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Mathematical modelling and well-posedness for Lithium-ion batteries

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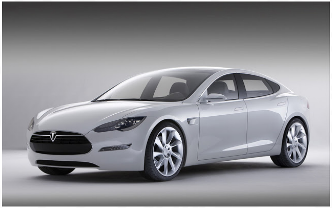
Plan of the talk

Outline

Outline

Lithium-ion batteries as a limiting vector

In several applications (electric cars, cell-phone technology, space exploration...) are limited by the charge density of electric batteries



Up to some minor modifications, the model currently being used is due to J. Newman in 1972[2].

However, there are still a vast number of open problems.

[2] J. Newman. *Electrochemical systems.* New Jersey: Prentice-Hall, 1972.

The infamous battery-catching-fire problem[3]

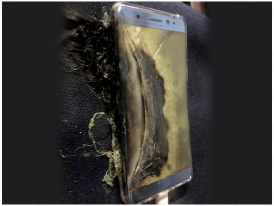


Figure: Burnt-out Samsung Note 7

The Samsung battery mystery:

> *In the case of batteries sourced from Amperex Technology Limited, some cells were missing insulation tape, and some batteries had sharp protrusions inside the cell that led to damage to the separator between the anode and cathode. The batteries also had thin separators in general, which increased the risks of separator damage and short circuiting.*

This alerts us of the need to understand in sharp detail battery dynamics. In particular, possible blow-up phenomena.

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[3] `https://www.wired.com/2017/01/why-the-samsung-galaxy-note-7-kept-exploding/`

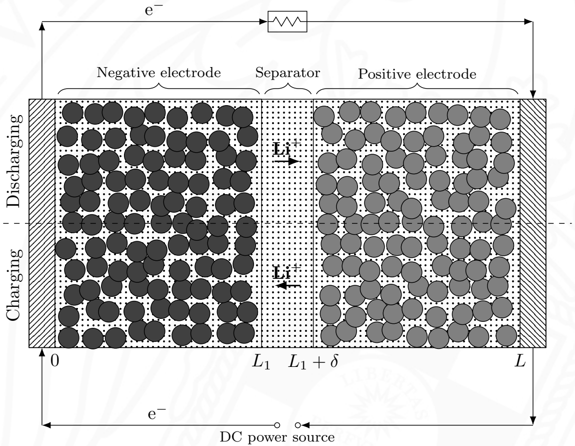
Outline

Outline

2. Mathematical Modeling
   - Basic electrochemical concepts
   - The Newman model
   - Writing of the model for existence and uniqueness theory

Outline

Basic electrochemical concepts



Schematic representation of a battery. On both sides of the cell the lined region represents the current collectors.

A typical Li-ion battery cell has three regions: A porous negative electrode, a porous positive electrode and an electron-blocking separator
Furthermore, the cell contains an electrolyte containing charge species that can move all along the cell.

Basic electrochemical concepts

– electrode: Intercalated Li compound usually made from Carbon, with $\mathrm{Li}_y\mathrm{C}_6$ active material. $y \in [0, 1]$ is the stoichiometry value
Discharge: Li^+ inside of solid $\mathrm{Li}_y\mathrm{C}_6$ particles diffuse to the surface where they react and transfer from the solid phase into the electrolyte phase. Charge: they follow the opposite way.

$$y\mathrm{Li}^+ + y\mathrm{e}^- + 6\mathrm{C} \longleftrightarrow \mathrm{Li}_y\mathrm{C}_6 \quad (0 \leq y \leq 1).$$

+ electrode: Usually a metal oxide or a blend of multiple metal oxides such as $\mathrm{Li}_{1-y}\mathrm{CoO}_2$, $\mathrm{Li}_{1-y}\mathrm{FePO}_4$ or $\mathrm{Li}_{1-y}\mathrm{Mn}_2\mathrm{O}_4$
Discharge: Li^+ travel via diffusion and migration through the electrolyte solution to the positive electrode where they react and insert into solid metal oxide particles. Charge: they follow the opposite way.

$$\mathrm{LiCoO}_2 \longleftrightarrow \mathrm{Li}_{1-y}\mathrm{CoO}_2 + y\mathrm{Li}^+ + y\mathrm{e}^- \quad (0 \leq y \leq 1),$$

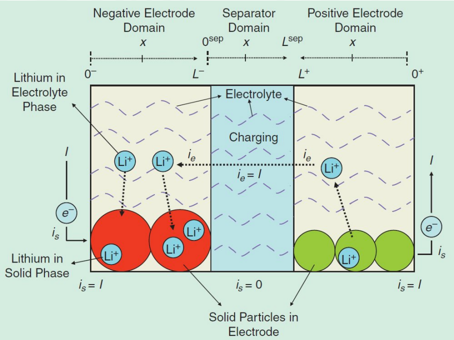
Total reaction equation:

$$\mathrm{LiCoO}_2 + 6\mathrm{C} \longleftrightarrow \mathrm{Li}_{1-y}\mathrm{CoO}_2 + \mathrm{Li}_y\mathrm{C}_6 \quad (0 \leq y \leq 1)$$

Outline

Mathematical model. 1D-model

A 1D electrochemical model is considered: x–direction: $x \in (0, L)$.
$L = L_1 + \delta + L_2$ being the cell width (m).



(from Chaturvedi et al (2010))

At each $x \in (0,L_1)\cup(L_1+\delta,L)$: generic spheric solid particle. Radius $R_{s,\pm}$

Mathematical model. 1D-model

Unknowns:

- Li concentration $c_{\mathrm{e}}(x,t)$ (mol / m^3) in the electrolyte
- Li concentration $c_{\mathrm{s}}(x;r,t)$ (mol / m^3) in the generic solid electrode particle at x
- Electric potential measured by a reference Lithium electrode $\varphi_{\mathrm{e}}(x,t)$ (V) in the electrolyte
- Electric potential $\phi_{\mathrm{s}}(x,t)$ (V) in the solid electrodes
- Temperature $T(t)$ (K) of the cell. It is usually considered as spatially homogeneous, although heat diffusion along the cell can be studied.

Validity of the 1D approximation: the characteristic lenth scale of a typical Li-ion cell along the X-axis is on the order of 100 μm, whereas the characteristic length scale for the remainder two axes is on the order of 100,000 μm or more

Mathematical model

Based on the works by John Newman and other authors:

Conservation of Li in the electrolyte phase

$$\begin{cases} \varepsilon_{\mathrm{e}} \dfrac{\partial c_{\mathrm{e}}}{\partial t} - \dfrac{\partial}{\partial x}\left(D_{\mathrm{e}} \varepsilon_{\mathrm{e}}^{p} \dfrac{\partial c_{\mathrm{e}}}{\partial x} \right) = \dfrac{1 - t_{+}^{0}}{F} j^{\mathrm{Li}}, & \text{in } (0, L) \times (0, t_{\mathrm{end}}), \\ \dfrac{\partial c_{\mathrm{e}}}{\partial x}(0, t) = \dfrac{\partial c_{\mathrm{e}}}{\partial x}(L, t) = 0, \quad t \in (0, t_{\mathrm{end}}), \\ c_{\mathrm{e}}(x, 0) = c_{\mathrm{e},0}(x), \quad x \in (0, L), \end{cases}$$

$$\varepsilon_{\mathrm{e}} = \varepsilon_{\mathrm{e}}(x) = \begin{cases} \varepsilon_{\mathrm{e},-} & \text{in } (0, L_1) \\ \varepsilon_{\mathrm{e,sep}} & \text{if } x \in (L_1, L_1 + \delta) \\ \varepsilon_{\mathrm{e},+} & \text{if } x \in (L_1 + \delta, L) \end{cases} \quad \text{volume fraction of the electrolyte}$$

p is the Bruggeman porosity exponent

D_{e} is the electrolyte phase Li diffusion coefficient ($\mathrm{m}^2\ \mathrm{s}^{-1}$)

t_{+}^{0} is the transference number of Li^{+} relative to the solvent velocity

j^{Li} reaction current resulting in production/consumption of Li ($\mathrm{A\ m}^{-3}$)

Flux of Lithium ions between phases

For j^{Li} the Butler-Volmer equation is used

$$j^{\mathrm{Li}} = j^{\mathrm{Li}}\Big(x, \phi_{\mathrm{s}}(x,t), \varphi_{\mathrm{e}}(x,t), c_{\mathrm{s}}(x; R_{\mathrm{s}}, t), c_{\mathrm{e}}(x,t), T(t)\Big)$$

$$j^{\mathrm{Li}}\Big(x, \phi_{\mathrm{s}}, \varphi_{\mathrm{e}}, c_{\mathrm{s}}, c_{\mathrm{e}}, T\Big) = \begin{cases} a_{\mathrm{s}} i_0 \left[\exp\left(\dfrac{\alpha_{\mathrm{a}} F}{R\,T}\eta\right) - \exp\left(\dfrac{-\alpha_{\mathrm{c}} F}{R\,T}\eta\right)\right] \\ \qquad \text{if } x \in (0, L_1) \cup (L_1 + \delta, L), \\ 0 \text{ if } x \in (L_1, L_1 + \delta) \end{cases}$$

$a_{\mathrm{s}} = a_{\mathrm{s}}(x) = \frac{3\varepsilon_{\mathrm{s}}(x)}{R_{\mathrm{s}}(x)}$ is the specific interfacial area of electrodes (m^{-1})

$$i_0 = i_0(x, c_{\mathrm{s}}, c_{\mathrm{e}}) = \begin{cases} k_-(c_{\mathrm{e}})^{\alpha_{\mathrm{a}}}(c_{\mathrm{s},-,\max} - c_{\mathrm{s}})^{\alpha_{\mathrm{a}}}(c_{\mathrm{s}})^{\alpha_{\mathrm{c}}} & \text{if } x \in (0, L_1), \\ k_+(c_{\mathrm{e}})^{\alpha_{\mathrm{a}}}(c_{\mathrm{s},+,\max} - c_{\mathrm{s}})^{\alpha_{\mathrm{a}}}(c_{\mathrm{s}})^{\alpha_{\mathrm{c}}} & \text{if } x \in (L_1 + \delta, L), \end{cases}$$

is the exchange current density of an electrode reaction ($\mathrm{A\ m}^{-2}$)
η is the surface overpotential (V) of an electrode reaction

The surface overpotential

$$\eta = \eta\Big(x, \phi_{\rm s}(x,t), \varphi_{\rm e}(x,t), c_{\rm s}(x; R_{\rm s}(x), t), c_{\rm e}(x,t), T(t)\Big),$$

$$\eta\Big(x, \phi_{\rm s}, \varphi_{\rm e}, c_{\rm s}, T\Big) = \begin{cases} \phi_{\rm s} - \varphi_{\rm e} - U(x, c_{\rm s}, T), \text{ if } x \in (0, L_1) \cup (L_1 + \delta, L), \\ 0 \text{ if } x \in (L_1, L_1 + \delta), \end{cases}$$

$U(x, c_{\rm s}, T)$ is the equilibrium potential (V) at the solid/electrolyte interface (i.e. OCV). A way of expressing U is

$$U(x, c, T) =$$

$$\begin{cases} U_- \left(\dfrac{c}{c_{{\rm s},-,\max}} \right) + \dfrac{\partial U_-}{\partial T} \left(\dfrac{c}{c_{{\rm s},-,\max}} \right) x \Big(T - T_{\rm ref} \Big) & \text{if } x \in (0, L_1), \\ U_+ \left(\dfrac{c}{c_{{\rm s},+,\max}} \right) + \dfrac{\partial U_+}{\partial T} \left(\dfrac{c}{c_{{\rm s},+,\max}} \right) x \Big(T - T_{\rm ref} \Big) & \text{if } x \in (L_1 + \delta, L). \end{cases}$$

where $U_-, U_+, \dfrac{\partial U_-}{\partial T} \dfrac{\partial U_-}{\partial T}$ are functions tipically obtained from fitting experimental data

Conservation of Li in the electrode solid phase

$$
\begin{cases}
\text{For each } x \in (0, L_1) \cup (L_1 + \delta, L): \\[1ex]
\dfrac{\partial c_{\mathrm{s}}}{\partial t} - \dfrac{D_{\mathrm{s}}}{r^2} \dfrac{\partial}{\partial r} \left(r^2 \dfrac{\partial c_{\mathrm{s}}}{\partial r} \right) = 0, \quad \text{in } (0, R_{\mathrm{s}}) \times (0, t_{\mathrm{end}}), \\[1ex]
\dfrac{\partial c_{\mathrm{s}}}{\partial r}(x; 0, t) = 0, \quad -D_{\mathrm{s}} \dfrac{\partial c_{\mathrm{s}}}{\partial r}(x; R_{\mathrm{s}}, t) = \dfrac{R_{\mathrm{s}}(x)}{3\varepsilon_{\mathrm{s}}(x) F} j^{\mathrm{Li}}, \quad t \in (0, t_{\mathrm{end}}), \\[1ex]
c_{\mathrm{s}}(x; r, 0) = c_{\mathrm{s},0}(x; r),
\end{cases}
$$

$D_{\mathrm{s}} = D_{\mathrm{s}}(x) = \begin{cases} D_{\mathrm{s},-} & \text{if } x \in (0, L_1), \\ D_{\mathrm{s},+} & \text{if } x \in (L_1 + \delta, L) \end{cases}$ is the solid phase Li diffusion coefficient ($\mathrm{m}^2\,\mathrm{s}^{-1}$)

