there exists a positive continuous function F^{Li} satisfying

$$(\bar{j}^{\text{Li}}(x, c_e, c_s, T, \eta) - \bar{j}^{\text{Li}}(x, c_e, c_s, T, \hat{\eta}))(\eta - \hat{\eta}) = F^{\text{Li}}(x, c_e, c_s, T, \eta, \hat{\eta})|\eta - \hat{\eta}|^2 \quad (2.5)$$

for all $x \in J_\delta$, $c_e > 0$, $c_s \in (0, c_{s,\max})$, $T > 0$ and $\eta, \hat{\eta} \in \mathbb{R}$.

Finally, on the temperature term F_T we will require the following:

Assumption 2.5. We have $F_T \in \mathcal{C}^1(K_Z; \mathbb{R})$ (in the sense of the Fréchet derivative).

2.2 Definition of weak solution

We introduce the natural space for radial solutions

$$H_r^1(0, R) = \{u : (0, R) \rightarrow \mathbb{R} \text{ measurable such that } u(r)r, u'(r)r \in L^2(0, R)\}$$

with the norm

$$\|u\|_{H_r^1(0, R)}^2 = \int_0^R |u(r)|^2 r^2 dr + \int_0^R |u'(r)|^2 r^2 dr$$

and the space

$$L^2(J_\delta; H_r^1(0, R_s(\cdot))) = \left\{ u : D_\delta \rightarrow \mathbb{R} \text{ measurable such that } \int_0^L \|u(x, \cdot)\|_{H_r^1(0, R_s(x))}^2 dx < +\infty \right\}.$$

Remark 2.6. Even though we will always present the variables as (x, t) , or $(r, t; x)$, it will sometimes be mathematically advantageous to consider maps $t \in [0, t_0] \mapsto u(\cdot, t) \in X$, where X will be a space of spatial functions, in which we will use the notations $\mathcal{C}([0, t_0]; X)$ or $L^2(0, t_0; X)$, depending on the regularity.

Definition 2.7. We define a weak solution of (1.5)–(1.9) as a quintuplet

$$(c_e, c_s, \varphi_e, \phi_s, T) \in L^2(0, t_{\text{end}}; \widetilde{K}_Z), \quad \widetilde{K}_Z = H^1(0, L) \times L^2(J_\delta; H_r^1(0, R_s(\cdot))) \times H^1(0, L) \times H^1(J_\delta) \times \mathbb{R},$$

such that

$$- \int_0^{t_{\text{end}}} \int_0^L c_e \frac{d\eta_e}{dt} \psi_e dx dt + \int_0^{t_{\text{end}}} \int_0^L D_e \frac{\partial c_e}{\partial x} \frac{d\psi_e}{dx} \eta_e dx dt = \int_0^{t_{\text{end}}} \int_0^L \alpha_e j^{\text{Li}} \eta_e \psi_e dx - \int_0^L c_{e,0} \eta(0) \psi_e dx$$

for all $\eta_e \in \mathcal{D}([0, t_{\text{end}})) = \{f \in \mathcal{C}^\infty([0, t_{\text{end}})) : \text{supp } f \subset [0, t_{\text{end}}) \text{ is compact}\}$ (see [25, 30]) and $\psi_e \in H^1(0, L)$. For a.e. $x \in J_\delta$,

$$- \int_0^{t_{\text{end}}} \int_0^{R_s(x)} c_s \frac{d\eta_s}{dt} \Psi_s r^2 dr dt + \int_0^{t_{\text{end}}} \int_0^{R_s(x)} D_s \eta_s \frac{\partial c_s}{\partial r} \frac{\partial \Psi_s}{\partial r} r^2 dr dt = - \int_0^{t_{\text{end}}} (R_s(x))^2 \alpha_s(x) j^{\text{Li}} \eta_s \Psi_s dt - \int_0^{R_s(x)} c_{s,0} \eta(0) \Psi_s r^2 dr$$

for all $\eta_s \in \mathcal{D}([0, t_{\text{end}}))$ and $\Psi_s \in H_r^1(0, R_s(x))$ radially symmetric. For every $t \in (0, t_{\text{end}})$,

$$\int_0^L \kappa \frac{\partial \varphi_e}{\partial x} \frac{d\psi_e}{dx} dx - \int_{J_\delta} j^{\text{Li}} \psi_e dx = \int_0^L \kappa \alpha_{\varphi_e} T \frac{\partial}{\partial x} (f_{\varphi_e}(c_e)) \frac{d\psi_e}{dx} dx \quad \text{for all } \psi_e \in H^1(0, L) \quad (2.6)$$

$$\int_{J_\delta} \sigma \frac{\partial \phi_s}{\partial x} \frac{d\psi_s}{dx} dx + \int_{J_\delta} j^{\text{Li}} \psi_s dx = \frac{I(t)}{A} (\psi_s(0) - \psi_s(L)) \quad \text{for all } \psi_s \in H^1(J_\delta) \quad (2.7)$$

and

$$T(t) = T_0 + \int_0^t (-\alpha_T(T(s) - T_{\text{amb}})) ds + \int_0^t F_T(c_e(\cdot, s), c_{s,B}(\cdot, s), \varphi_e(\cdot, s), \phi_s(\cdot, s), T(s)) ds.$$

2.3 Definition of weak-mild solution

Dealing directly with the weak formulation is technically very difficult. On the other hand, solutions in the classical sense (having all the necessary derivatives) may not exist. There is an intermediate type of solutions, known as “mild solutions”. As a general rule (and in particular this applies to our problem), any classical solution is a mild solution and any mild solution is a weak solution.

Let us introduce this kind of solutions in the simplest case: the heat equation. Consider the problem

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = f & \text{in } \Omega \times (0, t_{\text{end}}), \\ u = 0 & \text{on } \partial\Omega \times (0, t_{\text{end}}), \\ u(\cdot, 0) = u_0 & \text{in } \Omega, \end{cases} \quad (2.8)$$

in a bounded, smooth domain $\Omega \subset \mathbb{R}^N$. Let $u_0 \in L^2(\Omega)$ and $f \in L^2((0, t_{\text{end}}) \times \Omega)$. One can construct, as an intermediate step, the solution of the problem

$$\begin{cases} \frac{\partial v}{\partial t} - \Delta v = 0 & \text{in } \Omega \times (0, t_{\text{end}}), \\ v = 0 & \text{on } \partial\Omega \times (0, t_{\text{end}}), \\ v(\cdot, 0) = u_0 & \text{in } \Omega, \end{cases} \quad (2.9)$$

by considering the decomposition of $L^2(\Omega)$ in terms of eigenfunctions of $-\Delta$. Let us write the unique solution of (2.9) as $v(t) = S(t)u_0$. The operator $S(t)$ is a semigroup (see [10]), and has some interesting properties we will not discuss. A solution u of problem the non-homogeneous problem (2.8) can be written, for every $t \in [0, t_{\text{end}}]$, as

$$u(t) = S(t)u_0 + \int_0^t S(t-s)f(s) ds.$$

This kind of solution is known as a “mild solution”. As in [17], one can define the “Green operator” for problem (2.8) as the function

$$G_{t_{\text{end}}} : f \mapsto S(\cdot)u_0 + \int_0^\cdot S(\cdot-s)f(s) ds.$$

In our problem we will need to work with a suitable Green operator associated to each of the equations. Assuming Assumptions 2.2, we will define several Green operators.

For any $t_0 > 0$ we define (see [20]):

$$G_{c_e, t_0} : L^2((0, L) \times (0, t_0)) \rightarrow \mathcal{C}([0, t_0]; H^1(0, L)), \quad f \mapsto V,$$

as the solution of the problem

$$\begin{cases} \frac{\partial V}{\partial t} - \frac{\partial}{\partial x} \left(D_e \frac{\partial V}{\partial x} \right) = f, & (x, t) \in (0, L) \times (0, t_0), \\ \frac{\partial V}{\partial x}(0, t) = \frac{\partial V}{\partial x}(L, t) = 0, & t \in (0, t_0), \\ V(x, 0) = c_{e,0}(x), & x \in (0, L). \end{cases}$$

For system (1.6) we will need to do some extra work due to the fact that the equation is only “pseudo-two-dimensional”. First we define the solution of problem (1.6) for every x fixed,

$$G_{c_s, R, t_0} : \mathcal{C}([0, R]) \times \mathcal{C}([0, t_0]) \rightarrow \mathcal{C}([0, R] \times [0, t_0]), \quad (u_0, g) \mapsto V,$$

by solving the corresponding problem

$$\begin{cases} \frac{\partial V}{\partial t} - \frac{1}{r^2} \frac{\partial}{\partial r} (D_s r^2 V) = 0, & (y, t) \in (0, R) \times (0, t_0), \\ -D_s \frac{\partial V}{\partial r}(R, t) = g, & t \in (0, t_0), \\ V(r, 0) = u_0(r), & r \in (0, R). \end{cases}$$

The next step is to consider the dependence on x . Therefore, we construct the Green operator associated to problem (1.6) collecting all $x \in J_\delta$:

$$G_{c_s, t_0} : \mathcal{C}(J_\delta \times [0, t_0]) \rightarrow \mathcal{C}(D_\delta \times [0, t_0]), \quad g \mapsto W,$$

given by

$$W(r, x, t) = G_{c_s, R_s(x), t_0}(c_{s,0}(x, \cdot), g(x, \cdot))(r, t).$$

Finally, we consider the Green operator for system (1.9) as the function

$$G_{T, t_0} : \mathcal{C}([0, t_0]; Z) \rightarrow \mathcal{C}([0, t_0]), \quad (c_e, c_{s,B}, \varphi_e, \phi_s, T) \mapsto W$$

defined as

$$W(t) = T_0 + \int_0^t (-\alpha_T(T(s) - T_{\text{amb}}) + \int_0^t F_T(c_e(\cdot, s), c_{s,B}(\cdot, s), \varphi_e(\cdot, s), \phi_s(\cdot, s), T(s))) ds.$$

This operator is well defined and of class \mathcal{C}^1 due to Assumption 2.5. It will be useful to introduce the following

Nemistkij operators:

$$\begin{aligned} N_{j^{\text{Li}}} : K_Z &\rightarrow \mathcal{C}([0, L_1]) \cap \mathcal{C}([L_1, L_1 + \delta]) \cap \mathcal{C}([L_1 + \delta, L]), \\ (c_e, c_{s,B}, \varphi_e, \phi_s, T) &\mapsto j^{\text{Li}} \circ (c_e, c_{s,B}, \varphi_e, \phi_s, T), \\ N_{j^{\text{Li}}, t_0} : \mathcal{C}([0, t_0]; K_Z) &\rightarrow \mathcal{C}([0, t_0]; \mathcal{C}([0, L_1]) \cap \mathcal{C}([L_1, L_1 + \delta]) \cap \mathcal{C}([L_1 + \delta, L])), \\ (c_e, c_{s,B}, \varphi_e, \phi_s, T) &\mapsto j^{\text{Li}} \circ (c_e, c_{s,B}, \varphi_e, \phi_s, T). \end{aligned}$$

It is well known (see, e.g., [21]) that these operators are locally Lipschitz continuous and \mathcal{C}^1 (in the sense of the Fréchet derivative), properties that will be used in the proof of Theorem 1, due to the regularity of the elements of the composition (i.e. (2.2) and (2.3)).

Definition 2.8 (Weak-mild solution). We define a “weak-mild solution of problem (1.5)–(1.9)” as a quintuplet $(c_e, c_s, \varphi_e, \phi_s, T) \in \mathcal{C}([0, t_{\text{end}}]; K_Z)$ such that there exists $0 < t_{\text{end}} \leq t_{\text{end}}^I$ for which:

- (1) (φ_e, ϕ_s) is a weak solutions of system (1.7)–(1.8) for the functions c_e, c_s, T given in the quintuplet, in the sense that, for every $t \in [0, t_{\text{end}})$ the weak formulations (2.6) and (2.7) hold.
- (2) (c_e, c_s, T) is a mild solutions of system (1.5), (1.6), (1.9) for the functions φ_e, ϕ_s given in the quintuplet, in the sense that for every $t_0 < t_{\text{end}}$,

$$(c_e, c_s, T) = (G_{c_e, t_0}(\alpha_e N_{j^{\text{Li}}, t_0}), G_{c_s, t_0}(\alpha_s N_{j^{\text{Li}}, t_0}), G_{T, t_0}) \circ (c_e|_{t < t_0}, c_s|_{R=R_s(x), t < t_0}, \varphi_e|_{t < t_0}, \phi_s|_{t < t_0}, T|_{t < t_0}). \quad (2.10)$$

Definition 2.9 (Piecewise weak-mild solution). We define a “piecewise weak-mild solution” as a quintuplet $(c_e, c_s, \varphi_e, \phi_s, T)$ such that there exists a partition $\{t_0, \dots, t_N\}$ of $[0, t_{\text{end}}]$ such that in each interval $[t_i, t_{i+1}]$, $(c_e, c_s, \varphi_e, \phi_s, T)$ is a weak-mild solution in the previous sense, with $(c_e, c_s, T)(t_i)$ as initial condition in the interval $[t_i, t_{i+1}]$.

Remark 2.10. It is well known that for problems of type (2.8), any piecewise weak-mild solution is a weak solution.

Definition 2.11. Given a solution (in any of the previous senses) $(c_e, c_s, \varphi_e, \phi_s, T) \in \mathcal{C}([0, a], K_Z)$, we say that $(\widetilde{c_e}, \widetilde{c_s}, \widetilde{\varphi_e}, \widetilde{\phi_s}, \widetilde{T}) \in \mathcal{C}([0, b], K_Z)$ is an “extension” of $(c_e, c_s, \varphi_e, \phi_s, T)$ if it is also a solution (in the same sense), $b \geq a$ and

$$(\widetilde{c_e}, \widetilde{c_s}, \widetilde{\varphi_e}, \widetilde{\phi_s}, \widetilde{T})|_{t \leq a} = (c_e, c_s, \varphi_e, \phi_s, T).$$

We say that the extension is “proper” if $b > a$. We say that an extension is “maximal” if it does not admit a proper extension.

Notice that the contribution of c_s can be studied, basically, as a one-dimensional behavior on J_δ . More precisely, we consider the Green operator on the boundary of the balls $B_{R_s(x)}$, which we will show that contains all the necessary information

$$G_{c_{s,B}, t_0} : \mathcal{C}(\overline{J_\delta} \times [0, t_0]) \rightarrow \mathcal{C}(\overline{J_\delta} \times [0, t_0]), \quad g \mapsto W,$$

where

$$W(x, t) = (G_{c_{s,B}, t_0}(g))(R_s(x), x, t).$$

In this sense we can rewrite (2.10) in terms of the restriction $c_{s,B}$, instead of c_s , as follows:

Proposition 2.12. In Definitions 2.9 and 2.11, condition (2.10) is equivalent to the following property:

$$(c_e, c_{s,B}, T) \in \mathcal{C}([0, t_{\text{end}}]; X)$$

such that

$$(c_e, c_{s,B}, T) = (G_{c_e, t_0}(\alpha_e N_{j^{\text{Li}}, t_0}), G_{c_{s,B}, t_0}(\alpha_s N_{j^{\text{Li}}, t_0}), G_{T, t_0}) \circ (c_e|_{t < t_0}, c_{s,B}|_{t < t_0}, \varphi_e|_{t < t_0}, \phi_s|_{t < t_0}, T|_{t < t_0}). \quad (2.11)$$

Proof. It is trivial that (2.10) implies (2.11). Let us consider a quintuplet $(c_e, c_{s,B}, \varphi_e, \phi_s, T)$ that satisfies (2.11). Let us construct a solution $(c_e, c_s, \varphi_e, \phi_s, T)$ of (1.5)–(1.9) in the sense of Definition 2.8. Define, for any $t_0 < t_{\text{end}}$,

$$\widetilde{j^{\text{Li}}} = N_{j^{\text{Li}}, t_0}(c_e|_{t < t_0}, c_{s,B}|_{t < t_0}, \varphi_e|_{t < t_0}, \phi_s|_{t < t_0}, T|_{t < t_0}). \quad (2.12)$$

Define $c_s(x, r, t)$ to be the solution, for every $x \in J_\delta$, of the problem

$$\begin{cases} \frac{\partial c_s}{\partial t} - D_s \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_s}{\partial r} \right) = 0, & 0 < r < R_s(x), \\ c_s = c_{s,B}, & r = R_s(x), \\ \frac{\partial c_s}{\partial r} = 0, & r = 0, \\ c_s = c_{s,0}, & t = 0. \end{cases} \quad (2.13)$$

Since $c_s = c_{s,B}$ on $\partial B_{R_s(x)}$, due to (2.12), we have

$$\widetilde{j}^{\text{Li}}(x, t) = j^{\text{Li}}(x, c_e(x, t), c_s(R_s(x), x, t), \varphi_e(x, t), \phi_s(x, t), T(t)), \quad (x, t) \in J_\delta \times (0, t_0).$$

Furthermore, since $c_{s,B} = (G_{c_s, t_0} \widetilde{j}^{\text{Li}})|_{R=R_s(x)}$, it follows that c_s and $G_{c_s, t_0} \widetilde{j}^{\text{Li}}$ are solutions of the same parabolic problem (2.13) and, by the uniqueness of the solutions,

$$c_s = G_{c_s, t_0} \widetilde{j}^{\text{Li}}.$$

Therefore, $(c_e, c_s, \varphi_e, \phi_s, T)$ is a solution of (1.5)–(1.9) in the sense of Definition 2.8, up to time t_0 , which can be arbitrarily close to t_{end} . \square

2.4 Assumptions and results regarding Theorem 1

It was first shown in [31] that the uniqueness of solutions (φ_e, ϕ_s) of system (1.7)–(1.8) holds up to a constant relating the difference between φ_e and ϕ_s . To avoid this, we set the following assumption:

Assumption 2.13. As in (1.24), we define

$$\varphi_{e,\text{Li}} = \varphi_e - \alpha_{\varphi_e} T f_{\varphi_e}(c_e) \quad (2.14)$$

and assume that

$$\int_0^L \varphi_{e,\text{Li}} \, dx = 0. \quad (2.15)$$

This can be done because (φ_e, ϕ_s) is defined up to a constant.

Remark 2.14. We recall that $\mathcal{C}([a, b]) \subset H^1(a, b)$. Thus, since $0 < c_e \in H^1(a, b)$, we have $\min_{[0, L]} c_e > 0$, so $f_{\varphi_e}(c_e) \in H^1(0, L)$.

Remark 2.15. Another alternative to get the uniqueness of solution is to use the condition $\phi_s|_{x=0} = 0$, instead of (2.15), setting the value 0 of the potential in one of the walls.

The idea of the proof of Theorem 1 (which is done in Section 5) is the following. First we will show (see Proposition 2.16 and its proof in Section 3) that we can solve (1.7) and (1.8) to obtain (φ_e, ϕ_s) if c_s, c_e, T are given, extending to the nonlinear case the study for the linearized equation proved in [31]. Then we will apply a fixed point argument to the evolution problems (1.5), (1.6) and (1.9) to obtain the conclusion.

Proposition 2.16. Let $(c_e, c_{s,B}, T) \in K_X, I \in \mathbb{R}$ and let Assumptions 2.2–2.3 hold. Then there exist $\varphi_e \in H^1(0, L)$ and $\phi_s \in H^1(J_\delta)$ satisfying the elliptic equations (1.7) and (1.8) in the weak sense (2.6) and (2.7). Furthermore, given two solutions $(\varphi_e, \phi_s), (\widehat{\varphi_e}, \widehat{\phi_s})$, there exists a constant $C \in \mathbb{R}$ such that

$$\varphi_e - \widehat{\varphi_e} = \phi_s - \widehat{\phi_s} = C.$$

Hence we have uniqueness up to a constant. In particular, there exists a unique solution (φ_e, ϕ_s) satisfying Assumption 2.13.

Due to this proposition we know that the following functions are well defined:

$$G_\phi : K_X \times \mathbb{R} \rightarrow H^1(0, L) \times H^1(J_\delta), \quad (c_e, c_{s,B}, T, I) \mapsto (\varphi_e, \phi_s), \quad (2.16)$$

$$\widetilde{G}_\phi : K_X \times \mathbb{R} \rightarrow K_Z, \quad (c_e, c_{s,B}, T, I) \mapsto (c_e, c_{s,B}, G_\phi(c_e, c_{s,B}, T, I), T), \quad (2.17)$$

where $(\varphi_e, \phi_s) \in H^1(0, L) \times H^1(J_\delta)$ is the (unique) solution of (2.6)–(2.7) satisfying (2.15). Assuming now that I is a continuous function, i.e. $I \in \mathcal{C}([0, t_{\text{end}}^I])$, we define the Green operator, for $t_0 < t_{\text{end}}^I$,

$$\widetilde{G}_{\phi, t_0} : \mathcal{C}([0, t_0]; K_X) \rightarrow \mathcal{C}([0, t_0]; K_Z), \quad (c_e, c_{s,B}, T) \mapsto W,$$

where

$$W(t) = \widetilde{G}_\phi(c_e(t), c_{s,B}(t), T(t), I(t)).$$

In Section 3 we will prove that:

Proposition 2.17. *Let Assumptions 2.2–2.3 hold. Then the operator $\widetilde{G}_\phi : K_X \times \mathbb{R} \rightarrow K_Z$ is C^1 (in the sense of the Fréchet derivative).*

Remark 2.18. Since we will allow for charge and discharge cycles, we allow for I to be piecewise continuous, and this is why we define the piecewise weak-mild solution (see Definition 2.9).