$\varepsilon_{\mathrm{s}} = \varepsilon_{\mathrm{s}}(x) = \begin{cases} \varepsilon_{\mathrm{s},-} & \text{if } x \in (0, L_1), \\ \varepsilon_{\mathrm{s},+} & \text{if } x \in (L_1 + \delta, L), \end{cases}$ is the volume fraction of the active materials in the electrodes

Conservation of charge in the electrolyte phase

$$\begin{cases} \text{For each } t \in (0, t_{\mathrm{end}}) : \\ -\dfrac{\partial}{\partial x}\left(\varepsilon_{\mathrm{e}}^{p} \kappa \dfrac{\partial \varphi_{\mathrm{e}}}{\partial x}\right) + (1 - t_{+}^{0}) \dfrac{2R\,T}{F} \dfrac{\partial}{\partial x}\left(\varepsilon_{\mathrm{e}}^{p} \kappa \dfrac{\partial}{\partial x} \ln\left(c_{\mathrm{e}}\right)\right) = j^{\mathrm{Li}} \text{ in } (0, L), \\ \dfrac{\partial \varphi_{\mathrm{e}}}{\partial x}(0, t) = \dfrac{\partial \varphi_{\mathrm{e}}}{\partial x}(L, t) = 0, \end{cases}$$

$\kappa = \kappa\left(c_{\mathrm{e}}(x, t), T(t)\right)$ electrolyte ionic conductivity (S m^{-1})

Conservation of charge in the electrode solid phase

$$\begin{cases} \text{For each } t \in (0, t_{\text{end}}) : \\ -\varepsilon_{\text{s}} \sigma \dfrac{\partial^2 \phi_{\text{s}}}{\partial x^2} = - j^{\text{Li}} \text{ in } (0, L_1) \cup (L_1 + \delta, L), \\ -\varepsilon_{\text{s}}(0)\sigma(0) \dfrac{\partial \phi_{\text{s}}}{\partial x}(0, t) = -\varepsilon_{\text{s}}(L)\sigma(L) \dfrac{\partial \phi_{\text{s}}}{\partial x}(L, t) = \dfrac{I(t)}{A}, \\ \dfrac{\partial \phi_{\text{s}}}{\partial x}(L_1, t) = \dfrac{\partial \phi_{\text{s}}}{\partial x}(L_1 + \delta, t) = 0, \end{cases}$$

$\sigma = \sigma(x)$ electrical conductivity in electrodes (S m^{-1})

$I = I(t)$ is the applied current (A);

A (m^2) is the cross-sectional area (also the electrode plate area)

$\frac{I(t)}{A}$ is the applied current density (A m^{-2});

Heat transfer equation

$$\begin{cases} MC_p \dfrac{\mathrm{d}T}{\mathrm{d}t} = -hA_{\mathrm{s}}\Big(T - T_{\mathrm{amb}}\Big) + q_{\mathrm{r}} + q_{\mathrm{j}} + q_{\mathrm{c}} + q_{\mathrm{e}}, \ t \in (0, t_{\mathrm{end}}), \\ T(0) = T_0, \end{cases}$$

M (kg) is the mass of the battery
C_p (J kg^{-1} K^{-1}) is the specific heat capacity
h (W m^{-2} K^{-1}) is the heat transfer coefficient for convection
A_{s} (m^2) is the cell surface area exposed to the convective cooling medium (typically air)
T_{amb} is the (ambient) temperature of the cooling medium,

$q_{\rm r} = q_{\rm r}(t) = A \int_0^L j^{\rm Li} \eta \mathrm{d}x$ is the total reaction heat,

$$
\begin{aligned}
q_{\rm j}(t) &= A \int_0^{L_1} \varepsilon_{\rm s} \sigma \left(\frac{\partial \phi_{\rm s}}{\partial x} \right)^2 \mathrm{d}x + A \int_{L_1+\delta}^{L} \varepsilon_{\rm s} \sigma \left(\frac{\partial \phi_{\rm s}}{\partial x} \right)^2 \mathrm{d}x \\
&\quad + A \int_0^L \left[\varepsilon_{\rm e}^p \kappa \left(\frac{\partial \varphi_{\rm e}}{\partial x} \right)^2 + (t_+^0 - 1) \frac{2R\,T}{F} \varepsilon_{\rm e}^p \kappa \left(\frac{\partial \ln c_{\rm e}}{\partial x} \right) \left(\frac{\partial \varphi_{\rm e}}{\partial x} \right) \right] \mathrm{d}x
\end{aligned}
$$

is the ohmic heat due to the current carried in each phase and the limited conductivity of that phase,

$q_{\rm c} = q_{\rm c}(t) = I(t)^2 \frac{R_{\rm f}}{A}$ is the ohmic heat generated in the cell due to contact resistance between current collectors and electrodes, $R_{\rm f}$ (Ω m^2) is the film resistance of the electrodes

$$
\begin{aligned}
q_{\rm e} = q_{\rm e}(t) &= T A \left[\int_0^{L_1} j^{\rm Li} \frac{\partial U_-}{\partial T} \left(\frac{c_{\rm s}(x; R_{{\rm s},-}, t)}{c_{{\rm s},-,\max}} \right) \mathrm{d}x \right. \\
&\quad \left. + \int_{L_1+\delta}^{L} j^{\rm Li} \frac{\partial U_+}{\partial T} \left(\frac{c_{\rm s}(x; R_{{\rm s},+}, t)}{c_{{\rm s},+,\max}} \right) \mathrm{d}x \right]
\end{aligned}
$$

is the reversible heat caused by the reaction entropy change.

After solving the above model, we can get the state-of-charge

$$\mathrm{SOC}(t) = \frac{3}{L_1 (R_\mathrm{s})^3} \int_0^{L_1} \int_0^{R_{\mathrm{s},-}} r^2 \frac{c_\mathrm{s}(x;r,t)}{c_{\mathrm{s},-,\max}} \mathrm{d}r \mathrm{d}x$$

and the cell voltage

$$V(t) = \phi_\mathrm{s}(L,t) - \phi_\mathrm{s}(0,t) - \frac{R_\mathrm{f}}{A} I(t).$$

Outline

Complete model with simplified constants

For $(x,t) \in (0,L) \times (0,t_{\mathrm{end}})$

$$\begin{cases} \dfrac{\partial c_{\mathrm{e}}}{\partial t} - \dfrac{\partial}{\partial x}\left(D_{\mathrm{e}} \dfrac{\partial c_{\mathrm{e}}}{\partial x}\right) = \alpha_{\mathrm{e}} j^{\mathrm{Li}}, \\ \dfrac{\partial c_{\mathrm{e}}}{\partial x}(0,t) = \dfrac{\partial c_{\mathrm{e}}}{\partial x}(L,t) = 0, & t \in (0,t_{\mathrm{end}}), \\ c_{\mathrm{e}}(x,0) = c_{\mathrm{e},0}(x), & x \in (0,L), \end{cases} \tag{1}$$

For every $x \in (0,L_1) \cup (L_1+\delta, L)$ and $(r,t) \in (0,R_{\mathrm{s}}(x)) \times (0,t_{\mathrm{end}})$

$$\begin{cases} \dfrac{\partial c_{\mathrm{s}}}{\partial t} - \dfrac{D_s}{r^2}\dfrac{\partial}{\partial r}\left(r^2 \dfrac{\partial c_{\mathrm{s}}}{\partial r}\right) = 0, & \text{in ,} \\ \dfrac{\partial c_{\mathrm{s}}}{\partial r}(0,t;x) = 0, & t \in (0,t_{\mathrm{end}}), \\ -D_s \dfrac{\partial c_{\mathrm{s}}}{\partial r}(R_{\mathrm{s}}(x),t;x) = \alpha_s(x) j^{\mathrm{Li}} & t \in (0,t_{\mathrm{end}}), \\ c_{\mathrm{s}}(r,0;x) = c_{s,0}(r;x), & r \in (0,R_{\mathrm{s}}(x)), \end{cases} \tag{2}$$

We define $c_{\mathrm{s,B}}(x,t) = c_{\mathrm{s}}(R,t;x)$

For every $t > 0$, in $(0,L)$:

$$\begin{cases} -\dfrac{\partial}{\partial x}\left(\kappa \dfrac{\partial \varphi_{\mathrm{e}}}{\partial x}\right) + \alpha_{\varphi_{\mathrm{e}}} T \dfrac{\partial}{\partial x}\left(\kappa \dfrac{\partial}{\partial x}(f_{\varphi_{\mathrm{e}}}(c_{\mathrm{e}}))\right) = j^{\mathrm{Li}} \\ \dfrac{\partial \varphi_{\mathrm{e}}}{\partial x}(0,t) = \dfrac{\partial \varphi_{\mathrm{e}}}{\partial x}(L,t) = 0. \end{cases} \tag{3}$$

where $\kappa = \kappa(c_{\mathrm{e}}, T)$. For $x \in (0,L_1) \cup (L_1+\delta, L)$:

$$\begin{cases} -\dfrac{\partial}{\partial x}\left(\sigma \dfrac{\partial \phi_{\mathrm{s}}}{\partial x}\right) = -j^{\mathrm{Li}}, \\ \sigma(0)\dfrac{\partial \phi_{\mathrm{s}}}{\partial x}(0,t) = \sigma(L)\dfrac{\partial \phi_{\mathrm{s}}}{\partial x}(L,t) = -\dfrac{I(t)}{A}, \\ \dfrac{\partial \phi_{\mathrm{s}}}{\partial x}(L_1,t) = \dfrac{\partial \phi_{\mathrm{s}}}{\partial x}(L_1+\delta,t) = 0, \end{cases} \tag{4}$$

$$\begin{cases} \dfrac{\mathrm{d}T}{\mathrm{d}t}(t) = -\alpha_T(T(t) - T_{\mathrm{amb}}) + F_T, \\ T(0) = T_0, \end{cases} \tag{5}$$

A comment on divergence form equation

In [Ramos 2016], instead of equations (1), (3) and (4) the author consider the equations

$$
\begin{aligned}
\varepsilon_{\mathrm{e}} \frac{\partial c_{\mathrm{e}}}{\partial t} - \frac{\partial}{\partial x}\left(D_{\mathrm{e}} \varepsilon_{\mathrm{e}}^{p} \frac{\partial c_{\mathrm{e}}}{\partial x} \right) &= \alpha_e j^{\mathrm{Li}}, \quad \text{in } (0, L) \times (0, t_{\mathrm{end}}), \\
- \frac{\partial}{\partial x}\left(\varepsilon_{\mathrm{e}}^{p} \kappa \frac{\partial \varphi_{\mathrm{e}}}{\partial x} \right) + \alpha_{\varphi_{\mathrm{e}}} T \frac{\partial}{\partial x}\left(\varepsilon_{\mathrm{e}}^{p} \kappa \frac{\partial}{\partial x} (f_{\varphi_{\mathrm{e}}}(c_{\mathrm{e}})) \right) &= j^{\mathrm{Li}}, \quad \text{in } (0, L), \\
- \varepsilon_s \sigma \frac{\partial \phi_{\mathrm{s}}}{\partial x^2} = -j^{\mathrm{Li}}, \quad \text{in } (0, L_1) \cup (L_1 + \delta, L).
\end{aligned}
$$

where $\varepsilon_{\mathrm{e}} > 0$ 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 problem is not in divergence form.

Since the constant only jumps in two points, the problem can be written in three pieces with a matching boundary conditions, and techniques below apply.

The geometry

We simplify the domain notation by introducing the following sets:

$$J_\delta = (0, L_1) \cup (L_1 + \delta, L) \tag{6}$$

$$D_\delta = \bigcup_{x \in J_\delta} \{x\} \times [0, R_{\mathrm{s}}(x)]. \tag{7}$$

In fact, we will consider R_{s} constant in both $(0, L_1)$ and $(L_1 + \delta, L)$

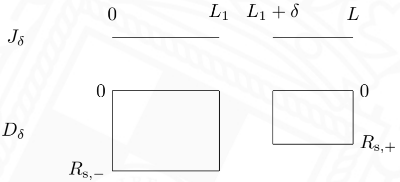


Figure: Domains J_δ (spatial domain of definition of $c_{\mathrm{e}}, \varphi_{\mathrm{e}}, \phi_{\mathrm{s}}$) and D_δ (spatial domain of definition of c_{s}). Notice that, since we are using a radial coordinate, every segment $\{x\} \times [0, R_{\mathrm{s}}(x)]$ in D_δ represents a ball $\{x\} \times B_{R_{\mathrm{s}}(x)}$ in $\{x\} \times \mathbb{R}^3$.

The flux function. General structure

The analytical expression of j^{Li} is given as follows, for $(c_{\text{e}}, c_{\text{s}}, \varphi_{\text{e}}, \phi_{\text{s}}, T) \in \mathbb{R}^5$:

$$j^{\text{Li}}(x, c_{\text{e}}, c_{\text{s}}, \varphi_{\text{e}}, \phi_{\text{s}}, T) = \begin{cases} \overline{j}^{\text{Li}}(x, c_{\text{e}}, c_{\text{s}}, T, \eta(x, c_{\text{e}}, c_{\text{s}}, \varphi_{\text{e}}, \phi_{\text{s}}, T)), & x \in J_\delta, \\ 0, & \text{otherwise}, \end{cases} \tag{8}$$

$$\eta(x, c_{\text{e}}, c_{\text{s}}, \varphi_{\text{e}}, \phi_{\text{s}}, T) = \phi_{\text{s}} - \varphi_{\text{e}} - U(x, c_{\text{e}}, c_{\text{s}}, T), \quad x \in J_\delta, \tag{9}$$

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.