The proof of the local existence of solutions will be based on finding a unique fixed point, in $\mathcal{C}([0, t_0]; K_X)$ for t_0 small enough, of the operator problem

$$(c_e, c_{s,B}, T) = (G_{c_e, t_0}(\alpha_a N_{j^{\text{Li}}, t_0}), G_{c_{s,B}, t_0}(\alpha_s N_{j^{\text{Li}}, t_0}), G_{T, t_0}) \circ \widetilde{G}_{\phi, t_0}(c_e, c_{s,B}, T).$$

2.5 Assumptions and remarks regarding Theorem 2

In Theorem 1 one of the reasons of a finite existence time could be that $c_{s,B} \rightarrow 0$, $c_{s,\max}$ or $c_e \rightarrow 0$. This conditions do not, a priori, pose a relevant physical problem since the battery may very well be completely full or empty. However, the generality of our setting allows for no better statement. Let us study the case which seems to be the most relevant for the modeling of Lithium-ion batteries by considering new assumptions.

Assumption 2.19. There exists a constant κ_1 such that $\kappa(c_e, T) \leq \kappa_1$ and $f_{\varphi_e}(\cdot) = \ln(\cdot)$.

Assumption 2.20. We have $c_{s,\max} < 1$ in the units considered to solve the problem.

This is purely technical, but it seems reasonable since, in empirical cases in the literature, one typically has $c_{s,\max} \sim 10^{-2} \text{ mol cm}^{-3}$. In particular, in [36] the authors take $c_{s,\max} = 1.6 \times 10^{-2} \text{ mol cm}^{-3}$.

Let us consider the following special nonlinear terms (which, for a broader generality, include some extra constants with respect to (1.12)–(1.16)), which we will take as assumption in Theorem 2.

Assumption 2.21. We assume that

$$\bar{j}^{\text{Li}}(x, c_e, c_s, T, \eta) = c_e^{\alpha_a} c_s^{\alpha_s} (c_{s,\max} - c_s)^{\beta_a} h\left(x, \frac{\eta}{T}\right),$$

$$h(x, s) = h_+(x, s) - h_-(x, s),$$

$$h_+(x, s) = \delta_1(x) \exp(\gamma_1 s),$$

$$h_-(x, s) = \delta_2(x) \exp(-\gamma_2 s),$$

$$\eta(x, c_e, c_s, \varphi_e, \phi_s, T) = \phi_s - \varphi_e - U(x, c_e, c_s, T),$$

where $\alpha_a, \alpha_s, \beta_a \in (0, 1)$, $\gamma_1, \gamma_2 > 0$ and $\delta_1(x), \delta_2(x) > 0$ are constant in each electrode. Notice that γ_1, γ_2 are constant but not dimensionless. Furthermore, we consider U slightly more general than in (1.17):

$$U(x, c_e, c_s, T) = -\lambda_{\min}(x, T) \ln c_s + \lambda_{\max}(x, T) \ln(c_{s,\max} - c_s) + \mu(x, T) \ln c_e + p(c_e, c_s, T), \quad (2.18)$$

where $\lambda_{\min}, \lambda_{\max}, \mu$ are given smooth nonnegative scalar functions and p is a continuous bounded function $[0, +\infty) \times [0, c_{s,\max}] \times (0, +\infty) \rightarrow \mathbb{R}$ with global bound denoted by $\|p\|_{L^\infty}$ (Figure 3 shows a typical graph of U).

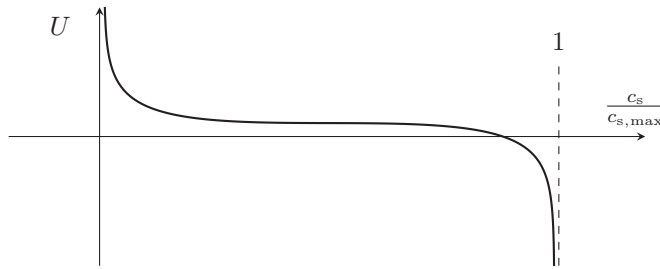


Figure 3: Possible representation of U .

Remark 2.22. It is a routine matter to check that this \bar{j}^{Li} satisfies Assumption 2.3.

Remark 2.23. Under Assumption 2.21 we can write $\bar{j}^{\text{Li}}(x, c_e, c_s, T, \eta(x, c_e, c_s, \varphi_e, \phi_s, T)) = \bar{j}_+^{\text{Li}} - \bar{j}_-^{\text{Li}}$, where

$$\bar{j}_+^{\text{Li}} = \delta_1(x) c_e^{\alpha_a} c_s^{\alpha_s} (c_{s,\max} - c_s)^{\beta_a} \exp\left(\frac{\gamma_1}{T} (\phi_s - \varphi_e - U(x, c_e, c_s, T))\right), \quad (2.19)$$

$$\bar{j}_-^{\text{Li}} = \delta_2(x) c_e^{\alpha_a} c_s^{\alpha_s} (c_{s,\max} - c_s)^{\beta_a} \exp\left(-\frac{\gamma_2}{T} (\phi_s - \varphi_e - U(x, c_e, c_s, T))\right). \quad (2.20)$$

Substituting (2.18) into (2.19)–(2.20), we have

$$\begin{aligned} \bar{j}_+^{\text{Li}} &= \delta_1(x) c_e^{\alpha_a - \gamma_1 \left(\alpha_{\varphi_e} + \frac{\mu(x, T)}{T}\right)} c_s^{\alpha_s + \gamma_1 \frac{\lambda_{\min}(x, T)}{T}} (c_{s,\max} - c_s)^{\beta_a - \gamma_1 \frac{\lambda_{\max}(x, T)}{T}} \\ &\quad \times \exp\left(\frac{\gamma_1}{T} (\phi_s - \varphi_{e,\text{Li}})\right) \exp\left(\frac{-\gamma_1}{T} p(c_e, c_s, T)\right), \end{aligned} \quad (2.21)$$

$$\begin{aligned} \bar{j}_-^{\text{Li}} &= \delta_1(x) c_e^{\alpha_a + \gamma_2 \left(\alpha_{\varphi_e} + \frac{\mu(x, T)}{T}\right)} c_s^{\alpha_s - \gamma_2 \frac{\lambda_{\min}(x, T)}{T}} (c_{s,\max} - c_s)^{\beta_a + \gamma_2 \frac{\lambda_{\max}(x, T)}{T}} \\ &\quad \times \exp\left(\frac{-\gamma_2}{T} (\phi_s - \varphi_{e,\text{Li}})\right) \exp\left(\frac{\gamma_2}{T} p(c_e, c_s, T)\right), \end{aligned} \quad (2.22)$$

On the exponents we will consider the following assumption (see Remark 2.26):

Assumption 2.24. For all $T > 0$ and $x \in [0, L]$,

$$\alpha_a - \gamma_1 \left(\alpha_{\varphi_e} + \frac{\mu(x, T)}{T}\right) \leq 1, \quad (2.23)$$

$$\alpha_a + \gamma_2 \left(\alpha_{\varphi_e} + \frac{\mu(x, T)}{T}\right) \geq 1, \quad (2.24)$$

$$\alpha_s + \gamma_1 \frac{\lambda_{\min}(x, T)}{T} \geq 1, \quad (2.25)$$

$$\beta_a + \gamma_2 \frac{\lambda_{\max}(x, T)}{T} \geq 1. \quad (2.26)$$

Remark 2.25. Notice that conditions (2.23)–(2.26) can be also written as

$$\begin{aligned} \lambda_{\min}(x, T) &\geq \frac{1 - \alpha_s}{\gamma_1} T > 0, & \lambda_{\max}(x, T) &\geq \frac{1 - \beta_a}{\gamma_2} T > 0, \\ \alpha_{\varphi_e} + \frac{\mu(x, T)}{T} &\geq \frac{1 - \alpha_a}{\gamma_2}, & \alpha_{\varphi_e} + \frac{\mu(x, T)}{T} &\geq \frac{\alpha_a - 1}{\gamma_1}. \end{aligned}$$

Theorem 2 gives a sufficient condition so that, under the structural consideration of a potential U similar to the one considered by Ramos–Please [32], should there be a blow-up of the solution, this is not caused by the non-physical behavior $c_e \rightarrow 0, +\infty$ or $c_s \rightarrow 0, c_{s,\max}$ as $t \rightarrow t_{\text{end}}$. Remark 2.26 gives an intuition of why this happens. On the other hand, if this conditions are not satisfied, then the toy models (2.27)–(2.28) suggest that if the sufficient conditions in Theorem 2 are not satisfied, then it could happen that $c_e \rightarrow 0, +\infty$ or $c_s \rightarrow 0, c_{s,\max}$. The suggestion of the potential in Ramos and Please [32] was motivated by physical consideration, and not by the mathematical theory. Nonetheless, this seems to be the exact right structure for the mathematical theory. This is a notion of robustness to this proposal.

Considering the parameters used by some authors (see, e.g., [36])

$$\alpha_s = \beta_a = \alpha_a = \frac{1}{2}, \quad \gamma_1 = \frac{\hat{\alpha}_a F}{R} = 5805.5 \text{ C K J}^{-1}, \quad \gamma_2 = \frac{\hat{\alpha}_c F}{R} = 5805.5 \text{ C K J}^{-1}$$

(where $\hat{\alpha}_a, \hat{\alpha}_c$ are non-dimensional charge transfer coefficients, F is the Faraday's constant and R is the universal gas constant), we have

$$\frac{1 - \alpha_s}{\gamma_1} = \frac{1 - \beta_a}{\gamma_2} = \frac{1 - \alpha_s}{\gamma_1} = \frac{1 - \alpha_s}{\gamma_2} = 8.61 \times 10^{-5} \text{ J C}^{-1} \text{ K}^{-1}.$$

Considering (1.17), as in [32], we have

$$\lambda_{\min} = \alpha(x)T, \quad \lambda_{\max} = \beta(x)T, \quad \mu(x) = \gamma(x)T.$$

So Assumption 2.24 translates into

$$\alpha(x), \beta(x) \geq 8.61 \times 10^{-5} \text{ J C}^{-1} \text{ K}^{-1}, \quad \gamma(x) \geq -\alpha_{\varphi_e} + 8.61 \times 10^{-5} \text{ J C}^{-1} \text{ K}^{-1}.$$

Remark 2.26. It is well known that equations of the form

$$u_t - \Delta u + u^q = f \geq 0 \quad (2.27)$$

with $q < 1$ can have a solution $u \not\equiv 0$ such that $\{x \in (0, L) : u(x, t) = 0\}$ has positive measure for all time t after an initial time t_0 . These regions are known as “dead cores” and a detailed analysis of this phenomenon can be found, for instance, in [14, 15]. On the other hand, if we study the equation

$$u_t - \Delta u = u^q + f, \quad (2.28)$$

we see that, if $q > 1$, then the solution can blow up $u \rightarrow +\infty$ for a finite time, whereas there is no blow-up if $q \leq 1$. As we will see in the proof of Theorem 2, we can bound c_e and c_s by solutions of problems of type (2.27), where conditions (2.23)–(2.26) define the exponents q appearing in (2.27) and (2.28). Taking into account these results, it seems that, if these conditions are not satisfied, it is likely that the solutions c_e or c_s reach 0 in finite time, which is a non-physical behavior.

2.6 Assumptions and remarks regarding Theorems 3 and 4

Tackling an example of global existence of solutions for the model seems to be a Herculean mission. However, if we assume some nicer behavior of the nonlinear term U , at least far from the natural “working” conditions of the system, then we can establish a result of global existence of solutions.

2.6.1 Truncated potential behavior

In this subsection we strive to make some small modifications to the problem so that we can show that the charge potentials do not blow up in finite time. First let us assume that for large difference of potentials the flux is constant. We slightly modify (2.21)–(2.22) to the following new hypothesis:

Assumption 2.27. Let $\bar{j}^{\text{Li}}(x, c_e, c_s, T, \eta(x, c_e, c_s, \varphi_e, \phi_s, T)) = \bar{j}_+^{\text{Li}} - \bar{j}_-^{\text{Li}}$, where

$$\bar{j}_+^{\text{Li}} = c_e^{\alpha_a - \gamma_1(\alpha_{\varphi_e} + \frac{\mu(x, T)}{T})} c_s^{\alpha_s + \gamma_1 \frac{\lambda_{\min}(x, T)}{T}} (c_{s, \max} - c_s)^{\beta_a - \gamma_1 \frac{\lambda_{\max}(x, T)}{T}} H\left(\frac{\gamma_1}{T}(\phi_s - \varphi_{e, \text{Li}})\right) \exp\left(\frac{-\gamma_1}{T}p(c_e, c_s, T)\right), \quad (2.29)$$

$$\bar{j}_-^{\text{Li}} = c_e^{\alpha_a + \gamma_2(\alpha_{\varphi_e} + \frac{\mu(x, T)}{T})} c_s^{\alpha_s - \gamma_2 \frac{\lambda_{\min}(x, T)}{T}} (c_{s, \max} - c_s)^{\beta_a + \gamma_2 \frac{\lambda_{\max}(x, T)}{T}} H\left(\frac{-\gamma_2}{T}(\phi_s - \varphi_{e, \text{Li}})\right) \exp\left(\frac{\gamma_2}{T}p(c_e, c_s, T)\right), \quad (2.30)$$

and H is a bounded smooth cut-off function of the exponential:

$$H(s) = \begin{cases} \exp(s), & s \leq s_\infty, \\ \zeta(s), & s > s_\infty, \end{cases}$$

where s_∞ is an arbitrarily large but fixed cut-off value, and ζ is such that $\zeta' > 0$.

Remark 2.28. Notice that (2.29)–(2.30) is (2.21)–(2.22) when $H(s) = \exp(s)$.

This modification allows us to prove Theorem 3 (see Section 7.1).

2.6.2 Truncated temperature behavior

Due to the delicate interconnectedness of the different terms in F_T , it is too difficult to prove a global existence theorem. Nonetheless, since many authors consider that the temperature is constant in the cell (see [13, 18, 33]), we will allow ourselves a substantial simplification on the structural assumption for F_T , in order to obtain the global uniqueness result avoiding the appearance of possible blow-up phenomena, which are related with the potential of Lithium batteries for thermal runaway and explosion under high temperature operation (see [36]).

Assumption 2.29. Assume that F_T is linear in T , i.e.

$$F_T = B_T(c_e, c_s, \varphi_e, \phi_s) + TA_T(c_e, c_s, \varphi_e, \phi_s),$$

and consider that B_T is a nonnegative bounded function $B_T \in [0, \bar{B}_T]$ and that A_T is bounded $A_T \in [\underline{A}_T, \bar{A}_T]$, where $\bar{B}_T, \underline{A}_T, \bar{A}_T \in \mathbb{R}$ are constant numbers.

This assumptions allow us to prove the result of global existence of solutions given in Theorem 4 (see Section 7.2).

Remark 2.30. The case $F_T \equiv 0$ is a particular case satisfying Assumptions 2.29, including the case of T just following Newton's law of cooling (if $\alpha_T \neq 0$) or $T \equiv T_0$, constant temperature (if $\alpha_T = 0$).

3 Green operator for the semilinear elliptic system (1.7)–(1.8). Proof of Propositions 2.16 and 2.17

The idea of the proof of Proposition 2.16 is to follow the idea for “low overpotentials” in [31], but replacing Lax–Milgram's theorem by the Brézis theory of “pseudo-monotone operators” (see [8]). Under some special assumptions, this result is sometimes referred to as Minty–Browder's theorem [11, 26] (see, e.g., [34]). Uniqueness up to a constant was already proved in [31].

Let us define, for a given $(c_e, c_{s,B}, T) \in K_X$, the following function:

$$\eta_0(x) = -\alpha_{\varphi_e} T f_{\varphi_e}(c_e(x)) - U(x, c_e(x), c_{s,B}(x), T), \quad x \in J_\delta,$$

which corresponds to $\eta|_{\phi_s - \varphi_{e,Li}=0}$. Since $(c_e, c_{s,B}, T)$ is known, we can define, for $x \in [0, L]$ and $\Phi \in \mathbb{R}$,

$$\underline{j}^{Li}(x, \Phi) = \begin{cases} \underline{j}^{Li}(x, c_e(x), c_{s,B}(x), T, \Phi + \eta_0(x)), & x \in J_\delta, \\ 0, & x \in (L_1, L_1 + \delta). \end{cases}$$

Notice that

$$\underline{j}^{Li}(x, \phi_s(x) - \varphi_{e,Li}(x)) = \underline{j}^{Li}(x, c_e(x), c_{s,B}(x), \varphi_e(x), \phi_s(x), T). \quad (3.1)$$

We also define

$$\underline{j}_0^{Li}(x) = \underline{j}^{Li}(x, 0),$$

which corresponds to $\underline{j}^{Li}|_{\phi_s - \varphi_{e,Li}=0}$.

Remark 3.1. Given $(c_e, c_{s,B}, T) \in K_X$, due to (2.2) and (2.3) we have $\underline{j}_0^{Li} \in L^\infty(0, L) \cap \mathcal{C}(\bar{J}_\delta)$.

Proof of Proposition 2.16. We rewrite (2.6)–(2.7) in terms of $\varphi_{e,\text{Li}}$, defining $\bar{\kappa}(x) = \kappa(c_e(x), T) \in \mathcal{C}([0, L])$, as

$$\int_0^L \bar{\kappa} \frac{\partial \varphi_{e,\text{Li}}}{\partial x} \frac{d\psi_e}{dx} dx - \int_{J_\delta} j^{\text{Li}} \psi_e dx = 0, \quad \int_{J_\delta} \sigma \frac{\partial \phi_s}{\partial x} \frac{d\psi_s}{dx} dx + \int_{J_\delta} j^{\text{Li}} \psi_s dx = -\frac{I}{A}(\psi_s(L) - \psi_s(0)), \quad (\psi_e, \psi_s) \in X_\phi.$$

Adding both equations, we obtain that (2.6)–(2.7) is equivalent to

$$\int_0^L \bar{\kappa} \frac{\partial \varphi_{e,\text{Li}}}{\partial x} \frac{d\psi_e}{dx} dx + \int_{J_\delta} \sigma \frac{\partial \phi_s}{\partial x} \frac{d\psi_s}{dx} dx + \int_{J_\delta} j^{\text{Li}}(\psi_s - \psi_e) dx = -\frac{I}{A}(\psi_s(L) - \psi_s(0)), \quad (\psi_e, \psi_s) \in X_\phi. \quad (3.2)$$

Let us define, for $x \in [0, L]$ and $\Phi \in \mathbb{R}$,

$$\widehat{j^{\text{Li}}}(x, \Phi) = \underline{j^{\text{Li}}}(x, \Phi) - j_0^{\text{Li}}(x). \quad (3.3)$$

Notice that $\widehat{j^{\text{Li}}}(x, 0) = 0$. We can rewrite (3.2) as

$$\begin{aligned} & \int_0^L \bar{\kappa} \frac{\partial \varphi_{e,\text{Li}}}{\partial x} \frac{d\psi_e}{dx} dx + \int_{J_\delta} \sigma \frac{\partial \phi_s}{\partial x} \frac{d\psi_s}{dx} dx + \int_{J_\delta} \widehat{j^{\text{Li}}}(x, \phi_s - \varphi_{e,\text{Li}})(\psi_s - \psi_e) dx \\ &= -\frac{I}{A}(\psi_s(L) - \psi_s(0)) - \int_{J_\delta} j_0^{\text{Li}}(x)(\psi_s - \psi_e) dx. \end{aligned}$$

Let us define the operator $A_1 : X_\Phi \rightarrow X_\Phi^*$ by

$$\langle A_1(\varphi_{e,\text{Li}}, \phi_s), (\psi_e, \psi_s) \rangle = \int_{J_\delta} \widehat{j^{\text{Li}}}(x, \phi_s - \varphi_{e,\text{Li}})(\psi_s - \psi_e) dx, \quad (\varphi_{e,\text{Li}}, \phi_s), (\psi_e, \psi_s) \in X_\Phi.$$

Since $H^1(J_\delta) \subset \mathcal{C}(\overline{J_\delta})$ and $(\varphi_{e,\text{Li}}, \phi_s) \in X_\Phi \rightarrow \widehat{j^{\text{Li}}}(x, \phi_s - \varphi_{e,\text{Li}}) \in \mathcal{C}(\overline{J_\delta})$ is bounded and continuous (due to (2.2) and (2.3)), it follows that the operator $A_1 : X_\Phi \rightarrow X_\Phi^*$ is bounded continuous. Furthermore, applying (3.1), (3.3) and Remark 2.4 (due to Assumption 2.3), we can show that A_1 is a monotone operator since, for all $(\varphi_{e,\text{Li}}, \phi_s), (\widetilde{\varphi_{e,\text{Li}}}, \widetilde{\phi_s}) \in X_\Phi$, we have that

$$\begin{aligned} & \langle A_1(\varphi_{e,\text{Li}}, \phi_s) - A_1(\widetilde{\varphi_{e,\text{Li}}}, \widetilde{\phi_s}), (\varphi_{e,\text{Li}}, \phi_s) - (\widetilde{\varphi_{e,\text{Li}}}, \widetilde{\phi_s}) \rangle \\ &= \int_{J_\delta} (\widehat{j^{\text{Li}}}(x, \phi_s - \varphi_{e,\text{Li}}) - \widehat{j^{\text{Li}}}(x, \widetilde{\phi_s} - \widetilde{\varphi_{e,\text{Li}}}))(\phi_s - \varphi_{e,\text{Li}} - (\widetilde{\phi_s} - \widetilde{\varphi_{e,\text{Li}}})) dx \\ &= \int_{J_\delta} (\underline{j^{\text{Li}}}(x, \phi_s - \varphi_{e,\text{Li}}) - \underline{j^{\text{Li}}}(x, \widetilde{\phi_s} - \widetilde{\varphi_{e,\text{Li}}}))(\phi_s - \varphi_{e,\text{Li}} - (\widetilde{\phi_s} - \widetilde{\varphi_{e,\text{Li}}})) dx \\ &= \int_{J_\delta} (\underline{j^{\text{Li}}}(x, c_e, c_{s,\text{B}}, \phi_s - \varphi_{e,\text{Li}} + \eta_0) - \underline{j^{\text{Li}}}(x, c_e, c_{s,\text{B}}, T, \widetilde{\phi_s} - \widetilde{\varphi_{e,\text{Li}}} + \eta_0))(\phi_s - \varphi_{e,\text{Li}} - (\widetilde{\phi_s} - \widetilde{\varphi_{e,\text{Li}}})) dx \\ &= \int_{J_\delta} F^{\text{Li}}(x, c_e(x), c_s(x), T, \eta(x), \widetilde{\eta}(x))(\phi_s - \varphi_{e,\text{Li}} - (\widetilde{\phi_s} - \widetilde{\varphi_{e,\text{Li}}}))^2 dx \end{aligned}$$

for all $(\varphi_{e,\text{Li}}, \phi_s), (\psi_e, \psi_s) \in X_\Phi$, due to (2.5) (which is true due to Assumption 2.3), where

$$\begin{aligned} \eta(x) &= \phi_s(x) - \varphi_{e,\text{Li}}(x) - \alpha_{\varphi_e} T f_{\varphi_e}(c_e) - U(x, c_e, c_s, T), \\ \widetilde{\eta}(x) &= \widetilde{\phi_s}(x) - \widetilde{\varphi_{e,\text{Li}}}(x) - \alpha_{\varphi_e} T f_{\varphi_e}(c_e) - U(x, c_e, c_s, T). \end{aligned}$$