The flux function. Butler-Volmer expression

$$\bar{j}^{\mathrm{Li}} = c_{\mathrm{e}}^{\alpha_a} c_{\mathrm{s}}^{\alpha_c} (c_{\mathrm{s,max}} - c_{\mathrm{s}})^{\alpha_a} h\left(x, \frac{1}{T}\eta\right) \tag{10}$$

$$h(x,\eta) = \delta_1(x)\exp(\alpha_a \eta) - \delta_2(x)\exp(-\alpha_c \eta), \tag{11}$$

$$f_{\varphi_{\mathrm{e}}}(c_{\mathrm{e}}) = \ln c_{\mathrm{e}}, \tag{12}$$

$$\alpha_a \in (0,1), \tag{13}$$

$$\alpha_c \in (0,1), \tag{14}$$

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

Function U was later proposed in [Ramos and Please 2015] as

$$U = -\alpha(x) T \ln c_{\mathrm{s}} + \beta(x) T \ln(c_{\mathrm{s,max}} - c_{\mathrm{s}}) + \gamma(x) T \ln c_{\mathrm{e}} + p(c_{\mathrm{e}}, c_{\mathrm{s}}, T), \tag{15}$$

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

Outline

Outline

3. Main results
   - Regularity assumptions of the nonlinear terms and initial data
   - Definition of weak-mild solution
   - Assumptions and results regarding Theorem 1
   - Assumptions and remarks regarding Theorem 2
   - Assumptions and remarks regarding Theorems 3 and 4

Main results I

Our aim in this talk is to present the results and techniques presented in

J. I. Díaz, D. Gómez-Castro, and A. M. Ramos. "On the well-posedness of a multiscale mathematical model for Lithium-ion batteries". In: *Advances in Nonlinear Analysis* To appear [2018], pp. 1–28. arXiv: 1802.06353

Main results II

Theorem 1 (Well-posedness with general flux and nature of the possible blow-up)

Let assumptions 1, 2, 3 and 4 hold. Then, if t_{end} is small enough, there exists a unique weak-mild solution by parts of (1)-(5) (in the sense of Definition 2 and satisfying Assumption 5).
Moveover, 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 $t \nearrow t_{\text{end}}$:

$$\min_{J_\delta \times [0,t]} c_{\text{s,B}} \to 0 \quad \text{or} \quad \max_{J_\delta \times [0,t]} c_{\text{s,B}} \to c_{\text{s,max}} \quad \text{or} \quad \min_{[0,L]\times[0,t]} c_{\text{e}} \to 0$$
$$\text{or} \quad \max_{[0,t]\times[0,L]} c_{\text{e}} \to +\infty \quad \text{or} \quad \min_{[0,t]} T \to 0 \quad \text{or} \quad \max_{[0,t]} T \to +\infty. \tag{16}$$

Main results III

Theorem 2 (Well-posedness for the Butler-Volmer flux and nature of the possible blow-up)

Let Assumptions 1, 2, 4, 6, 7, 8 and 9 hold. Then, if t_{end} is small enough, there exists a unique weak-mild solution by parts of (1)-(5) (in the sense of Definition 2 and satisfying assumption 5). This solution admits a unique maximal extension in time with $t_{\text{end}} \le t_{\text{end}}^I$.
Moveover, if $t_{\text{end}} < t_{\text{end}}^I$ then, as $t \nearrow t_{\text{end}}$ either

$$\max_{J_\delta \times [0,t]} |\phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}}| \to +\infty \quad \text{or} \quad \min_{[0,t]} T \to 0 \quad \text{or} \quad \max_{[0,t]} T \to +\infty. \tag{17}$$

Furthermore,

$$0 < c_{\mathrm{s}} < c_{\mathrm{s,max}} \quad \text{and} \quad c_{\mathrm{e}} > 0, \qquad \forall\, 0 \le t < t_{\text{end}}. \tag{18}$$

Main results IV

Theorem 3 (Blow up behaviour when j^{Li} is bounded with respect to $\phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}}$)

Let Assumptions 1, 2, 4, 6, 7, 9 and 10 hold. Then, if t_{end} is small enough, there exists a unique weak-mild solution by parts of (1) - (5) (in the sense of Definition 2 and satisfying Assumption 5). This solution admits a unique maximal extension in time with $t_{\mathrm{end}} \leq t_{\mathrm{end}}^I$. If $t_{\mathrm{end}} < t_{\mathrm{end}}^I$, as $t \to t_{\mathrm{end}}$ then either

$$\min_{[0,t]} T \to 0 \quad \text{or} \quad \max_{[0,t]} T \to +\infty. \tag{19}$$

Finally, by assuming some additional conditions (see Assumptions 10, 11) 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:

Main results V

Theorem 4 (Global existence in a modified case)

Let assumptions 1, 2, 4, 6, 7, 9, 10 and 11 hold. Then, there exists a unique weak-mild solution by parts of (1) - (5), defined for $t \in [0, t^I_{\text{end}}]$ (in the sense of Definition 1 and satisfying Assumption 5).

Outline

3 Main results
- Regularity assumptions of the nonlinear terms and initial data
- Definition of weak-mild solution
- Assumptions and results regarding Theorem 1
- Assumptions and remarks regarding Theorem 2
- Assumptions and remarks regarding Theorems 3 and 4

Regularity assumptions I

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

Assumptions 1

Let us take the data:

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

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

$$
\mathcal{C}_{\mathrm{part}}([a,b]) = \{ f : [a,b] \to \mathbb{R} : \exists\, a = t_0 < t_1 < \cdots < t_N = b \text{ such that } f \in \mathcal{C}([t_{i-1}, t_i]) \}. \tag{20}
$$

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

Regularity assumptions II

Assumptions 2

$D_\mathrm{e} \in L^\infty(0,L), \kappa \in \mathcal{C}^2((0,+\infty)^2), \sigma \in L^\infty(J_\delta), D_\mathrm{e} \geq D_{e,0} > 0,$
$\kappa \geq \kappa_0 > 0, \sigma \geq \sigma_0 > 0$ and $f_{\varphi_\mathrm{e}} \in \mathcal{C}^2((0,+\infty)).$

Regularity assumptions III

Let us define the open convex sets where we expect to find the solutions:

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

where $H^1(a,b)$ is the usual Sobolev space over the interval (a,b) (see, e.g., [Brézis 2010; Ramos 2012]). It is important to point out that $H^1(a,b) \hookrightarrow \mathcal{C}([a,b])$. Finally, we define

$$
X_\phi = \left\{ (u,v) \in H^1(0,L) \times H^1(J_\delta) : \int_0^L u(x)\, \mathrm{d}x = 0 \right\}, \tag{21}
$$

the natural space in which we will look for the pair $(\varphi_{\mathrm{e}}, \phi_{\mathrm{s}})$.

Regularity assumptions IV

Instead of narrowly focusing on (10)-(14) we shall state an assumption (sufficient to prove Theorem 1) satisfied by a broader family of functions:

Assumptions 3

For the flux function we assume:

$$\bar{j}^{\mathrm{Li}} \in \mathcal{C}^2(J_\delta \times (0,+\infty) \times (0, c_{\mathrm{s,max}}) \times (0,+\infty) \times \mathbb{R}), \tag{22}$$

$$U \in \mathcal{C}^2(J_\delta \times (0,+\infty) \times (0, c_{\mathrm{s,max}}) \times (0,+\infty)), \tag{23}$$

such that

$$\frac{\partial \bar{j}^{\mathrm{Li}}}{\partial \eta}(x, c_{\mathrm{e}}, c_{\mathrm{s}}, T, \eta) > 0, \tag{24}$$

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

Regularity assumptions V

Remark 1

In particular, it follows from Assumption 3 (in particular due to (22) and (24) applying the Mean Value Theorem) that there exists a positive continuous function F^{Li} satisfying

$$\left(\bar{j}^{\mathrm{Li}}(x, c_{\mathrm{e}}, c_{\mathrm{s}}, T, \eta) - \bar{j}^{\mathrm{Li}}(x, c_{\mathrm{e}}, c_{\mathrm{s}}, T, \hat{\eta})\right)(\eta - \hat{\eta}) = F^{\mathrm{Li}}\left(x, c_{\mathrm{e}}, c_{\mathrm{s}}, T, \eta, \hat{\eta}\right)|\eta - \hat{\eta}|^2, \quad (25)$$

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

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

Assumptions 4

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

Outline

3. Main results
   - Regularity assumptions of the nonlinear terms and initial data
   - Definition of weak-mild solution
   - Assumptions and results regarding Theorem 1
   - Assumptions and remarks regarding Theorem 2
   - Assumptions and remarks regarding Theorems 3 and 4

An introduction to mild solutions I

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

$$\begin{cases} \dfrac{\partial u}{\partial t} - \Delta u = f & \text{in } \Omega \times (0, t_{\text{end}}), \\ u = 0 & \text{on } \partial\Omega \times (0, t_{\text{end}}), \\ u(\cdot, 0) = u_0, & \text{in } \Omega, \end{cases} \tag{26}$$

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 following problem

$$\begin{cases} \dfrac{\partial v}{\partial t} - \Delta v = 0 & \text{in } \Omega \times (0, t_{\text{end}}), \\ v = 0 & \text{on } \partial\Omega \times (0, t_{\text{end}}), \\ v(\cdot, 0) = u_0, & \text{in } \Omega, \end{cases} \tag{27}$$

by considering the decomposition of $L^2(\Omega)$ in terms of eigenfunctions of $-\Delta$.

An introduction to mild solutions II

Let us write the unique solution of (27) as $v(t) = S(t)u_0$. The operator $S(t)$ is a semigroup (see [Brézis 2010]), and has some interesting properties we will not discuss. A solution u of problem the non homogeneous problem (26) can be written, for every $t \in [0, t_{\text{end}}]$, as

$$u(t) = S(t)u_0 + \int_0^t S(t-s)f(s)\,\mathrm{d}s. \tag{28}$$

This kind of solution is known as a "mild solution". As in [Díaz and Vrabie 1989], one can define the "Green operator" for problem (26) as the function

$$G_{t_{\text{end}}} : f \mapsto S(\cdot)u_0 + \int_0^{\cdot} S(\cdot - s)f(s)\,\mathrm{d}s. \tag{29}$$

Mild solutions of each equation with RHS known I

In our problem we will need to work with a suitable Green operator associated to each of the equations. Assuming Assumptions 2, we will define several Green operators.
For any $t_0 > 0$ we define (see [Friedman 1964]):

$$\begin{aligned} G_{c_e, t_0} : L^2((0,L)\times(0,t_0)) &\to \mathcal{C}([0,t_0]; H^1(0,L)), \\ f &\mapsto V, \end{aligned}$$

as the solution of the problem

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

Mild solutions of each equation with RHS known II

For system (2) we will need to do some extra work due to the fact that the equation is only “pseudo 2D”. First we define the solution of problem (2) for every x fixed

$$\begin{aligned} G_{c_s,R,t_0} : \mathcal{C}([0,R]) \times \mathcal{C}([0,t_0]) &\to \mathcal{C}([0,R]\times[0,t_0]), \\ (u_0, g) &\mapsto V, \end{aligned}$$

by solving the corresponding problem

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

Mild solutions of each equation with RHS known III

The next step is to consider the dependence on x. Therefore we construct the Green operator associated to problem (2) collecting all $x \in J_\delta$:

$$\begin{aligned} G_{c_s, t_0} : \mathcal{C}(J_\delta \times [0, t_0]) &\to \mathcal{C}(D_\delta \times [0, t_0]), \\ g &\mapsto W, \end{aligned}$$

given by

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

Mild solutions of each equation with RHS known IV

Finally, we consider the Green operator for the system (5) as the function

$$\begin{aligned} G_{T,t_0} : \mathcal{C}([0,t_0];Z) &\to \mathcal{C}([0,t_0]), \\ (c_\mathrm{e}, c_{\mathrm{s,B}}, \varphi_\mathrm{e}, \phi_\mathrm{s}, T) &\mapsto W \end{aligned}$$

defined as

$$\begin{aligned} W(t) = T_0 + \int_0^t (-\alpha_T (T(s) - T_\mathrm{amb}) \\ + \int_0^t F_T(c_\mathrm{e}(\cdot,s), c_{\mathrm{s,B}}(\cdot,s), \varphi_\mathrm{e}(\cdot,s), \phi_\mathrm{s}(\cdot,s), T(s)))\, \mathrm{d}s. \end{aligned}$$

This operator is well-defined and of class $\mathcal{C}^1$ due to Assumption 4.