Therefore, for all $(\psi_e, \psi_s) \in X_\Phi$,

$$\langle A_1(\phi_s, \varphi_{e,\text{Li}}) - A_1(\widetilde{\phi_s}, \widetilde{\varphi_{e,\text{Li}}}), (\phi_s, \varphi_{e,\text{Li}}) - (\widetilde{\phi_s}, \widetilde{\varphi_{e,\text{Li}}}) \rangle \geq C \int_{J_\delta} (\phi_s - \varphi_{e,\text{Li}} - (\widetilde{\phi_s} - \widetilde{\varphi_{e,\text{Li}}}))^2 dx, \quad (3.4)$$

where

$$C = C(c_e, c_s, T, \phi_s - \varphi_{e,\text{Li}}, (\widetilde{\phi_s} - \widetilde{\varphi_{e,\text{Li}}})) = \min_{x \in J_\delta} \int_{J_\delta} F^{\text{Li}}(x, c_e(x), c_s(x), T, \eta(x), \widetilde{\eta}(x)) > 0.$$

Let the operator $\mathcal{A} : X_\phi \rightarrow X_\phi^*$ be defined by

$$\langle \mathcal{A}(\phi_s, \varphi_{e,\text{Li}}), (\psi_s, \psi_e) \rangle = \int_0^L \tilde{\kappa} \frac{\partial \varphi_{e,\text{Li}}}{\partial x} \frac{d\psi_e}{dx} dx + \int_{J_\delta} \sigma \frac{\partial \phi_s}{\partial x} \frac{d\psi_s}{dx} dx + \langle A_1(\phi_s, \varphi_{e,\text{Li}}), (\psi_s, \psi_e) \rangle.$$

Then \mathcal{A} is a bounded, continuous, monotone operator. Moreover, it is coercive due to the Poincaré–Wirtinger inequality $\|\varphi_{e,\text{Li}}\|_{L^2(0,L)} \leq C\|\nabla \varphi_{e,\text{Li}}\|_{L^2(0,L)}$ and inequality (3.4). Hence, there exists a unique solution of system (1.7)–(1.8), due to the Minty–Browder theorem. \square

Remark 3.2. Of course, if (φ_e, ϕ_s) is a solution of system (1.7)–(1.8) and C is a constant, then $(\varphi_e + C, \phi_s + C)$ is also a solution. However, there exists only one solution in X_ϕ .

Remark 3.3. The main part of the proof above was to apply the monotonicity of j^{Li} with respect to $\phi_s - \varphi_{e,\text{Li}}$. The idea behind this monotonicity method has to do with the convexity of the associated energy functional.

We have so far proved that the map G_ϕ given by (2.16) is well defined. We prove now, applying the Implicit Function Theorem, that this map is \mathcal{C}^1 .

Proof of Proposition 2.17. We will apply the Implicit Function Theorem for the Banach space-valued mapping $F : \hat{X} \times \hat{Y} \rightarrow \hat{Z}$, to solve for an operator $\widehat{G}_\phi : U \subset \hat{X} \rightarrow \hat{Y}$ in an expression of the form

$$F(\hat{x}, \widehat{G}_\phi(\hat{x})) = 0 \quad \text{for all } \hat{x} \in U. \quad (3.5)$$

The choice of functional spaces will be

$$\hat{X} = \mathcal{C}_{>\kappa_0}([0, L]) \times \mathbb{R} \times K_X, \quad \hat{Y} = X_\phi, \quad \hat{Z} = X_\phi^*,$$

with

$$\mathcal{C}_{>\kappa_0}([0, L]) = \{\tilde{\kappa} \in \mathcal{C}([0, L]) : \tilde{\kappa} > \kappa_0\} \quad \text{for some } \kappa_0 > 0.$$

We will then check that

$$G_\phi(c_e, c_{s,B}, T, I) = \widehat{G}_\phi(\kappa(c_e, T), I, c_e, c_{s,B}, T) + (\alpha_{\varphi_e} Tf_{\varphi_e}(c_e), 0),$$

due to the definition of $\varphi_{e,\text{Li}}$ (see (2.14)). Notice that \hat{X} is an open set of a Banach space, and therefore we can consider the Implicit Function Theorem (see, e.g., [24]) in this setting. We will use the notation

$$\hat{x} = (\tilde{\kappa}, I, c_e, c_{s,B}, T) \in \hat{X}, \quad \hat{y} = (\varphi_{e,\text{Li}}, \phi_s) = (u, v) \in \hat{Y}.$$

We consider the maps $A_1, A_2, A_3, A_4 : \hat{X} \times \hat{Y} \rightarrow \hat{Z}$, given by

$$\begin{aligned} A_1(\hat{x}, \hat{y})(\psi_e, \psi_s) &= A_1(\hat{x}, u)(\psi_e) = \int_0^L \tilde{\kappa}(x) u'(x) \psi_e'(x) dx, \\ A_2(\hat{x}, \hat{y})(\psi_e, \psi_s) &= A_2(v)(\psi_s) = \int_{J_\delta} \sigma(x) v'(x) \psi_s'(x) dx, \\ \bar{\eta}_0(x, \hat{x}(x)) &= -\alpha_{\varphi_e} Tf_{\varphi_e}(c_e(x)) - U(x, c_e(x), c_{s,B}(x), T), \\ A_3(\hat{x}, \hat{y})(\psi_e, \psi_s) &= \int_{J_\delta} j^{\text{Li}}(x, \hat{x}(x), v(x) - u(x) + \bar{\eta}_0(x, \hat{x}(x))) \cdot (\psi_s(x) - \psi_e(x)) dx, \\ A_4(\hat{x}, \hat{y})(\psi_e, \psi_s) &= A_4(I)(\psi_s) = \frac{I}{A}(\psi_s(L) - \psi_s(0)), \\ F &= A_1 + \dots + A_4. \end{aligned}$$

Our definition of weak solution is precisely

$$F(\hat{x}, \hat{y}) = 0_{\hat{Z}}.$$

The function A_4 is linear and continuous, therefore \mathcal{C}^∞ . It is automatic to see that

$$D_{\hat{y}} A_4 = 0.$$

On the other hand, A_1, A_2 are multilinear and continuous, and therefore of class \mathcal{C}^1 . In particular, for $\hat{y} = (u, v), \hat{\bar{y}} = (\bar{u}, \bar{v}) \in X_\Phi$ we have

$$\begin{aligned} D_u A_1(\bar{\kappa}, u)(\bar{u}) &= A_1(\bar{\kappa}, \bar{u}), \\ D_v A_2(u)(\bar{v}) &= A_2(\bar{v}). \end{aligned}$$

Since $\frac{\partial \bar{J}^{\text{Li}}}{\partial \eta}$ is of class \mathcal{C}^1 (see (2.2) in Assumption 2.3), so is A_3 and

$$D_{(u,v)} A_3(\hat{x}, u, v)(\bar{u}, \bar{v})(\psi_e, \psi_s) = \int_{J_\delta} g(\bar{v} - \bar{u})(\psi_s - \psi_e) dx,$$

where, for $x \in J_\delta$,

$$g(x) = \frac{\partial \bar{J}^{\text{Li}}}{\partial \eta}(x, \hat{x}(x), v(x) - u(x) + \bar{\eta}_0(x, \hat{x}(x))).$$

Let $\hat{x}^0 = (\bar{\kappa}, c_e, c_{s,B}, T) \in \hat{X}$, and let $\hat{y}^0 = (u^0, v^0) = (\varphi_{e,\text{Li}}, \phi_s) \in X_\Phi$ be the solution found in Proposition 2.16. Then $g(x) > 0$ is in $\mathcal{C}(\bar{J}_\delta)$. Therefore, there exists a constant g_0 such that $g(x) \geq g_0 > 0$ in J_δ . Then

$$D_{(u,v)} F(\hat{x}^0, \hat{y}^0) : (\bar{u}, \bar{v}) \in X_\Phi \rightarrow X_\Phi^*,$$

understood as a bilinear form

$$G((\bar{u}, \bar{v}), (\psi_e, \psi_s)) = \int_0^L \bar{\kappa} \bar{u}' \psi_e' + \int_{J_\delta} \sigma \bar{v}' \psi_s' + \int_{J_\delta} g(x)(\bar{u} - \bar{v})(\psi_s - \psi_e),$$

is continuous and coercive in $X_\Phi \times X_\Phi$. Therefore, by Lax–Milgram’s theorem $D_{(u,v)} F(\hat{x}^0, \hat{y}^0)$ is bijective. Then, by the Implicit Function Theorem applied to F , there exists a unique \mathcal{C}^1 function $\widehat{G}_\Phi : U \rightarrow X_\Phi$, defined in a neighborhood U of \hat{x}^0 in \hat{X} , such that (3.5) holds.

Since $(c_e, T) \in H^1(0, L) \times \mathbb{R} \mapsto \kappa(c_e, T) \in \mathcal{C}([0, L])$ is also \mathcal{C}^1 (the function κ is of class \mathcal{C}^2 due to Assumption 2.2), we have that the map

$$(c_e, c_{s,B}, T, I) \in K_X \times \mathbb{R} \xrightarrow{J} (\kappa(c_e, T), I, c_e, c_{s,B}, T) \in \hat{X}$$

is \mathcal{C}^1 . Let us choose a point $(c_e^0, c_{s,B}^0, T^0, I^0) \in K_X \times \mathbb{R}$, and let $\hat{x}_0 = (\kappa(c_e^0, T^0), I^0, c_e^0, c_{s,B}^0, T^0) \in \hat{X}$. Let $U \subset \hat{X}$ be a suitable neighborhood of \hat{x}_0 so that $\widehat{G}_\Phi : U \rightarrow X_\Phi$ is defined satisfying (3.5). Taking the neighborhood of $(c_e^0, c_{s,B}^0, T^0, I^0)$ given by $V = J^{-1}(U) \subset K_X \times \mathbb{R}$, the composition

$$(c_e, c_{s,B}, T, I) \in V \xrightarrow{J} (\kappa(c_e, T), I, c_e, c_{s,B}, T) \in U \xrightarrow{\widehat{G}_\Phi} (\varphi_{e,\text{Li}}, \phi_s) \in X_\Phi$$

is \mathcal{C}^1 . We finally consider the following translation (which is also of class \mathcal{C}^1):

$$\tau : V \times X_\Phi \rightarrow H^1(0, L) \times H^1(J_\delta), \quad (c_e, c_{s,B}, T, I, \varphi_{e,\text{Li}}, \phi_s) \mapsto (\varphi_e, \phi_s) = (\varphi_{e,\text{Li}} + \alpha_{\varphi_e} T f_{\varphi_e}(c_e), \phi_s).$$

Due to the uniqueness (up to a constant) result we proved in Proposition 2.16,

$$\tau \circ (Id, \widehat{G}_\Phi \circ J) : V \subset K_X \times \mathbb{R} \rightarrow H^1(0, L) \times H^1(J_\delta)$$

is the map $G_\Phi|_V$ (as constructed in (2.16) through Proposition 2.16). Thus, G_Φ is of class \mathcal{C}^1 in a neighborhood of $(c_e^0, c_{s,B}^0, T^0, I^0)$. Since this argument holds over any point $(c_e^0, c_{s,B}^0, T^0, I^0) \in K_X \times \mathbb{R}$, we have shown that G_Φ is of class \mathcal{C}^1 over $K_X \times \mathbb{R}$. This implies that \widehat{G}_Φ is also \mathcal{C}^1 and it concludes the proof. \square

Therefore, as an immediate consequence of Proposition 2.17, we have the following lemma in terms of the space of piecewise continuous functions $\mathcal{C}_{\text{part}}$ defined by (2.1):

Lemma 3.4. *Let $I \in \mathcal{C}([0, t_0])$. Then the operator $\widetilde{G}_{\Phi,t} : \mathcal{C}([0, t_0], K_X) \rightarrow \mathcal{C}([0, t_0], K_Z)$ is locally Lipschitz continuous. If $I \in \mathcal{C}_{\text{part}}([0, t_0])$, then $\widetilde{G}_{\Phi,t} : \mathcal{C}([0, t_0], K_X) \rightarrow \mathcal{C}_{\text{part}}([0, t_0], K_Z)$ is locally Lipschitz continuous.*

4 Regularity of the Green operators $G_{c_e,t}$ and $G_{c_s,B,t}$

The regularity of $G_{c_e,t}$ is a well-known property:

$$G_{c_e,t_0} : L^2((0, t_0) \times (0, L)) \rightarrow \mathcal{C}([0, t_0]; H^1(0, L)).$$

This operator has a nice representation formula

$$(G_{c_e,t_0}f)(t) = S(t)c_{e,0} + \int_0^t S(t-s)f(s) ds,$$

where $S(t)u_0$ is the solution of

$$\begin{cases} \frac{\partial u}{\partial t} - \frac{\partial}{\partial x} \left(D_e \frac{\partial c_e}{\partial x} \right) = 0 & \text{in } (0, L) \times \mathbb{R}, \\ \frac{\partial u}{\partial x} = 0 & \text{in } \{0, L\} \times \mathbb{R}, \\ u(0) = u_0, \quad t = 0. \end{cases}$$

A number of properties can easily be derived from this expression. For instance, the continuous dependence with respect to the data:

$$\|G_{c_e,t_0}f - G_{c_e,t_0}g\|_{\mathcal{C}([0,t_0];H^1(0,L))} \leq \rho(t_0)\|f - g\|_{L^2(0,t_0;H^1(0,L))},$$

where ρ is an increasing, continuous function such that $\rho(0) = 0$.

The term $G_{c_s,B,t}$ is a little trickier. First we recall (see [3, 28]) that, for any $q > 2$,

$$G_{c_s,R,t_0} : \mathcal{C}((0, R)) \times L^q(0, t_0) \rightarrow \mathcal{C}([0, t_0] \times [0, R])$$

and

$$\|G_{c_s,R,t_0}(u_0, g)\|_{L^\infty(0,t_0;L^\infty(B_R))} \leq C(\|u_0\|_{L^\infty(B_R)} + \|g\|_{L^q(0,t_0)}).$$

Therefore, due to the linearity of the equation, for x, y in the same connected component of J_δ , we have

$$\|G_{c_s,R,t_0}(u_0, g) - G_{c_s,R,t_0}(v_0, h)\|_{L^\infty(0,T;L^\infty(B_R))} \leq C(\|u_0 - v_0\|_{L^\infty(B_R)} + \|g - h\|_{L^q(0,T)}).$$

This solves the problem of continuity of $G_{c_s}g$ with respect to x via the continuous dependence of the operator. Since $c_{s,0}$ is continuous, working in each component we can prove directly that

$$G_{c_s,B,t_0} : \mathcal{C}(\overline{J_\delta}; L^q(0, t_0)) \rightarrow \mathcal{C}(\overline{J_\delta} \times [0, t_0])$$

is Lipschitz continuous. Furthermore, it is easy to check that

$$G_{c_s,B,t_0} : \mathcal{C}(\overline{J_\delta} \times [0, t_0]) \rightarrow \mathcal{C}(\overline{J_\delta} \times [0, t_0]).$$

We also have the following time estimate, for $t_0 \geq 0$,

$$\|G_{c_s,B,t_0}g - G_{c_s,B,t_0}h\|_{L^\infty([0,t_0] \times J_\delta)} \leq Ct_0^{\frac{1}{q}}\|g - h\|_{L^\infty((0,t_0) \times J_\delta)}.$$

By defining the vectorial Green operator for the evolutionary part

$$\mathbf{G}_t = (G_{c_e,t}G_{c_s,t}, G_{T,t}) : \mathcal{C}([0, t]; Y) \rightarrow \mathcal{C}([0, t]; X),$$

due to the previous results, we have

$$\|\mathbf{G}_t\mathbf{y} - \mathbf{G}_t\hat{\mathbf{y}}\|_{\mathcal{C}([0,t];X)} \leq \rho(t)\|\mathbf{y} - \hat{\mathbf{y}}\|_{\mathcal{C}([0,t];Y)}, \quad (4.1)$$

where ρ is a continuous function such that $\rho(0) = 0$.

5 Proof of Theorem 1

First, let us assume that I is continuous. Let us define the function

$$\mathbf{f}(c_e, c_{s,B}, \varphi_e, \phi_s, T) = (\alpha_e(x)N_{jLi}(c_e, c_{s,B}, \varphi_e, \phi_s, T), \alpha_{\phi_s}N_{jLi}(c_e, c_{s,B}, \varphi_e, \phi_s, T), -hA_s(T - T_{amb}) + F_T).$$

It is clear that $\mathbf{f} : K_X \rightarrow Y$ is locally Lipschitz continuous (due to the definition and regularity of N_{jLi} and F_T). Let us define, for any $t > 0$,

$$\mathbf{f}_t : \mathcal{C}([0, t]; K_X) \rightarrow \mathcal{C}([0, t]; Y)$$

by $\mathbf{f}_t(\mathbf{x})(s) = \mathbf{f}(\mathbf{x}(s))$ for $s \in [0, t]$. This operator is also locally Lipschitz continuous. Let $\mathbf{x} = (c_e, c_{s,B}, T)$. Then we can rewrite the fixed point problem (2.11) (which was our definition of a weak-mild solution of (1.5)–(1.9)) as

$$\mathbf{x} = \mathbf{G}_t \circ \mathbf{f}_t \circ \widetilde{G}_{\phi,t}(\mathbf{x}). \quad (5.1)$$

Since $\mathbf{f}_t \circ \widetilde{G}_{\phi,t} : \mathcal{C}([0, t_0], K_X) \rightarrow \mathcal{C}([0, t_0], Y)$ is locally Lipschitz continuous (due to Lemma 3.4), we can set a bounded neighborhood $\mathbf{U} \subset K_X$ around $\mathbf{x}(0) = (c_e(0), c_{s,B}(0), T(0)) \in K_X$ and a bounded set $\mathbf{V} \subset Y$ such that the composition

$$\mathbf{f}_t \circ \widetilde{G}_{\phi,t_0} : \mathcal{C}([0, t_0], \mathbf{U}) \rightarrow \mathcal{C}([0, t_0], \mathbf{V})$$

is globally Lipschitz continuous. Due to the continuity of \mathbf{G}_t and the fact that $\mathbf{G}_0 \equiv \mathbf{x}(0) \in K_X$, there exists $t_1 > 0$ such that

$$\mathbf{G}_{t_1} : \mathcal{C}([0, t_1], \mathbf{V}) \rightarrow \mathcal{C}([0, t_1], \mathbf{U}).$$

Therefore, due to (4.1), we obtain that, for $t_2 = \min\{t_0, t_1\} > 0$,

$$\mathbf{G}_{t_2} \circ \mathbf{f}_t \circ \widetilde{G}_{\phi,t_2} : \mathcal{C}([0, t_2], \mathbf{U}) \rightarrow \mathcal{C}([0, t_2], \mathbf{U})$$

is a contracting map. Then we can apply the Banach Fixed Point Theorem to find a unique solution of problem (5.1). If I is \mathcal{C}_{part} , then one can simply paste the mild solutions from the different time partitions. In this sense there exists a unique “piecewise weak-mild solution”.

By applying classical results, there exists a maximal existence time $t_{end} \leq t_{end}^I$. If $t_{end} < t_{end}^I$, then we have $d(\mathbf{x}(t), \partial K_X) \rightarrow 0$ or $\|\mathbf{x}(t)\|_X \rightarrow +\infty$ as $t \rightarrow t_{end}$. This is equivalent to (1.26) and the proof is complete.

6 Proof of Theorem 2

There are a number of papers studying the semilinear equation $u_t - \Delta u = f(u)$ with Robin-type boundary conditions, and its eventual possible blow-up, depending on the growth of f . Some of the most classical results are due to Amann [1] (for some more recent works, see e.g., [29]).