Netmiskii operators I

It will be useful to introduce the following Nemistkij operators:

$$\begin{aligned} N_{j^{\mathrm{Li}}} : K_Z &\to \mathcal{C}([0, L_1]) \cap \mathcal{C}([L_1, L_1+\delta]) \cap \mathcal{C}([L_1+\delta, L]) \\ (c_{\mathrm{e}}, c_{s,B}, \varphi_{\mathrm{e}}, \phi_{\mathrm{s}}, T) &\mapsto j^{\mathrm{Li}} \circ (c_{\mathrm{e}}, c_{s,B}, \varphi_{\mathrm{e}}, \phi_{\mathrm{s}}, T) \end{aligned}$$

$$\begin{aligned} N_{j^{\mathrm{Li}}, t_0} : \mathcal{C}([0, t_0]; K_Z) &\to \mathcal{C}([0, t_0]; \mathcal{C}([0, L_1]) \cap \mathcal{C}([L_1, L_1+\delta]) \cap \mathcal{C}([L_1+\delta, L])) \\ (c_{\mathrm{e}}, c_{s,B}, \varphi_{\mathrm{e}}, \phi_{\mathrm{s}}, T) &\mapsto j^{\mathrm{Li}} \circ (c_{\mathrm{e}}, c_{s,B}, \varphi_{\mathrm{e}}, \phi_{\mathrm{s}}, T). \end{aligned}$$

It is well known (see, e.g., [Henry 1981]) 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. (22) and (23)).

Weak-mild solution of the coupled model I

Definition 1 (Weak-mild solution)

We define a "weak-mild solution of (1)–(5)" as a quintuplet $(c_\mathrm{e}, c_\mathrm{s}, \varphi_\mathrm{e}, \phi_\mathrm{s}, T) \in C([0, t_\mathrm{end}); K_Z)$ such that there exists $0 < t_\mathrm{end} \leq t^I_\mathrm{end}$ for which:

1. $(\varphi_\mathrm{e}, \phi_\mathrm{s})$ is a weak solutions of system (3)–(4) for the functions $c_\mathrm{e}, c_\mathrm{s}, T$ given in the quintuplet, in the sense that, for every $t \in [0, t_\mathrm{end})$ the weak formulations

$$\int_0^L \kappa \frac{\partial \varphi_\mathrm{e}}{\partial x} \frac{\mathrm{d}\psi_\mathrm{e}}{\mathrm{d}x}\,\mathrm{d}x - \int_{J_\delta} j^{\mathrm{Li}} \psi_\mathrm{e}\,\mathrm{d}x = \int_0^L \kappa \alpha_{\varphi_\mathrm{e}} T \frac{\partial}{\partial x}(f_{\varphi_\mathrm{e}}(c_\mathrm{e})) \frac{\mathrm{d}\psi_\mathrm{e}}{\mathrm{d}x}\,\mathrm{d}x, \qquad \forall\, \psi_\mathrm{e} \in H^1(0, L) \tag{30}$$

$$\int_{J_\delta} \sigma \frac{\partial \phi_\mathrm{s}}{\partial x} \frac{\mathrm{d}\psi_\mathrm{s}}{\mathrm{d}x}\,\mathrm{d}x + \int_{J_\delta} j^{\mathrm{Li}} \psi_\mathrm{s}\,\mathrm{d}x = \frac{I(t)}{A}(\psi_\mathrm{s}(0) - \psi_\mathrm{s}(L)), \qquad \forall\, \psi_\mathrm{s} \in H^1(J_\delta) \tag{31}$$

2. $(c_\mathrm{e}, c_\mathrm{s}, T)$ is a mild solutions of the system (1), (2), (5) for the functions $\varphi_\mathrm{e}, \phi_\mathrm{s}$ given in the quintuplet, in the sense that for every $t_0 < t_\mathrm{end}$:

$$\begin{aligned}(c_\mathrm{e}, c_\mathrm{s}, T) = &\left(G_{c_\mathrm{e}, t_0}\left(\alpha_\mathrm{e} N_{j^{\mathrm{Li}}, t_0}\right), G_{c_\mathrm{s}, t_0}\left(\alpha_\mathrm{s} N_{j^{\mathrm{Li}}, t_0}\right), G_{T, t_0}\right) \\ &\circ (c_\mathrm{e}|_{t<t_0}, c_\mathrm{s}|_{R=R_\mathrm{s}(x), t<t_0}, \varphi_\mathrm{e}|_{t<t_0}, \phi_\mathrm{s}|_{t<t_0}, T|_{t<t_0}).\end{aligned} \tag{32}$$

Further comments on weak-mild solutions I

Definition 2 (Piecewise weak-mild solution)

We define a "piecewise weak-mild solution" as a quintuplet $(c_\mathrm{e}, c_\mathrm{s}, \varphi_\mathrm{e}, \phi_\mathrm{s}, T)$ such that there exists a partition $\{t_0, \cdots, t_N\}$ of $[0, t_\mathrm{end}]$ such that in $[t_i, t_{i+1}]$ $(c_\mathrm{e}, c_\mathrm{s}, \varphi_\mathrm{e}, \phi_\mathrm{s}, T)$ is a weak-mild solution in the previous sense, with $(c_\mathrm{e}, c_\mathrm{s}, T)(t_i)$ as initial condition in the interval $[t_i, t_{i+1}]$.

Remark 2

It is well known that for problems of type (26), any piecewise weak-mild solution is a weak solution.

Further comments on weak-mild solutions II

Definition 3

Given a solution (in any of the previous senses) $(c_{\mathrm{e}}, c_{\mathrm{s}}, \varphi_{\mathrm{e}}, \phi_{\mathrm{s}}, T) \in \mathcal{C}([0,a), K_Z)$, we say that $(\tilde{c}_{\mathrm{e}}, \tilde{c}_{\mathrm{s}}, \tilde{\varphi}_{\mathrm{e}}, \tilde{\phi}_{\mathrm{s}}, \tilde{T}) \in \mathcal{C}([0,b), K_Z)$ is an "extension" of $(c_{\mathrm{e}}, c_{\mathrm{s}}, \varphi_{\mathrm{e}}, \phi_{\mathrm{s}}, T)$ if it is also a solution (in the same sense), $b \geq a$ and

$$(\tilde{c}_{\mathrm{e}}, \tilde{c}_{\mathrm{s}}, \tilde{\varphi}_{\mathrm{e}}, \tilde{\phi}_{\mathrm{s}}, \tilde{T})|_{t \leq a} = (c_{\mathrm{e}}, c_{\mathrm{s}}, \varphi_{\mathrm{e}}, \phi_{\mathrm{s}}, T).$$

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.

Further comments on weak-mild solutions III

Notice that the contribution of c_s can be studied, basically, as a 1D behaviour on J_δ.

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

where

$$W(x,t) = (G_{c_\mathrm{s},t_0}(g))(R_\mathrm{s}(x),x,t).$$

In this sense we can rewrite (32) in terms of the restriction $c_{\mathrm{s,B}}$, instead of c_s, as follows:

Proposition 1

In Definitions 2 and 3, condition (32) *is equivalent to the following property:* $(c_\mathrm{e}, c_{\mathrm{s,B}}, T) \in \mathcal{C}([0,t_{\mathrm{end}}); X)$ *such that*

$$\begin{aligned} (c_\mathrm{e}, c_{s,B}, T) = {} & \left(G_{c_\mathrm{e},t_0}\left(\alpha_\mathrm{e} N_{j^{\mathrm{Li}},t_0}\right), G_{c_{\mathrm{s,B}},t_0}\left(\alpha_\mathrm{s} N_{j^{\mathrm{Li}},t_0}\right), G_{T,t_0}\right) \\ & \circ \left(c_\mathrm{e}|_{t<t_0}, c_{\mathrm{s,B}}|_{t<t_0}, \varphi_\mathrm{e}|_{t<t_0}, \phi_\mathrm{s}|_{t<t_0}, T|_{t<t_0}\right). \end{aligned} \tag{33}$$

Outline

Idea of the proof I

The idea of the proof of Theorem 1 is the following:

1. we will show (see Proposition 2) that we can solve (3) and (4) to obtain $(\varphi_{\mathrm{e}}, \phi_{\mathrm{s}})$ if $c_{\mathrm{s}}, c_{\mathrm{e}}, T$ are given, extending to the nonlinear case the study for the linearized equation proved in [Ramos 2016]
2. we will apply a fixed point argument to the evolution problems (1), (2) and (5) to obtain the conclusion.

The problem for φ_e and ϕ_s I

It was first shown in [Ramos 2016] that the uniqueness of solutions (φ_e, ϕ_s) of system (3)–(4) holds up to a constant relating the difference between φ_e and ϕ_s. To avoid this we set the following assumption:

Assumptions 5

We define

$$\varphi_{e,Li} = \varphi_e - \alpha_{\varphi_e} T f_{\varphi_e}(c_e), \tag{34}$$

and assume that

$$\int_0^L \varphi_{e,Li} \, dx = 0. \tag{35}$$

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

The problem for φ_{e} and ϕ_{s} II

Remark 3

We recall that $H^1(a,b) \subset \mathcal{C}([a,b])$. Thus, since $0 < c_{\mathrm{e}} \in H^1(a,b)$ then, $\min_{[0,L]} c_{\mathrm{e}} > 0$, so $f_{\varphi_{\mathrm{e}}}(c_{\mathrm{e}}) \in H^1(0,L)$.

Remark 4

Another alternative to get the uniqueness of solution is to use the condition $\phi_{\mathrm{s}}|_{x=0} = 0$, instead of (35), setting the value 0 of the potential in one of the walls.

The problem for φ_{e} and ϕ_{s} III

Proposition 2

Let $(c_{\mathrm{e}}, c_{\mathrm{s,B}}, T) \in K_X$, $I \in \mathbb{R}$ *and let Assumptions 2, 3 hold. Then there exists* $\varphi_{\mathrm{e}} \in H^1(0,L)$ *and* $\phi_s \in H^1(J_\delta)$ *satisfying the elliptic equations* (3) *and* (4) *in the weak sense* (30) *and* (31)*. Furthermore, given two solutions* $(\varphi_{\mathrm{e}}, \phi_{\mathrm{s}}), (\hat{\varphi}_{\mathrm{e}}, \hat{\phi}_{\mathrm{s}})$ *there exists a constant* $C \in \mathbb{R}$ *such that*

$$\varphi_{\mathrm{e}} - \widehat{\varphi_{\mathrm{e}}} = \phi_{\mathrm{s}} - \widehat{\phi}_{\mathrm{s}} = C.$$

Hence we have uniqueness up to a constant. In particular, there exists a unique solution $(\varphi_{\mathrm{e}}, \phi_{\mathrm{s}})$ *satisfying Assumption 5.*

▸ Proof

The problem for φ_{e} and ϕ_{s} IV

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

$$\begin{aligned} G_\phi : \quad K_X \times \mathbb{R} &\rightarrow H^1(0,L) \times H^1(J_\delta) \\ (c_{\mathrm{e}}, c_{\mathrm{s,B}}, T, I) &\mapsto (\varphi_{\mathrm{e}}, \phi_{\mathrm{s}}), \end{aligned} \tag{36}$$

$$\begin{aligned} \widetilde{G}_\phi : \quad K_X \times \mathbb{R} &\rightarrow K_Z \\ (c_{\mathrm{e}}, c_{\mathrm{s,B}}, T, I) &\mapsto (c_{\mathrm{e}}, c_{\mathrm{s,B}}, G_\phi(c_{\mathrm{e}}, c_{\mathrm{s,B}}, T, I), T), \end{aligned} \tag{37}$$

where $(\varphi_{\mathrm{e}}, \phi_{\mathrm{s}}) \in H^1(0,L) \times H^1(J_\delta)$ is the (unique) solution of (30)–(31) satisfying (35). Assuming now that I is a continuous function, i.e. $I \in \mathcal{C}([0, t_{\mathrm{end}}^I])$, we define the Green operator, for $t_0 < t_{\mathrm{end}}^I$:

$$\begin{aligned} \widetilde{G}_{\phi,t_0} : \mathcal{C}([0,t_0]; K_X) &\rightarrow \mathcal{C}([0,t_0]; K_Z) \\ (c_{\mathrm{e}}, c_{\mathrm{s,B}}, T) &\mapsto W, \end{aligned}$$

where

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

The problem for φ_{e} and ϕ_{s} V

Proposition 3

Let Assumptions 2, 3 hold. Then, the operator $\widetilde{G}_\phi : K_X \times \mathbb{R} \to K_Z$ is C^1 (in the sense of the Fréchet derivative).

▸ Proof

Remark 5

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).

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

$$(c_{\mathrm{e}}, c_{\mathrm{s,B}}, T) = \left(G_{c_{\mathrm{e}},t_0}\left(\alpha_{\mathrm{a}} N_{j^{\mathrm{Li}},t_0}\right), G_{c_{\mathrm{s,B}},t_0}\left(\alpha_{\mathrm{s}} N_{j^{\mathrm{Li}},t_0}\right), G_{T,t_0}\right) \circ \widetilde{G}_{\phi,t_0}(c_{\mathrm{e}}, c_{\mathrm{s,B}}, T).$$

Outline

Assumptions and remarks regarding Theorem 2 I

In Theorem 1 one of the reasons of a finite existence time could be that $c_{\mathrm{s,B}} \to 0, c_{\mathrm{s,max}}$ or $c_{\mathrm{e}} \to 0$. This conditions do not, a priori, pose a relevant physical problem since the battery may very well be completely full or empty.

Assumptions 6

There exists a constant κ_1 such that $\kappa(c_{\mathrm{e}}, T) \leq \kappa_1$ and $f_{\varphi_{\mathrm{e}}}(\cdot) = \ln(\cdot)$.

Assumptions 7

$c_{\mathrm{s,max}} < 1$ in the units considered to solve the problem.