Let us assume that the solution $(c_e, c_{s,B}, \varphi_e, \phi_s, T)$ is defined in $[0, t_0)$, where $0 < t_0 < t_{end}^I$, and assume that (1.27) does not hold as $t \nearrow t_0$. We will show that (1.26) does not hold, and therefore $t_{end} > t_0$. We can think of the problem written in the following way:

$$\frac{\partial c_e}{\partial t} - \frac{\partial}{\partial x} \left(D_e \frac{\partial c_e}{\partial x} \right) + C_1 c_e^{\alpha_a + \gamma_2} \left(\alpha_{\varphi_e} + \frac{\mu(\bar{T})}{T} \right) = C_2 c_e^{\alpha_a - \gamma_1} \left(\alpha_{\varphi_e} + \frac{\mu(\bar{T})}{T} \right) \geq 0,$$

where C_1 and C_2 are functions which we will show can be estimated. We can define

$$\begin{aligned} \bar{\mu} &= \max_{[0,L] \times [0,t_0]} \left(\alpha_{\varphi_e} + \frac{\mu(x, T(t))}{T(t)} \right), \\ \underline{\mu} &= \min_{[0,L] \times [0,t_0]} \left(\alpha_{\varphi_e} + \frac{\mu(x, T(t))}{T(t)} \right) \geq 1, \\ \bar{C}_1 &= \max_{x \in J_\delta} (\delta_1 + \delta_2) \left(\max_{[0,L]} \alpha_e \right) \exp \left(\frac{\gamma_1 + \gamma_2}{\min_{[0,t_0]} T(t)} (\|\psi_s - \varphi_e\|_{L^\infty} + \|p\|_{L^\infty}) \right). \end{aligned}$$

Notice that, since $c_{s,\max} < 1$, we can conclude that $0 \leq C_1, C_2 \leq \bar{C}_1$. Finally, we can define some increasing continuous functions β_1, β_2 such that $\beta_1(0) = \beta_2(0) = 0$, with β_2 Lipschitz continuous and

$$\begin{aligned} \max\{s^{\alpha_a - \gamma_1 \underline{\mu}}, s^{\alpha_a - \gamma_1 \bar{\mu}}\} &\leq \beta_1(s) \leq 1 + s, \\ \beta_2(s) &\geq \max\{s^{\alpha_a + \gamma_2 \bar{\mu}}, s^{\alpha_a + \gamma_2 \underline{\mu}}\}, \end{aligned}$$

so that we can construct the supersolution \bar{c}_e and subsolution \underline{c}_e defined as solutions, respectively, of

$$\begin{cases} \frac{\partial \bar{c}_e}{\partial t} - \frac{\partial}{\partial x} \left(D_e \frac{\partial \bar{c}_e}{\partial x} \right) = \bar{C} \beta_1(\bar{c}_e), & (x, t) \in (0, L) \times (0, t_{\text{end}}), \\ \bar{c}_e(0) = c_{e,0}, & t = 0, \\ \partial_n \bar{c}_e = 0, & x \in \{0, L\}, \\ \frac{\partial \underline{c}_e}{\partial t} - \frac{\partial}{\partial x} \left(D_e \frac{\partial \underline{c}_e}{\partial x} \right) + \bar{C} \beta_2(\underline{c}_e) = 0, & (x, t) \in (0, L) \times (0, t_{\text{end}}), \\ \underline{c}_e(0) = c_{e,0}, & t = 0, \\ \partial_n \underline{c}_e = 0, & x \in \{0, L\}. \end{cases}$$

Using the conditions on the exponents given by Assumption 2.24, we deduce that $\bar{c}_e, \underline{c}_e$ are continuous, globally defined in time and

$$\min_{[0, L] \times [0, t_0]} \underline{c}_e > 0, \quad \max_{[0, L] \times [0, t_0]} \bar{c}_e < +\infty.$$

We also have that

$$\begin{cases} \frac{\partial c_s}{\partial t} - \frac{D_s}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_s}{\partial r} \right) = 0, & (x, r, t) \in D_\delta \times (0, t_0), \\ \frac{\partial c_s}{\partial r} + C_3 c_s^{\alpha_s + \gamma_1 \frac{\lambda_{\min}(x, T)}{T}} = \alpha_{c_s} j_-^{\text{Li}} \geq 0, & r = R_s(x), \\ c_s = c_{s,0} & t = 0, \end{cases}$$

where C_3 is a suitable function, such that if we define

$$\begin{aligned} \underline{\lambda}_{\min} &= \min_{[0, L] \times [0, t_0]} \frac{\lambda_{\min}(x, T(t))}{T(t)}, \\ \bar{\lambda}_{\min} &= \max_{[0, L] \times [0, t_0]} \frac{\lambda_{\min}(x, T(t))}{T(t)}, \\ \bar{C}_3 &= \max_{x \in J_\delta} (\delta_1 + \delta_2) \left(\max_{[0, L]} \alpha_s \right) \left(\max_{a \in \{\alpha_a \pm \gamma_{1,2} \underline{\mu}, \alpha_a \pm \gamma_{1,2} \bar{\mu}\}} \|c_e\|_{L^\infty}^\alpha \right) \\ &\quad \times \exp \left(\frac{1}{\min_{[0, t_0]} T(t)} \max\{\gamma_1, \gamma_2\} (\|\psi_s - \varphi_e\|_{L^\infty} + \|p\|_{L^\infty}) \right), \end{aligned}$$

then $0 \leq C_3 \leq \bar{C}_3$. Now, let β_3 be a monotone increasing locally Lipschitz continuous function such that $\beta_3(0) = 0$ and

$$\beta_3(s) \geq \max\{s^{\alpha_{c_s} + \gamma_1 \underline{\lambda}_{\min}}, s^{\alpha_{c_s} + \gamma_1 \bar{\lambda}_{\min}}\}.$$

We construct the subsolution \underline{c}_s , for every $t_0 < +\infty$, as the solution of

$$\begin{cases} \frac{\partial \underline{c}_s}{\partial t} - \frac{D_s}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \underline{c}_s}{\partial r} \right) = 0, & (x, y, t) \in (x, r, t) \in D_\delta \times (0, t_0), \\ \partial_n \underline{c}_s + \bar{C}_3 \sigma(\underline{c}_s) = 0, & r = R_s(x), \\ \underline{c}_s(x, y, t) = \min_{\sigma \in J_\delta} c_{s,0}(\sigma, y), & t = 0, \end{cases}$$

so that, by the comparison principle, we have that $0 < \underline{c}_s \leq c_s$ (by applying Assumptions 2.24). Finally, if we write

$$\begin{cases} \frac{\partial}{\partial t} (c_{s,\max} - c_s) - \frac{D_s}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial (c_{s,\max} - c_s)}{\partial r} \right) = 0, & (x, y, t) \in (x, r, t) \in D_\delta \times (0, t_0), \\ \frac{\partial}{\partial r} (c_{s,\max} - c_s) + C_4 (c_{s,\max} - c_s)^{\beta_a + \gamma_2 \frac{\lambda_{\max}(T)}{T}} = j_+^{\text{Li}} \geq 0, & r = R_s(x), \\ c_{s,\max} - c_s = c_{s,\max} - c_{s,0}, & t = 0, \end{cases} \quad (6.1)$$

since $0 \leq C_4 \leq \bar{C}_3$, if we introduce

$$\underline{\lambda}_{\max} = \min_{[0,L] \times [0,t_0]} \frac{\lambda_{\max}(x, T(t))}{T(t)}, \quad \bar{\lambda}_{\max} = \max_{[0,L] \times [0,t_0]} \frac{\lambda_{\max}(x, T(t))}{T(t)}$$

and define β_4 as a monotone increasing locally Lipschitz continuous function such that $\beta_4(0) = 0$ and

$$\beta_4(s) \geq \max\{s^{\alpha_{c_s} + \gamma_2 \bar{\lambda}_{\max}}, s^{\alpha_{c_s} + \gamma_2 \bar{\lambda}_{\max}}\},$$

then, by defining \bar{c}_s as the solution of

$$\begin{cases} \frac{\partial \bar{c}_s}{\partial t} - \frac{D_s}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \bar{c}_s}{\partial r} \right) = 0, & (x, y, t) \in D_\delta^{3D} \times (0, t_0), \\ \frac{\partial}{\partial r} \bar{c}_s + \bar{C}_3 \beta_4(\bar{c}_s) = 0, & |y| = R_s(x), \\ \bar{c}_s(x, y, t) = \min_{\sigma \in J_\delta} (c_{s,\max} - c_{s,0}(\sigma, y)), & t = 0, \end{cases}$$

we arrive at the definition of the searched function $\bar{c}_s = c_{s,\max} - \bar{c}_s$. We have $\bar{c}_s > 0$ (due to Assumption 2.24) and \bar{c}_s is a subsolution of (6.1). Hence $\bar{c}_s \leq c_{s,\max} - c_s$. Therefore, $c_s \leq \bar{c}_s < c_{s,\max}$. Putting these two bounding solutions together, we conclude $0 < \bar{c}_s \leq c_s \leq \bar{c}_s < c_{s,\max}$. Hence (1.26) does not hold as $t \nearrow t_0$. Applying Theorem 1, we obtain that $t_{\text{end}} > t_0$. Therefore, either $t_{\text{end}} = t_{\text{end}}^I$ or (1.27).

7 Proof of a global in time existence result

7.1 On the truncated potential case. Proof of Theorem 3

Assume that (1.28) does not hold as $t \rightarrow t_0$ with $0 < t_0 < t_{\text{end}}^I$. We can substitute the constants in the proof of Proposition 3

$$\begin{aligned} \bar{C}_1 &= \max_{x \in J_\delta} (\delta_1 + \delta_2) \left(\max_{[0,L]} \alpha_e \right) \exp \left(\frac{\gamma_1 + \gamma_2}{\min_{[0,t_0]} T} \|p\|_{L^\infty} \right), \\ \bar{C}_3 &= \max_{x \in J_\delta} (\delta_1 + \delta_2) \left(\max_{[0,L]} \alpha_s \right) \left(\max_{\alpha \in \{\alpha_a \pm \gamma_{1,2} \underline{\mu}, \alpha_a \pm \gamma_{1,2} \bar{\mu}\}} \|c_e\|_{L^\infty}^\alpha \right) \|H\|_{L^\infty} \exp \left(\frac{\gamma_1 + \gamma_2}{\min_{[0,t_0]} T} \|p\|_{L^\infty} \right) \end{aligned}$$

and repeat the argument. We get good bounds for $c_e, c_{s,B}$ for $t \in [0, t_0]$, which do not depend on $\|\phi_s - \varphi_{e,\text{Li}}\|_{L^\infty}$. Hence, applying Lemma 3.4, we can obtain some estimates of ϕ_s and $\varphi_{e,\text{Li}}$ in $[0, t_0]$. Therefore, by Theorem 2, we have that $t_{\text{end}} > t_0$. Hence, by contraposition, if $t_{\text{end}} < t_{\text{end}}^I$, then (1.28) must hold.

7.2 On the truncated temperature case. Proof of Theorem 4

It is immediate to establish global sub- and supersolutions for T , which ensure (1.28) does not happen, and hence we get the global existence of solutions.

8 Final remarks

8.1 Mass conservation and derived properties

We begin by analyzing the compatibility conditions for the elliptic problems with Neumann boundary conditions. The compatibility conditions for the existence of ϕ_s are

$$\int_0^{L_1} j^{\text{Li}} dx = + \frac{I(t)}{A}, \quad \int_{L_1+\delta}^L j^{\text{Li}} dx = - \frac{I(t)}{A}.$$

Hence, we deduce that

$$\int_0^L j^{\text{Li}} dx = 0.$$

This is also the compatibility condition for system (1.8).