This is purely technical, but it seems reasonable since, in empirical cases in the literature, typically $c_{\mathrm{s,max}} \sim 10^{-2}$ mol cm^{-3}. In particular, in [Smith and Wang 2006] the authors take $c_{\mathrm{s,max}} = 1.6 \times 10^{-2}$ mol cm^{-3}.

Assumptions and remarks regarding Theorem 2 II

Assumptions 8

$$\bar{j}^{\mathrm{Li}}(x, c_{\mathrm{e}}, c_{\mathrm{s}}, T, \eta) = c_{\mathrm{e}}^{\alpha_{\mathrm{a}}} c_{\mathrm{s}}^{\alpha_{\mathrm{s}}} (c_{\mathrm{s,max}} - c_{\mathrm{s}})^{\beta_{\mathrm{a}}} h\left(x, \frac{\eta}{T}\right),$$
$$h(x,s) = h_+(x,s) - h_-(x,s),$$
$$h_+(x,s) = \delta_1(x)\exp(\gamma_1 s),$$
$$h_-(x,s) = \delta_2(x)\exp(-\gamma_2 s),$$
$$\eta(x, c_{\mathrm{e}}, c_{\mathrm{s}}, \varphi_{\mathrm{e}}, \phi_{\mathrm{s}}, T) = \phi_{\mathrm{s}} - \varphi_{\mathrm{e}} - U(x, c_{\mathrm{e}}, c_{\mathrm{s}}, T).$$

where $\alpha_{\mathrm{a}}, \alpha_{\mathrm{s}}, \beta_{\mathrm{a}} \in (0,1)$, $\gamma_1, \gamma_2 > 0$ and $\delta_1(x), \delta_2(x) > 0$ are constant in each electrode. Furthermore, we consider U slightly more general than (15):

$$U(x, c_{\mathrm{e}}, c_{\mathrm{s}}, T) = -\lambda_{\min}(x,T)\ln c_{\mathrm{s}} + \lambda_{\max}(x,T)\ln(c_{\mathrm{s,max}} - c_{\mathrm{s}}) + \mu(x,T)\ln c_{\mathrm{e}} + p(c_{\mathrm{e}}, c_{\mathrm{s}}, T), \tag{38}$$

where $\lambda_{\min}, \lambda_{\max}, \mu$ are given smooth nonnegative scalar functions and p is a continuous bounded function.

Assumptions and remarks regarding Theorem 2 I

Figure: Possible representation of U

Assumptions and remarks regarding Theorem 2 II

Remark 6

Under these assumptions we have

$$\begin{aligned} \bar{j}^{\mathrm{Li}}_{+} &= \delta_1(x) c_{\mathrm{e}}^{\alpha_{\mathrm{a}} - \gamma_1 \left(\alpha \varphi_{\mathrm{e}} + \frac{\mu(x,T)}{T} \right)} c_{\mathrm{s}}^{\alpha_{\mathrm{s}} + \gamma_1 \frac{\lambda_{\min}(x,T)}{T}} (c_{\mathrm{s},\max} - c_{\mathrm{s}})^{\beta_{\mathrm{a}} - \gamma_1 \frac{\lambda_{\max}(x,T)}{T}} \\ &\quad \times \exp\left(\frac{\gamma_1}{T} (\phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}}) \right) \exp\left(\frac{-\gamma_1}{T} p(c_{\mathrm{e}}, c_{\mathrm{s}}, T) \right), \end{aligned} \tag{39}$$

$$\begin{aligned} \bar{j}^{\mathrm{Li}}_{-} &= \delta_1(x) c_{\mathrm{e}}^{\alpha_{\mathrm{a}} + \gamma_2 \left(\alpha \varphi_{\mathrm{e}} + \frac{\mu(x,T)}{T} \right)} c_{\mathrm{s}}^{\alpha_{\mathrm{s}} - \gamma_2 \frac{\lambda_{\min}(x,T)}{T}} (c_{\mathrm{s},\max} - c_{\mathrm{s}})^{\beta_{\mathrm{a}} + \gamma_2 \frac{\lambda_{\max}(x,T)}{T}} \\ &\quad \times \exp\left(\frac{-\gamma_2}{T} (\phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}}) \right) \exp\left(\frac{\gamma_2}{T} p(c_{\mathrm{e}}, c_{\mathrm{s}}, T) \right), \end{aligned} \tag{40}$$

Assumptions and remarks regarding Theorem 2 III

Assumptions 9

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

$$\alpha_{\mathrm{a}} - \gamma_1 \left(\alpha_{\varphi_{\mathrm{e}}} + \frac{\mu(x,T)}{T} \right) \leq 1 \tag{41}$$

$$\alpha_{\mathrm{a}} + \gamma_2 \left(\alpha_{\varphi_{\mathrm{e}}} + \frac{\mu(x,T)}{T} \right) \geq 1 \tag{42}$$

$$\alpha_{\mathrm{s}} + \gamma_1 \frac{\lambda_{\min}(x,T)}{T} \geq 1, \tag{43}$$

$$\beta_{\mathrm{a}} + \gamma_2 \frac{\lambda_{\max}(x,T)}{T} \geq 1. \tag{44}$$

Outline

3. Main results
   - Regularity assumptions of the nonlinear terms and initial data
   - Definition of weak-mild solution
   - Assumptions and results regarding Theorem 1
   - Assumptions and remarks regarding Theorem 2
   - Assumptions and remarks regarding Theorems 3 and 4

Truncated potential behaviour I

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.

Truncated potential behaviour II

Assumptions 10

Let $\bar{j}^{\mathrm{Li}}(x, c_\mathrm{e}, c_\mathrm{s}, T, \eta(x, c_\mathrm{e}, c_\mathrm{s}, \varphi_\mathrm{e}, \phi_\mathrm{s}, T)) = \bar{j}_+^{\mathrm{Li}} - \bar{j}_-^{\mathrm{Li}}$ where

$$\begin{aligned}\bar{j}_+^{\mathrm{Li}} &= c_\mathrm{e}^{\alpha_\mathrm{a} - \gamma_1 \left(\alpha_{\varphi_\mathrm{e}} + \frac{\mu(x,T)}{T} \right)} c_\mathrm{s}^{\alpha_\mathrm{s} + \gamma_1 \frac{\lambda_{\min}(x,T)}{T}} (c_{\mathrm{s},\max} - c_\mathrm{s})^{\beta_\mathrm{a} - \gamma_1 \frac{\lambda_{\max}(x,T)}{T}} \\ &\quad \times H\left(\frac{\gamma_1}{T} (\phi_\mathrm{s} - \varphi_{\mathrm{e,Li}}) \right) \exp\left(\frac{-\gamma_1}{T} p(c_\mathrm{e}, c_\mathrm{s}, T) \right), \end{aligned} \tag{45}$$

$$\begin{aligned}\bar{j}_-^{\mathrm{Li}} &= c_\mathrm{e}^{\alpha_\mathrm{a} + \gamma_2 \left(\alpha_{\varphi_\mathrm{e}} + \frac{\mu(x,T)}{T} \right)} c_\mathrm{s}^{\alpha_\mathrm{s} - \gamma_2 \frac{\lambda_{\min}(x,T)}{T}} (c_{\mathrm{s},\max} - c_\mathrm{s})^{\beta_\mathrm{a} + \gamma_2 \frac{\lambda_{\max}(x,T)}{T}} \\ &\quad \times H\left(\frac{-\gamma_2}{T} (\phi_\mathrm{s} - \varphi_{\mathrm{e,Li}}) \right) \exp\left(\frac{\gamma_2}{T} p(c_\mathrm{e}, c_\mathrm{s}, T) \right), \end{aligned} \tag{46}$$

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

$$H(s) = \begin{cases} \exp(s), & s \le s_\infty, \\ \zeta(s), & s > s_\infty, \end{cases} \tag{47}$$

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

Truncated temperature behaviour I

Due to the 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 [Chaturvedi et al. 2010; Farrell and Please 2005; Ranom 2014]), 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.

Assumptions 11

Assume that F_T is linear in T

$$F_T = B_T(c_\mathrm{e}, c_\mathrm{s}, \varphi_\mathrm{e}, \phi_\mathrm{s}) + T A_T(c_\mathrm{e}, c_\mathrm{s}, \varphi_\mathrm{e}, \phi_\mathrm{s}), \tag{48}$$

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

Outline

Outline

4. Proof of Theorem 1
   - Green operator G_Φ
   - Regularity of the Green operators $G_{c_{\mathrm{e}},t}$ and $G_{c_{\mathrm{s,B}},t}$
   - Proof of Theorem 1

Outline

4. Proof of Theorem 1
   - Green operator G_Φ
   - Regularity of the Green operators $G_{c_{\mathrm{e}},t}$ and $G_{c_{\mathrm{s,B}},t}$
   - Proof of Theorem 1

Green operator for the semilinear elliptic system I

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

$$\eta_0(x) = -\alpha_{\varphi_{\mathrm{e}}} T f_{\varphi_{\mathrm{e}}}(c_e(x)) - U(x, c_{\mathrm{e}}(x), c_{\mathrm{s,B}}(x), T), \qquad \forall x \in J_\delta,$$

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

$$\underline{j}^{\mathrm{Li}}(x, \Phi) = \begin{cases} \overline{j}^{\mathrm{Li}}(x, c_{\mathrm{e}}(x), c_{\mathrm{s,B}}(x), T, \Phi + \eta_0(x)) & x \in J_\delta, \\ 0 & x \in (L_1, L_1 + \delta). \end{cases} \tag{49}$$

Notice that

$$\underline{j}^{\mathrm{Li}}(x, \phi_{\mathrm{s}}(x) - \varphi_{\mathrm{e,Li}}(x)) = j^{\mathrm{Li}}(x, c_{\mathrm{e}}(x), c_{\mathrm{s,B}}(x), \varphi_{\mathrm{e}}(x), \phi_{\mathrm{s}}(x), T). \tag{50}$$

We also define

$$j_0^{\mathrm{Li}}(x) = \underline{j}^{\mathrm{Li}}(x, 0) \tag{51}$$

Green operator for the semilinear elliptic system II

which corresponds to $j^{\mathrm{Li}}|_{\phi_{\mathrm{s}}-\varphi_{\mathrm{e,Li}}=0}$.

Remark 7

Given $(c_{\mathrm{e}}, c_{\mathrm{s,B}}, T) \in K_X$, due to (22) and (23) we have $j_0^{\mathrm{Li}} \in L^\infty(0,L) \cap \mathcal{C}(\overline{J_\delta})$.

Proof of Proposition 2 I

We rewrite (30)–(31) in terms of $\varphi_{\mathrm{e,Li}}$, defining $\tilde\kappa(x) = \kappa(c_{\mathrm{e}}(x), T) \in \mathcal{C}([0, L])$, as

$$
\begin{aligned}
&\int_0^L \tilde\kappa \frac{\partial \varphi_{\mathrm{e,Li}}}{\partial x} \frac{\mathrm{d}\psi_{\mathrm{e}}}{\mathrm{d}x} - \int_{J_\delta} j^{\mathrm{Li}} \psi_{\mathrm{e}} \,\mathrm{d}x = 0,\\
&\int_{J_\delta} \sigma \frac{\partial \phi_{\mathrm{s}}}{\partial x} \frac{\mathrm{d}\psi_{\mathrm{s}}}{\mathrm{d}x} \,\mathrm{d}x + \int_{J_\delta} j^{\mathrm{Li}} \psi_{\mathrm{s}} \,\mathrm{d}x = -\frac{I}{A}(\psi_{\mathrm{s}}(L) - \psi_{\mathrm{s}}(0)), \qquad \forall (\psi_{\mathrm{e}}, \psi_{\mathrm{s}}) \in X_\phi.
\end{aligned}
$$

Adding both equations we obtain that (30)–(31) is equivalent to

$$
\int_0^L \tilde\kappa \frac{\partial \varphi_{\mathrm{e,Li}}}{\partial x} \frac{\mathrm{d}\psi_{\mathrm{e}}}{\mathrm{d}x} \,\mathrm{d}x + \int_{J_\delta} \sigma \frac{\partial \phi_{\mathrm{s}}}{\partial x} \frac{\mathrm{d}\psi_{\mathrm{s}}}{\mathrm{d}x} \,\mathrm{d}x + \int_{J_\delta} j^{\mathrm{Li}} (\psi_{\mathrm{s}} - \psi_{\mathrm{e}}) \,\mathrm{d}x = -\frac{I}{A}(\psi_{\mathrm{s}}(L) - \psi_{\mathrm{s}}(0)) \tag{52}
$$

$\forall (\psi_{\mathrm{e}}, \psi_{\mathrm{s}}) \in X_\phi$. Let us define, for $x \in [0, L]$ and $\Phi \in \mathbb{R}$,

$$
\widehat{j^{\mathrm{Li}}}(x, \Phi) = \underline{j}^{\mathrm{Li}}(x, \Phi) - j_0^{\mathrm{Li}}(x). \tag{53}
$$

Notice that $\widehat{j^{\mathrm{Li}}}(x, 0) = 0$.

Proof of Proposition 2 II

We can rewrite (52) as

$$\int_0^L \tilde\kappa \frac{\partial \varphi_{\mathrm{e,Li}}}{\partial x}\frac{\mathrm{d}\psi_{\mathrm{e}}}{\mathrm{d}x}\,\mathrm{d}x + \int_{J_\delta} \sigma \frac{\partial \phi_{\mathrm{s}}}{\partial x}\frac{\mathrm{d}\psi_{\mathrm{s}}}{\mathrm{d}x}\,\mathrm{d}x + \int_{J_\delta} \widehat{j^{\mathrm{Li}}}(x, \phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}})(\psi_{\mathrm{s}} - \psi_{\mathrm{e}})\,\mathrm{d}x$$
$$= -\frac{I}{A}(\psi_{\mathrm{s}}(L) - \psi_{\mathrm{s}}(0)) - \int_{J_\delta} j_0^{\mathrm{Li}}(x)(\psi_{\mathrm{s}} - \psi_{\mathrm{e}})\,\mathrm{d}x.$$

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

$$\langle A_1(\varphi_{\mathrm{e,Li}}, \phi_{\mathrm{s}}), (\psi_{\mathrm{e}}, \psi_{\mathrm{s}})\rangle = \int_{J_\delta} \widehat{j^{\mathrm{Li}}}(x, \phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}})(\psi_{\mathrm{s}} - \psi_{\mathrm{e}})\,\mathrm{d}x,$$

for all $(\varphi_{\mathrm{e,Li}}, \phi_{\mathrm{s}}), (\psi_{\mathrm{e}}, \psi_{\mathrm{s}}) \in X_\phi$. Since $H^1(J_\delta) \subset \mathcal{C}(\overline{J_\delta})$ and $(\varphi_{\mathrm{e,Li}}, \phi_{\mathrm{s}}) \in X_\phi \to \widehat{j^{\mathrm{Li}}}(x, \phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}}) \in \mathcal{C}(\overline{J_\delta})$ is bounded and continuous (due to (22) and (23)) we have that $A_1 : X_\phi \to X_\phi^*$ is bounded continuous.

Proof of Proposition 2 III

Furthermore, applying (50), (53) and Remark 1 (due to Assumption 3), we can show that A_1 is a monotone operator since, for all $(\varphi_{\mathrm{e,Li}}, \phi_{\mathrm{s}}), (\widetilde{\varphi_{\mathrm{e,Li}}}, \widetilde{\phi_{\mathrm{s}}}) \in X_\phi$ we have that

$$
\begin{aligned}
&\langle A_1(\varphi_{\mathrm{e,Li}}, \phi_{\mathrm{s}}) - A_1(\widetilde{\varphi_{\mathrm{e,Li}}}, \tilde{\phi}_{\mathrm{s}}), (\varphi_{\mathrm{e,Li}}, \phi_{\mathrm{s}}) - (\widetilde{\varphi_{\mathrm{e,Li}}}, \tilde{\phi}_{\mathrm{s}}) \rangle \\
&\quad = \int_{J_\delta} \left(\widehat{j^{\mathrm{Li}}}(x, \phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}}) - \widehat{j^{\mathrm{Li}}}(x, \widetilde{\phi_{\mathrm{s}}} - \widetilde{\varphi_{\mathrm{e,Li}}}) \right) \left(\phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}} - (\widetilde{\phi_{\mathrm{s}}} - \widetilde{\varphi_{\mathrm{e,Li}}}) \right) \mathrm{d}x \\
&\quad = \int_{J_\delta} \left(\underline{j}^{\mathrm{Li}}(x, \phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}}) - \underline{j}^{\mathrm{Li}}(x, \widetilde{\phi_{\mathrm{s}}} - \widetilde{\varphi_{\mathrm{e,Li}}}) \right) \left(\phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}} - (\widetilde{\phi_{\mathrm{s}}} - \widetilde{\varphi_{\mathrm{e,Li}}}) \right) \mathrm{d}x \\
&\quad = \int_{J_\delta} \left(\bar{j}^{\mathrm{Li}}(x, c_{\mathrm{e}}, c_{\mathrm{s,B}}, \phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}} + \eta_0) - \bar{j}^{\mathrm{Li}}(x, c_{\mathrm{e}}, c_{\mathrm{s,B}}, T, \widetilde{\phi_{\mathrm{s}}} - \widetilde{\varphi_{\mathrm{e,Li}}} + \eta_0) \right) \\
&\qquad\qquad \times \left(\phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}} - (\widetilde{\phi_{\mathrm{s}}} - \widetilde{\varphi_{\mathrm{e,Li}}}) \right) \mathrm{d}x \\
&\quad = \int_{J_\delta} F^{\mathrm{Li}}(x, c_{\mathrm{e}}(x), c_{\mathrm{s}}(x), T, \eta(x), \widetilde{\eta}(x)) \left(\phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}} - (\widetilde{\phi_{\mathrm{s}}} - \widetilde{\varphi_{\mathrm{e,Li}}}) \right)^2 \mathrm{d}x
\end{aligned}
$$

Proof of Proposition 2 IV

for all $(\varphi_{\mathrm{e,Li}}, \phi_{\mathrm{s}}), (\psi_{\mathrm{e}}, \psi_{\mathrm{s}}) \in X_\phi$, due to (25) (which is true due to Assumption 3), where

$$\eta(x) = \phi_{\mathrm{s}}(x) - \varphi_{\mathrm{e,Li}}(x) - \alpha_{\varphi_{\mathrm{e}}} T f_{\varphi_{\mathrm{e}}}(c_{\mathrm{e}}) - U(x, c_{\mathrm{e}}, c_{\mathrm{s}}, T),$$
$$\widetilde{\eta}(x) = \widetilde{\phi}_{\mathrm{s}}(x) - \widetilde{\varphi_{\mathrm{e,Li}}}(x) - \alpha_{\varphi_{\mathrm{e}}} T f_{\varphi_{\mathrm{e}}}(c_{\mathrm{e}}) - U(x, c_{\mathrm{e}}, c_{\mathrm{s}}, T).$$

Therefore, for all $(\psi_{\mathrm{e}}, \psi_{\mathrm{s}}) \in X_\phi$,

$$\langle A_1(\phi_{\mathrm{s}}, \varphi_{\mathrm{e,Li}}) - A_1(\widetilde{\phi}_{\mathrm{s}}, \widetilde{\varphi_{\mathrm{e,Li}}}), (\phi_{\mathrm{s}}, \varphi_{\mathrm{e,Li}}) - (\widetilde{\phi}_{\mathrm{s}}, \widetilde{\varphi_{\mathrm{e,Li}}}) \rangle \geq C \int_{J_\delta} \left(\phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}} - (\widetilde{\phi}_{\mathrm{s}} - \widetilde{\varphi_{\mathrm{e,Li}}}) \right)^2 \tag{54}$$

where

$$C = C\left(c_{\mathrm{e}}, c_{\mathrm{s}}, T, \phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}}, (\widetilde{\phi}_{\mathrm{s}} - \widetilde{\varphi_{\mathrm{e,Li}}})\right) = \min_{x \in J_\delta} \int_{J_\delta} F^{\mathrm{Li}}(x, c_{\mathrm{e}}(x), c_{\mathrm{s}}(x), T, \eta(x), \widetilde{\eta}(x)) > 0.$$

Proof of Proposition 2 V

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

$$\langle \mathcal{A}(\phi_{\rm s}, \varphi_{\rm e,Li}), (\psi_{\rm s}, \psi_{\rm e}) \rangle = \int_0^L \tilde\kappa \frac{\partial \varphi_{\rm e,Li}}{\partial x} \frac{{\rm d}\psi_{\rm e}}{{\rm d}x} \,{\rm d}x + \int_{J_\delta} \sigma \frac{\partial \phi_{\rm s}}{\partial x} \frac{{\rm d}\psi_{\rm s}}{{\rm d}x} \,{\rm d}x + \langle A_1(\phi_{\rm s}, \varphi_{\rm e,Li}), (\psi_{\rm s}, \psi_{\rm e}) \rangle. \tag{55}$$

Then $\mathcal{A}$ is a bounded, continuous, monotone operator. Moreover, it is coercive due to the Poincaré-Wirtinger inequality $\|\varphi_{\rm e,Li}\|_{L^2(0,L)} \le C \|\nabla \varphi_{\rm e,Li}\|_{L^2(0,L)}$ and (54). Hence, there exists a unique solution of the system (3)-(4), due to the Minty-Browder theorem. □

Remark 8

Of course if $(\varphi_{\rm e}, \phi_{\rm s})$ is a solution of the system (3)-(4) and C is a constant then $(\varphi_{\rm e} + C, \phi_{\rm s} + C)$ is also a solution. However, there exists only one solution in X_ϕ.

Proof of Proposition 2 VI

Remark 9

The main part of the proof above was to apply the monotonicity of j^{Li} with respect to $\phi_{\mathrm{s}} - \varphi_{\mathrm{e,Li}}$. 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 (36) is well-defined. We prove now, applying the Implicit Function Theorem, that this map is $\mathcal{C}^1$.

Proof of Proposition 3 I

We will apply the implicit function theorem for the Banach space-valued mapping $F : \widehat{X} \times \widehat{Y} \to \widehat{Z}$, to solve for an operator $\widehat{G}_\phi : U \subset \widehat{X} \to \widehat{Y}$ in an expression of the form

$$F(\widehat{x}, \widehat{G}_\phi(\widehat{x})) = 0, \qquad \text{for all } \widehat{x} \in U. \tag{56}$$

The choice of functional spaces will be

$$\widehat{X} = \mathcal{C}_{>k_0}([0, L]) \times \mathbb{R} \times K_X, \qquad \widehat{Y} = X_\phi, \qquad \widehat{Z} = X_\phi^*, \tag{57}$$

with

$$\mathcal{C}_{>\kappa_0}([0, L]) = \{\tilde{\kappa} \in \mathcal{C}([0, L]) : \tilde{\kappa} > \kappa_0\}, \quad \text{for some } \kappa_0 > 0. \tag{58}$$

We will then check that

$$G_\phi(c_{\mathrm{e}}, c_{\mathrm{s,B}}, T, I) = \widehat{G}_\phi(\kappa(c_{\mathrm{e}}, T), I, c_{\mathrm{e}}, c_{\mathrm{s,B}}, T) + (\alpha_{\varphi_{\mathrm{e}}} T f_{\varphi_{\mathrm{e}}}(c_{\mathrm{e}}), 0), \tag{59}$$

Proof of Proposition 3 II

due to the definition of $\varphi_{\mathrm{e,Li}}$ (see (34)). Notice that $\widehat{X}$ is an open set of a Banach space, and therefore we can consider the Implicit Function Theorem (see, e.g., [Lang 2012]) in this setting. We will use the notation

$$\widehat{x} = (\tilde{\kappa}, I, c_{\mathrm{e}}, c_{\mathrm{s,B}}, T) \in \widehat{X}, \qquad \widehat{y} = (\varphi_{\mathrm{e,Li}}, \phi_{\mathrm{s}}) = (u, v) \in \widehat{Y}.$$

Proof of Proposition 3 III

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

$$A_1(\widehat{x}, \widehat{y})(\psi_{\mathrm{e}}, \psi_{\mathrm{s}}) = A_1(\widehat{x}, u)(\psi_{\mathrm{e}}) = \int_0^L \tilde{\kappa}(x) u'(x) \psi_{\mathrm{e}}'(x) \,\mathrm{d}x$$

$$A_2(\widehat{x}, \widehat{y})(\psi_{\mathrm{e}}, \psi_{\mathrm{s}}) = A_2(v)(\psi_{\mathrm{s}}) = \int_{J_\delta} \sigma(x) v'(x) \psi_{\mathrm{s}}'(x) \,\mathrm{d}x$$

$$\overline{\eta}_0(x, \widehat{x}(x)) = -\alpha_{\varphi_{\mathrm{e}}} T f_{\varphi_{\mathrm{e}}}(c_e(x)) - U(x, c_{\mathrm{e}}(x), c_{\mathrm{s,B}}(x), T)$$

$$A_3(\widehat{x}, \widehat{y})(\psi_{\mathrm{e}}, \psi_{\mathrm{s}}) = \int_{J_\delta} \overline{j}^{\mathrm{Li}}(x, \widehat{x}(x), v(x) - u(x) + \overline{\eta}_0(x, \widehat{x}(x))) \cdot (\psi_{\mathrm{s}}(x) - \psi_{\mathrm{e}}(x)) \,\mathrm{d}x$$

$$A_4(\widehat{x}, \widehat{y})(\psi_{\mathrm{e}}, \psi_{\mathrm{s}}) = A_4(I)(\psi_{\mathrm{s}}) = \frac{I}{A}(\psi_{\mathrm{s}}(L) - \psi_{\mathrm{s}}(0))$$

$$F = A_1 + \cdots + A_4.$$

Our definition of weak solution is precisely

$$F(\widehat{x}, \widehat{y}) = 0_{\widehat{Z}}. \tag{60}$$

Proof of Proposition 3 IV

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

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

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

$$D_u A_1(\tilde{\kappa}, u)(\bar{u}) = A_1(\tilde{\kappa}, \bar{u})$$
$$D_v A_2(u)(\bar{v}) = A_2(\bar{v})$$

Since $\frac{\partial \bar{j}^{\mathrm{Li}}}{\partial \eta}$ is of class C^1 (see (22) in Assumption 3), then A_3 is also of class C^1 and

$$D_{(u,v)} A_3(\widehat{x}, u, v)(\bar{u}, \bar{v})(\psi_{\mathrm{e}}, \psi_{\mathrm{s}}) = \int_{J_\delta} g(\bar{v} - \bar{u})(\psi_{\mathrm{s}} - \psi_{\mathrm{e}}) \, \mathrm{d}x.$$

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

$$g(x) = \frac{\partial \bar{j}^{\mathrm{Li}}}{\partial \eta}(x, \widehat{x}(x), v(x) - u(x) + \overline{\eta}_0(x, \widehat{x}(x))).$$

Proof of Proposition 3 V

Let $\widehat{x}^0 = (\tilde\kappa, c_{\mathrm{e}}, c_{\mathrm{s,B}}, T) \in \widehat{X}$, and let $\widehat{y}^0 = (u^0, v^0) = (\varphi_{\mathrm{e,Li}}, \phi_{\mathrm{s}}) \in X_\phi$ be the solution found in Proposition 2. Then $g(x) > 0$ is in $\mathcal{C}(\overline{J_\delta})$. Therefore, there exists a constant g_0 such that $g(x) \ge g_0 > 0$ in J_δ. Then

$$D_{(u,v)} F(\widehat{x}^0, \widehat{y}^0) : (\bar u, \bar v) \in X_\phi \to X_\phi^*$$

understood as a bilinear form

$$G((\bar u, \bar v), (\psi_{\mathrm{e}}, \psi_{\mathrm{s}})) = \int_0^L \tilde\kappa \bar u' \psi_{\mathrm{e}}' + \int_{J_\delta} \sigma \bar v' \psi_{\mathrm{s}}' + \int_{J_\delta} g(x)(\bar u - \bar v)(\psi_{\mathrm{s}} - \psi_{\mathrm{e}}),$$

is continuous and coercive in $X_\phi \times X_\phi$. Therefore, by Lax-Milgram's theorem $D_{(u,v)} F(\widehat{x}^0, \widehat{y}^0)$ is bijective. Then, by the Implicit Function Theorem applied to F, there exists a unique C^1 function $\widehat{G}_\phi : U \to X_\phi$, defined in a neighbourhood U of $\widehat{x}^0$ in $\widehat{X}$, such that (56) holds.