Let us take a look at the mass balance condition. From system (1.6) we observe that

$$\frac{d}{dt} \left(\int_0^L c_e dx \right) = \int_0^L \left(\frac{\partial}{\partial t} c_e \right) dx = \int_0^L \alpha_e j^{\text{Li}} dx + D_e \left(\frac{\partial c_e}{\partial x}(L) - \frac{\partial c_e}{\partial x}(0) \right) = 0.$$

Thus, as expected, the mathematical model satisfies that the total concentration in the electrolyte is constant. Since $c_e \geq 0$ (we have constructed the convex spaces K_X and K_Z so that the solution of the mathematical model satisfies this condition, which is consistent with the physics of the problem since it is a concentration), this conclusion also implies that $\|c_e\|_{L^1(0,L)}$ is constant. In other words, as a whole, the electrolyte is saturated of Lithium. Any Lithium contribution from an electrode is immediately compensated somewhere else.

In fact, if one considers the Lithium concentration in the anode and cathode, for the pseudo-two-dimensional (P2D) model considered here, one gets

$$\begin{aligned} \frac{d}{dt} \left(4\pi \int_0^{L_1} \int_0^{R_{s,-}} c_s r^2 dr dx \right) &= 4\pi \int_0^{L_1} \int_0^{R_{s,-}} \frac{\partial c_s}{\partial t} r^2 dr dx = 4\pi \int_0^{L_1} \int_0^{R_{s,-}} D_s \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_s}{\partial r} \right) dr dx \\ &= -4\pi \int_0^{L_1} R_{s,-}^2 \alpha_{s,-} j^{\text{Li}} dx = -4\pi \frac{R_{s,-}^2 \alpha_{s,-} I(t)}{A}, \end{aligned}$$

and, analogously,

$$\frac{d}{dt} \left(4\pi \int_{L_1+\delta}^L \int_0^{R_{s,+}} c_s r^2 dr dx \right) = +4\pi \frac{R_{s,+}^2 \alpha_{s,+} I(t)}{A}.$$

If

$$R_{s,+}^2 \alpha_{s,+} = R_{s,-}^2 \alpha_{s,-},$$

then the P2D model satisfies that any loss of Lithium in its anode is instantaneously received by its cathode and viceversa. Otherwise, there would appear to be a net variation in the total amount of Lithium in the solid phase.

The state of the charge at time t of the cell, $\text{SOC}(t)$, can then be estimated as a normalized average of the mass of Lithium in one of the electrodes, typically the negative one (see [31]):

$$\text{SOC}(t) = \frac{3}{L_1(R_{s,-})^3} \int_0^{L_1} \int_0^{R_{s,-}} r^2 \frac{c_s(r, t; x)}{c_{s,\max}} dr dx.$$

8.2 Model validation and identification of parameters

In order to validate the model and identify suitable parameters, it is often necessary to compare the solutions of the model with real-world data and minimize some error functional using suitable parameter identification techniques and minimization algorithms (see, e.g., [19, 22, 23]). Since internal properties of the battery, such as the spatial distribution of Lithium ions, cannot be measured during operation, it is standard to measure only the temperature T (on the outside of the battery, but it is a safe assumption that the temperature is spatially homogeneous) and the output voltage V (see, for example, [5, 37]), which can be estimated by using (1.23).

9 Conclusions

In this work, we have shown that the system of equations (1.5)–(1.9) has a unique solution (under some mild conditions). In the most general setting, only local in time existence result can be shown, and the nature of the possible blow-up is characterized. The most difficult part of the study of an eventual possible blow-up is the structure of the open circuit potential U . By considering the model of U given by (2.18), which was proposed in [32], we can rule out some non-physical behaviors as the possible causes of blow-up, by making some assumptions on the coefficients. Finally, for the sake of mathematical completeness, we provide some extra conditions that allow for global uniqueness in time and make some comments regarding the conservation of Lithium in the model and the model validation.

Funding: The research of the authors was partially supported by the Spanish Ministry of Economy, Industry and Competitiveness under projects MTM2014-57113-P and MTM2015-64865-P. The research of D. Gómez-Castro was supported by a FPU Grant from the Ministerio de Educación, Cultura y Deporte (Spain). All the authors are members of the Research Group MOMAT (Ref. 910480) of the UCM.

References

- [1] H. Amann, On abstract parabolic fundamental solutions, *J. Math. Soc. Japan* **39** (1987), no. 1, 93–116.
- [2] S. N. Antontsev, J. I. Díaz and S. Shmarev, *Energy Methods for Free Boundary Problems: Applications to Nonlinear PDEs and Fluid Mechanics*, Birkhäuser, Boston, 2002.
- [3] W. Arendt, C. J. K. Batty and F. Neubrander, *Vector-valued Laplace Transforms and Cauchy Problems*, Monogr. Math., Springer, Basel, 2013.
- [4] R. Bermejo, J. Carpio, J. I. Díaz and L. Tello, Mathematical and numerical analysis of a nonlinear diffusive climate energy balance model, *Math. Comput. Model.* **49** (2009), no. 5–6, 1180–1210.
- [5] C. R. Birkel and D. A. Howey, Model identification and parameter estimation for LiFePO₄ batteries, in: *IET Hybrid and Electric Vehicles Conference 2013—HEVC 2013* IET, London (2013), 1–6.
- [6] C. R. Birkel, E. McTurk, M. R. Roberts, P. G. Bruce and D. A. Howey, A parametric open circuit voltage model for Lithium ion batteries, *J. Electrochem. Soc.* **162** (2015), no. 12, A2271–A2280.
- [7] A. M. Bizeray, D. A. Howey and C. W. Monroe, Resolving a discrepancy in diffusion potentials, with a case study for Li-ion batteries, *J. Electrochem. Soc.* **163** (2016), no. 8, E223–E229.
- [8] H. Brézis, Équations et inéquations non linéaires dans les espaces vectoriels en dualité, *Ann. Inst. Fourier* **18** (1968), no. 1, 115–175.
- [9] H. Brézis, Is there failure of the inverse function theorem?, in: *Morse Theory, Minimax Theory and Their Applications to Nonlinear Differential Equations* (Beijing 1999), New Stud. Adv. Math. 1 International Press, Somerville (1999), 23–33.
- [10] H. Brézis, *Functional Analysis, Sobolev Spaces and Partial Differential Equations*, Springer, New York, 2010.
- [11] F. E. Browder, Nonlinear monotone operators and convex sets in Banach spaces, *Bull. Amer. Math. Soc.* **71** (1965), no. 5, 780–785.
- [12] A. C. Casal, J. I. Díaz and J. M. Vegas, Blow-up in some ordinary and partial differential equations with time-delay, *Dynam. Systems Appl.* **18** (2009), no. 1, 29–46.
- [13] N. A. Chaturvedi, R. Klein, J. Christensen, J. Ahmed and A. Kojic, Algorithms for advanced battery-management systems, *IEEE Control Syst.* **30** (2010), no. 3, 49–68.
- [14] J. I. Díaz, *Nonlinear Partial Differential Equations and Free Boundaries*, Pitman, London, 1985.
- [15] J. I. Díaz, Qualitative study of nonlinear parabolic equations: An introduction, *Extracta Math.* **16** (2001), no. 3, 303–342.
- [16] J. I. Díaz and G. Hetzer, A functional quasilinear reaction-diffusion equation arising in climatology, in: *Partial Differential Equations and Applications. Papers Dedicated to Jacques-Louis Lions*, Gauthier-Villars, Paris (1998), 461–480.
- [17] J. I. Díaz and I. I. Vrabie, Propriétés de compacité de l'opérateur de Green généralisé pour l'équation des milieux poreux, *C. R. Math. Acad. Sci. Sér. I. Math.* **309** (1989), no. 4, 221–223.
- [18] T. W. Farrell and C. P. Please, Primary alkaline battery cathodes, *J. Electrochem. Soc.* **152** (2005), no. 10, A1930–A1941.
- [19] A. Fraguera, J. A. Infante, A. M. Ramos and J. M. Rey, A uniqueness result for the identification of a time-dependent diffusion coefficient, *Inverse Problems* **29** (2013), no. 12, Article ID 125009.
- [20] A. Friedman, *Partial Differential Equations of Parabolic Type*, Dover, Mineola, 1964.
- [21] D. Henry, *Geometric Theory of Semilinear Parabolic Equations*, Lecture Notes in Math. 840, Springer, Berlin, 1981.

- [22] J. Infante, M. Molina-Rodríguez and A. M. Ramos, On the identification of a thermal expansion coefficient, *Inverse Probl. Sci. Eng.* **23** (2015), no. 8, 1405–1424.
- [23] B. Ivorra, B. Mohammadi and A. M. Ramos, A multi-layer line search method to improve the initialization of optimization algorithms, *European J. Oper. Res.* **247** (2015), no. 3, 711–720.
- [24] S. Lang, *Fundamentals of Differential Geometry*, Springer, New York, 2012.
- [25] J. L. Lions, *Quelques Méthodes de Résolution pour les Problèmes aux Limites non Linéaires*, Dunod, Paris, 1969.
- [26] G. J. Minty, On a “monotonicity” method for the solution of nonlinear equations in Banach spaces, *Proc. Nat. Acad. Sci. USA* **50** (1963), no. 6, 1038–1041.
- [27] J. Newman, *Electrochemical Systems*, Prentice-Hall, New Jersey, 1972.
- [28] R. Nittka, Inhomogeneous parabolic Neumann problems, *Czechoslovak Math. J.* **64** (2014), no. 3, 703–742.
- [29] C.-V. Pao, *Nonlinear Parabolic and Elliptic Equations*, Springer, New York, 2012.
- [30] A. M. Ramos, *Introducción al análisis matemático del método de elementos finitos*, Editorial Complutense, Madrid, 2012.
- [31] A. M. Ramos, On the well-posedness of a mathematical model for Lithium-ion batteries, *Appl. Math. Model.* **40** (2016), no. 1, 115–125.
- [32] A. M. Ramos and C. P. Please, Some comments on the Butler–Volmer equation for modeling Lithium-ion batteries, preprint (2015), <https://arxiv.org/abs/1503.05912>.
- [33] R. Ranom, *Mathematical modelling of Lithium ion batteries*, Ph.D. thesis, University of Southampton, Southampton, 2014.
- [34] M. Renardy and R. C. Rogers, *An Introduction to Partial Differential Equations*, Springer, New York, 2006.
- [35] G. Richardson, A. M. Ramos, R. Ranom and C. Please, Charge transport modelling of Lithium ion batteries, in preparation.
- [36] K. Smith and C.-Y. Wang, Power and thermal characterization of a Lithium-ion battery pack for hybrid-electric vehicles, *J. Power Sources* **160** (2006), no. 1, 662–673.
- [37] L. Zhang, L. Wang, G. Hinds, C. Lyu, J. Zheng and J. Li, Multi-objective optimization of Lithium-ion battery model using genetic algorithm approach, *J. Power Sources* **270** (2014), 367–378.