Proof of Proposition 3 VI

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

$$(c_{\mathrm{e}}, c_{\mathrm{s,B}}, T, I) \in K_X \times \mathbb{R} \overset{J}{\longmapsto} (\kappa(c_{\mathrm{e}}, T), I, c_{\mathrm{e}}, c_{\mathrm{s,B}}, T) \in \widehat{X}$$

is C^1. Let us choose a point $(c_{\mathrm{e}}^0, c_{\mathrm{s,B}}^0, T^0, I^0) \in K_X \times \mathbb{R}$, and let $\widehat{x}_0 = (\kappa(c_{\mathrm{e}}^0, T^0), I^0, c_{\mathrm{e}}^0, c_{\mathrm{s,B}}^0, T^0) \in \widehat{X}$. Let $U \subset \widehat{X}$ be a suitable neighbourhood of $\widehat{x}_0$ so that $\widehat{G}_\phi : U \to X_\phi$ is defined satisfying (56). Taking the neighbourhood of $(c_{\mathrm{e}}^0, c_{\mathrm{s,B}}^0, T^0, I^0)$ given by $V = J^{-1}(U) \subset K_X \times \mathbb{R}$, the composition

$$(c_{\mathrm{e}}, c_{\mathrm{s,B}}, T, I) \in V \overset{J}{\longmapsto} (\kappa(c_{\mathrm{e}}, T), I, c_{\mathrm{e}}, c_{\mathrm{s,B}}, T) \in U \overset{\widehat{G}_\phi}{\longmapsto} (\varphi_{\mathrm{e,Li}}, \phi_{\mathrm{s}}) \in X_\phi$$

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

$$\begin{aligned} \tau : V \times X_\phi \quad &\longrightarrow \quad H^1(0,L) \times H^1(J_\delta) \\ (c_{\mathrm{e}}, c_{\mathrm{s,B}}, T, I, \varphi_{\mathrm{e,Li}}, \phi_{\mathrm{s}}) \quad &\longmapsto \quad (\varphi_{\mathrm{e}}, \phi_{\mathrm{s}}) = (\varphi_{\mathrm{e,Li}} + \alpha_{\varphi_{\mathrm{e}}} T f_{\varphi_{\mathrm{e}}}(c_{\mathrm{e}}), \phi_{\mathrm{s}}). \end{aligned}$$

Proof of Proposition 3 VII

Due to the uniqueness (up to a constant) result we proved in Proposition 2,

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

is the map $G_\phi|_V$ (as constructed in (36) through Proposition 2). Thus, G_ϕ is of class C^1 in a neighbourhood of $(c_{\mathrm{e}}^0, c_{\mathrm{s,B}}^0, T^0, I^0)$. Since this argument holds over any point $(c_{\mathrm{e}}^0, c_{\mathrm{s,B}}^0, T^0, I^0) \in K_X \times \mathbb{R}$, we have shown that G_ϕ is of class $\mathcal{C}^1$ over $K_X \times \mathbb{R}$. This implies that $\widetilde{G}_\phi$ is also $\mathcal{C}^1$ and it concludes the proof. $\square$

Lemma 4.1

Let $I \in \mathcal{C}([0, t_0])$ then $\widetilde{G}_{\phi,t} : \mathcal{C}([0, t_0], K_X) \to \mathcal{C}([0, t_0], K_Z)$ is locally Lipschitz continuous. If $I \in \mathcal{C}_{\mathrm{part}}([0, t_0])$ then $\widetilde{G}_{\phi,t} : \mathcal{C}([0, t_0], K_X) \to \mathcal{C}_{\mathrm{part}}([0, t_0], K_Z)$ is locally Lipschitz continuous.

Outline

4. Proof of Theorem 1
   - Green operator G_Φ
   - Regularity of the Green operators $G_{c_\mathrm{e},t}$ and $G_{c_{\mathrm{s,B}},t}$
   - Proof of Theorem 1

Green operators $G_{c_\mathrm{e},t}$ and $G_{c_{\mathrm{s,B}},t}$ I

The regularity of $G_{c_\mathrm{e},t}$ is a well-known property:

$$G_{c_\mathrm{e},t_0} : L^2((0,t_0)\times(0,L)) \to \mathcal{C}([0,t_0];H^1(0,L)).$$

This operator has a nice representation formula

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

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

$$\begin{cases} \dfrac{\partial u}{\partial t} - \dfrac{\partial}{\partial x}\left(D_\mathrm{e} \dfrac{\partial c_\mathrm{e}}{\partial x}\right) = 0, & (0,L)\times\mathbb{R}, \\ \dfrac{\partial u}{\partial x} = 0, & \{0,L\}\times\mathbb{R}, \\ u(0) = u_0, & t = 0. \end{cases}$$

Green operators $G_{c_e,t}$ and $G_{c_{s,B},t}$ II

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

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

where ρ is and increasing, continuous function such that $\rho(0) = 0$.
The term $G_{c_{s,B},t}$ is a little trickier. First we recall (see [Arendt, Batty, and Neubrander 2013; Nittka 2014]) that, for any $q > 2$:

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

and

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

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

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

Green operators $G_{c_{\mathrm{e}},t}$ and $G_{c_{\mathrm{s,B}},t}$ III

This solves the problem of continuity of $G_{c_{\mathrm{s}}} g$ 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

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

is Lipschitz continuous. Furthermore it is easy to check that

$$G_{c_{\mathrm{s,B}},t_0} : \mathcal{C}(\overline{J_\delta} \times [0,t_0]) \to \mathcal{C}(\overline{J_\delta} \times [0,t_0]).$$

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

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

By defining the vectorial Green operator for the evolutionary part

$$\mathbf{G}_t = (G_{c_{\mathrm{e}},t} G_{c_{\mathrm{s}},t}, G_{T,t}) : \mathcal{C}([0,t];Y) \to \mathcal{C}([0,t];X),$$

Green operators $G_{c_{\mathrm{e}},t}$ and $G_{c_{\mathrm{s,B}},t}$ IV

due to the previous results, we have

$$\|\mathbf{G}_t\mathbf{y} - \mathbf{G}_t\hat{\mathbf{y}}\|_{\mathcal{C}([0,t];X)} \le \rho(t)\|\mathbf{y} - \hat{\mathbf{y}}\|_{\mathcal{C}([0,t];Y)}, \tag{61}$$

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

Outline

4. Proof of Theorem 1
   - Green operator G_Φ
   - Regularity of the Green operators $G_{c_e,t}$ and $G_{c_{s,B},t}$
   - Proof of Theorem 1

Proof of Theorem 1 I

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

$$\mathbf{f}(c_{\mathrm{e}}, c_{\mathrm{s,B}}, \varphi_{\mathrm{e}}, \phi_{\mathrm{s}}, T) = \Big(\alpha_e(x) N_{j^{\mathrm{Li}}}(c_{\mathrm{e}}, c_{\mathrm{s,B}}, \varphi_{\mathrm{e}}, \phi_{\mathrm{s}}, T), \\ \alpha_{\phi_{\mathrm{s}}} N_{j^{\mathrm{Li}}}(c_{\mathrm{e}}, c_{\mathrm{s,B}}, \varphi_{\mathrm{e}}, \phi_{\mathrm{s}}, T), \\ -hA_s(T - T_{\mathrm{amb}}) + F_T \Big).$$

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

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

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 $\mathbf{x} = (c_{\mathrm{e}}, c_{\mathrm{s,B}}, T)$. Then we can rewrite the fixed point problem (33) (which was our definition of weak-mild solution of (1)-(5)) as

$$\mathbf{x} = \mathbf{G}_t \circ \mathbf{f}_t \circ \widetilde{G}_{\phi,t}(\mathbf{x}). \tag{62}$$

Proof of Theorem 1 II

Since $\mathbf{f}_t \circ \widetilde{G}_{\phi,t} : \mathcal{C}([0,t_0],K_X) \to \mathcal{C}([0,t_0],Y)$ is locally Lipschitz continuous (due to Lemma 4.1), we can set a bounded neighbourhood $\mathbf{U} \subset K_X$ around $\mathbf{x}(0) = (c_{\mathrm{e}}(0), c_{\mathrm{s,B}}(0), T(0)) \in K_X$, and a bounded set $\mathbf{V} \subset Y$, such that the composition

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

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

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

Therefore, due to (61), we obtain that, for $t_2 = \min\{t_0,t_1\} > 0$ we have that

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

is a contracting map.

Then, we can apply the Banach fixed point theorem to find a unique solution of problem (62). If I is $\mathcal{C}_{\mathrm{part}}$ then one can simply paste the mild solutions from the

Proof of Theorem 1 III

different time partitions. In this sense there exists a unique “piecewise weak-mild solution”.

Applying classical results, there exists a maximal existence time $t_{\text{end}} \le t_{\text{end}}^I$. If $t_{\text{end}} < t_{\text{end}}^I$ then $d(\mathbf{x}(t), \partial K_X) \to 0$ or $\|\mathbf{x}(t)\|_X \to +\infty$ as $t \to t_{\text{end}}$. This is equivalent to (16) and the proof is complete. $\square$

Outline

Outline

Proof of Theorem 2 I

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 [Amann 1987] (for some more recent works, see e.g., [Pao 2012]).

Let us assume that the solution $(c_\mathrm{e}, c_{\mathrm{s,B}}, \varphi_\mathrm{e}, \phi_\mathrm{s}, T)$ is defined in $[0, t_0)$, where $0 < t_0 < t^I_{\mathrm{end}}$, and assume that (17) does not hold as $t \nearrow t_0$. We will show that (16) does not hold, and therefore $t_{\mathrm{end}} > t_0$. We can think of the problem written in the following way

$$\frac{\partial c_\mathrm{e}}{\partial t} - \frac{\partial}{\partial x}\left(D_\mathrm{e} \frac{\partial c_\mathrm{e}}{\partial x} \right) + C_1 c_\mathrm{e}^{\alpha_\mathrm{a} + \gamma_2 \left(\alpha_{\varphi_\mathrm{e}} + \frac{\mu(\hat{T})}{\hat{T}} \right)} = C_2 c_\mathrm{e}^{\alpha_\mathrm{a} - \gamma_1 \left(\alpha_{\varphi_\mathrm{e}} + \frac{\mu(\hat{T})}{\hat{T}} \right)} \geq 0,$$

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

Proof of Theorem 2 II

We can define

$$\overline{\mu} = \max_{[0,L]\times[0,t_0]} \left(\alpha_{\varphi_{\mathrm{e}}} + \frac{\mu(x,T(t))}{T(t)} \right),$$

$$\underline{\mu} = \min_{[0,L]\times[0,t_0]} \left(\alpha_{\varphi_{\mathrm{e}}} + \frac{\mu(x,T(t))}{T(t)} \right) \geq 1,$$

$$\overline{C}_1 = \max_{x\in J_\delta} (\delta_1 + \delta_2) \left(\max_{[0,L]} \alpha_{\mathrm{e}} \right) \exp \left(\frac{\gamma_1 + \gamma_2}{\min_{[0,t_0]} T(t)} (\|\psi_{\mathrm{s}} - \varphi_{\mathrm{e}}\|_{L^\infty} + \|p\|_{L^\infty}) \right).$$

Notice that, since $c_{\mathrm{s,max}} < 1$, we can conclude that $0 \leq C_1, C_2 \leq \overline{C}_1$. 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

$$\max\{s^{\alpha_{\mathrm{a}} - \gamma_1 \underline{\mu}}, s^{\alpha_{\mathrm{a}} - \gamma_1 \overline{\mu}}\} \leq \beta_1(s) \leq 1 + s,$$

$$\beta_2(s) \geq \max\{s^{\alpha_{\mathrm{a}} + \gamma_2 \overline{\mu}}, s^{\alpha_{\mathrm{a}} + \gamma_2 \underline{\mu}}\},$$

Proof of Theorem 2 III

so that we can construct the supersolution $\overline{c_{\rm e}}$ and subsolution $\underline{c_{\rm e}}$ defined as solutions, respectively, of

$$\begin{cases} \dfrac{\partial \overline{c_{\rm e}}}{\partial t} - \dfrac{\partial}{\partial x}\left(D_{\rm e} \dfrac{\partial \overline{c_{\rm e}}}{\partial x} \right) = \overline{C} \beta_1(\overline{c_{\rm e}}) & (x,t) \in (0,L) \times (0, t_{\rm end}), \\ \overline{c_{\rm e}}(0) = c_{e,0} & t = 0, \\ \partial_n \overline{c_{\rm e}} = 0 & x \in \{0, L\}, \end{cases}$$

$$\begin{cases} \dfrac{\partial \underline{c_{\rm e}}}{\partial t} - \dfrac{\partial}{\partial x}\left(D_{\rm e} \dfrac{\partial \underline{c_{\rm e}}}{\partial x} \right) + \overline{C} \beta_2(\underline{c_{\rm e}}) = 0 & (x,t) \in (0,L) \times (0, t_{\rm end}), \\ \underline{c_{\rm e}}(0) = c_{e,0} & t = 0, \\ \partial_n \underline{c_{\rm e}} = 0 & x \in \{0, L\}. \end{cases}$$

Using the conditions on the exponents given by Assumptions 9, we deduce that $\overline{c_{\rm e}}, \underline{c_{\rm e}}$ are continuous, globally defined in time and

$$\min_{[0,L]\times[0,t_0]} \underline{c_{\rm e}} > 0 \qquad \max_{[0,L]\times[0,t_0]} \overline{c_{\rm e}} < +\infty.$$

Proof of Theorem 2 IV

We also have that

$$\begin{cases} \dfrac{\partial c_{\mathrm{s}}}{\partial t} - \dfrac{D_{\mathrm{s}}}{r^2}\dfrac{\partial}{\partial r}\left(r^2 \dfrac{\partial c_{\mathrm{s}}}{\partial r}\right) = 0, & (x, r, t) \in D_\delta \times (0, t_0), \\ \dfrac{\partial c_{\mathrm{s}}}{\partial r} + C_3 c_{\mathrm{s}}^{\alpha_{\mathrm{s}} + \gamma_1 \frac{\lambda_{\min}(x,T)}{T}} = \alpha_{c_{\mathrm{s}}} j_-^{\mathrm{Li}} \ge 0, & r = R_{\mathrm{s}}(x), \\ c_{\mathrm{s}} = c_{\mathrm{s},0} & t = 0, \end{cases}$$

Proof of Theorem 2 V

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

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

$$\overline{\lambda}_{\min} = \max_{[0,L]\times[0,t_0]} \frac{\lambda_{\min}(x, T(t))}{T(t)}$$

$$\overline{C}_3 = \max_{x\in J_\delta} (\delta_1 + \delta_2) \left(\max_{[0,L]} \alpha_{\mathrm{s}} \right) \left(\max_{\alpha \in \{\alpha_{\mathrm{a}} \pm \gamma_{1,2}\underline{\mu}, \alpha_{\mathrm{a}} \pm \gamma_{1,2}\overline{\mu}\}} \|c_{\mathrm{e}}\|^{\alpha}_{L^\infty} \right)$$

$$\times \exp \left(\frac{1}{\min_{[0,t_0]} T(t)} \max\{\gamma_1, \gamma_2\} (\|\psi_{\mathrm{s}} - \varphi_{\mathrm{e}}\|_{L^\infty} + \|p\|_{L^\infty}) \right),$$

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

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

Proof of Theorem 2 VI

We construct the subsolution $\underline{c_\mathrm{s}}$, for every $t_0 < +\infty$, as the solution of

$$\begin{cases} \dfrac{\partial \underline{c_\mathrm{s}}}{\partial t} - \dfrac{D_\mathrm{s}}{r^2}\dfrac{\partial}{\partial r}\left(r^2 \dfrac{\partial \underline{c_\mathrm{s}}}{\partial r}\right) = 0, & (x,y,t) \in (x,r,t) \in D_\delta \times (0,t_0), \\ \partial_n \underline{c_\mathrm{s}} + \overline{C}_3 \sigma(\underline{c_\mathrm{s}}) = 0, & r = R_\mathrm{s}(x), \\ \underline{c_\mathrm{s}}(x,y,t) = \displaystyle\min_{\sigma \in J_\delta} c_{\mathrm{s},0}(\sigma, y) & t = 0, \end{cases}$$

so that, by the comparison principle, we have that $0 < \underline{c_\mathrm{s}} \le c_\mathrm{s}$, (by applying Assumptions 9). Finally, if we write

$$\begin{cases} \dfrac{\partial}{\partial t}(c_{\mathrm{s,max}} - c_\mathrm{s}) - \dfrac{D_\mathrm{s}}{r^2}\dfrac{\partial}{\partial r}\left(r^2 \dfrac{\partial (c_{\mathrm{s,max}} - c_\mathrm{s})}{\partial r}\right) = 0 & (x,y,t) \in D_\delta \times (0,t_0), \\ \dfrac{\partial}{\partial r}(c_{\mathrm{s,max}} - c_\mathrm{s}) + C_4 (c_{\mathrm{s,max}} - c_\mathrm{s})^{\beta_\mathrm{a} + \gamma_2 \frac{\lambda_{\mathrm{max}}(T)}{T}} = j_+^{\mathrm{Li}} \ge 0 & r = R_\mathrm{s}(x), \\ c_{\mathrm{s,max}} - c_\mathrm{s} = c_{\mathrm{s,max}} - c_{\mathrm{s},0} & t = 0, \end{cases} \tag{63}$$

Proof of Theorem 2 VII

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

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

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

$$\beta_4(s) \geq \max\left\{ s^{\alpha_{c_s} + \gamma_2 \underline{\lambda}_{\max}}, s^{\alpha_{c_s} + \gamma_2 \overline{\lambda}_{\max}} \right\}$$

then, by defining $\tilde{c_{\mathrm{s}}}$ as the solution of

$$\begin{cases} \dfrac{\partial \tilde{c_{\mathrm{s}}}}{\partial t} - \dfrac{D_{\mathrm{s}}}{r^2} \dfrac{\partial}{\partial r}\left(r^2 \dfrac{\partial \tilde{c_{\mathrm{s}}}}{\partial r} \right) = 0 & (x,y,t) \in D_\delta^{3D} \times (0,t_0), \\ \dfrac{\partial}{\partial r} \tilde{c_{\mathrm{s}}} + \overline{C}_3 \beta_4(\tilde{c_{\mathrm{s}}}) = 0 & |y| = R_{\mathrm{s}}(x) \\ \tilde{c_{\mathrm{s}}}(x,y,t) = \min\limits_{\sigma \in J_\delta} (c_{\mathrm{s},\max} - c_{\mathrm{s},0}(\sigma, y)) & t = 0, \end{cases}$$

Proof of Theorem 2 VIII

we arrive to the definition of the searched function $\overline{c_s} = c_{s,\max} - \tilde{c_s}$. We have that $\tilde{c_s} > 0$ (due to Assumption 9) and $\tilde{c_s}$ is a subsolution of (63). Hence $\tilde{c_s} \leq c_{s,\max} - c_s$. Therefore we have that $c_s \leq \overline{c_s} < c_{s,\max}$. Putting these two bounding solutions together we conclude

$$0 < \underline{c_s} \leq c_s \leq \overline{c_s} < c_{s,\max}.$$

Hence (16) does not hold as $t \nearrow t_0$. Applying Theorem 1 we obtain that $t_{\mathrm{end}} > t_0$. Therefore, either $t_{\mathrm{end}} = t^I_{\mathrm{end}}$ or (17). $\square$

Outline

Outline

6. Proof of Theorems 3 and 4
   - On the truncated potential case. Proof of Theorem 3
   - On the truncated temperature case. Proof of Theorem 4

Outline

On the truncated potential case. Proof of Theorem 3

Proof of Theorem 3.

Assume that (19) does not hold as $t \to t_0$ with $0 < t_0 < t^I_{\text{end}}$. We can substitute the constants in the proof of Proposition 3

$$\overline{C}_1 = \max_{x \in J_\delta} (\delta_1 + \delta_2) \left(\max_{[0,L]} \alpha_{\text{e}} \right) \exp \left(\frac{\gamma_1 + \gamma_2}{\min_{[0,t_0]} T} \|p\|_{L^\infty} \right), \tag{64}$$

$$\begin{aligned} \overline{C}_3 = {} & \max_{x \in J_\delta} (\delta_1 + \delta_2) \left(\max_{[0,L]} \alpha_{\text{s}} \right) \left(\max_{\alpha \in \{\alpha_{\text{a}} \pm \gamma_{1,2} \underline{\mu}, \alpha_{\text{a}} \pm \gamma_{1,2} \overline{\mu}\}} \|c_{\text{e}}\|^{\alpha}_{L^\infty} \right) \\ & \times \|H\|_{L^\infty} \exp \left(\frac{\gamma_1 + \gamma_2}{\min_{[0,t_0]} T} \|p\|_{L^\infty} \right), \end{aligned} \tag{65}$$

and repeat the argument. We get good bounds for $c_{\text{e}}, c_{\text{s,B}}$ for $t \in [0, t_0]$, which do not depend on $\|\phi_{\text{s}} - \varphi_{\text{e,Li}}\|_{L^\infty}$. Hence, applying Lemma 4.1 we can obtain some estimates of ϕ_{s} and $\varphi_{\text{e,Li}}$ in $[0, t_0]$. Therefore, by Theorem 2, we have that $t_{\text{end}} > t_0$. Hence, by contraposition, if $t_{\text{end}} < t^I_{\text{end}}$ then (19) must hold. $\square$

Outline

6. Proof of Theorems 3 and 4
   - On the truncated potential case. Proof of Theorem 3
   - On the truncated temperature case. Proof of Theorem 4

On the truncated temperature case. Proof of Theorem 4

Proof of Theorem 4.

It is immediate to establish global sub and supersolutions for T, which ensure (19) does not happen, and hence we get the global existence of solutions. $\square$

References I

- H. Amann. "On abstract parabolic fundamental solutions". In: *Journal of the Mathematical Society of Japan* 39.1 (1987), pp. 93–116.
- W. Arendt, C. J. K. Batty, and F. Neubrander. *Vector-valued Laplace Transforms and Cauchy Problems.* Monographs in Mathematics. Basel: Springer, 2013.
- H. Brézis. *Functional Analysis, Sobolev Spaces and Partial Differential Equations.* New York: Springer, 2010.
- N. A. Chaturvedi, R. Klein, J. Christensen, J. Ahmed, and A. Kojic. "Algorithms for advanced battery-management systems". In: *Control Systems, IEEE* 30.3 (2010), pp. 49–68.
- J. I. Díaz, D. Gómez-Castro, and A. M. Ramos. "On the well-posedness of a multiscale mathematical model for Lithium-ion batteries". In: *Advances in Nonlinear Analysis* To appear (2018), pp. 1–28. arXiv: 1802.06353.

References II

J. I. Díaz and I. I. Vrabie. "Propriétés de compacité de l'opérateur de Green généralisé pour l'équation des milieux poreux". In: *Comptes Rendus de l'Académie des Sciences. Série I. Mathématique* 309.4 (1989), pp. 221–223.

T. W. Farrell and C. P. Please. "Primary Alkaline Battery Cathodes". In: *Journal of The Electrochemical Society* 152.10 (2005), A1930.

A. Friedman. *Partial differential equations of parabolic type.* Mineola, NY: Courier Dover Publications, 1964.

D. Henry. *Geometric Theory of Semilinear Parabolic Equations.* Vol. 840. Lecture Notes in Mathematics. Berlin: Springer, 1981.

S. Lang. *Fundamentals of differential geometry.* Vol. 191. New York: Springer, 2012.

J. Newman. *Electrochemical systems.* New Jersey: Prentice-Hall, 1972.

References III

- R. Nittka. "Inhomogeneous parabolic Neumann problems". In: *Czechoslovak Mathematical Journal* 64.3 (2014), pp. 703–742.
- C.-V. Pao. *Nonlinear parabolic and elliptic equations*. New York: Springer, 2012.
- A. M. Ramos. *Introducción al análisis matemático del método de elementos finitos*. Madrid: Editorial Complutense, 2012.
- A. M. Ramos. "On the well-posedness of a mathematical model for lithium-ion batteries". In: *Applied Mathematical Modelling* 40.1 (2016), pp. 115–125.
- A. M. Ramos and C. P. Please. "Some comments on the Butler-Volmer equation for modeling Lithium-ion batteries". In: *Preprint arXiv:1503.05912* (2015), pp. 1–14.
- R. Ranom. "Mathematical Modelling of Lithium Ion Batteries". PhD thesis. Southampton, 2014.

References IV

K. Smith and C.-Y. Wang. “Power and thermal characterization of a lithium-ion battery pack for hybrid-electric vehicles”. In: *Journal of Power Sources* 160.1 (2006), pp. 662–673.