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



Angel Manuel Ramos

Instituto de Matemática Interdisciplinar, Departamento de Matemática Aplicada, Facultad de Ciencias Matemáticas, Universidad Complutense de Madrid, Plaza de Ciencias 3, Madrid 28040, Spain

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ABSTRACT

We discuss the well-posedness of a mathematical model that is used in the literature for the simulation of lithium-ion batteries. First, a mathematical model based on a macrohomogeneous approach is presented, following previous work. Then it is shown, from a physical and a mathematical point of view, that a boundary condition widely used in the literature is not correct. Although the errors could be just sign typos (which can be explained as carelessness in the use of d/dx versus d/dn , with n the outward unit vector) and authors using this model probably use the correct boundary condition when they solve it in order to do simulations, readers should be aware of the right choice. Therefore, the deduction of the correct boundary condition is done here, and a mathematical study of the well-posedness of the corresponding problem is presented.

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1. Introduction

Lithium-ion batteries have become very popular in recent years as a source of energy in multiple portable electronic devices. A mathematical model showing the key factors of the battery operation can be very helpful for the design and optimization of new models and also for the real-time control of battery performance.

On the basis of a macrohomogeneous approach developed by Newman [1], several mathematical models have been developed for these purposes [2–11], and include the main physics present in charge/discharge processes. A fully mathematical model is presented in Section 2, including a system of boundary value problems for the conservation of lithium and conservation of charge in the solid and electrolyte phases, together with an initial value problem for the conservation of energy. In the literature [9,10,12,8,6,7], one can find numerical computations of the model (or simplifications of it), with parameters corresponding to actual devices, that help to highlight the structure of this highly coupled model and show the relevance to the applications.

In recent years, several authors have written articles in different journals including a boundary condition that is not correct (see Remark 5). Although the authors probably used the correct boundary condition when solving the model in order to do simulations, the reader should be aware of the right choice. In this article it is shown why that condition is not only physically incorrect (see Section 3) but also mathematically incorrect, since it is proved (see Section 4, Remark 7) that the corresponding system of boundary value problems modeling the conservation of charge does not have any solution (therefore the system is not well-posed). Some results regarding the uniqueness and existence of a solution (with the correct boundary condition) for a simplified version of the model are given in Section 4.

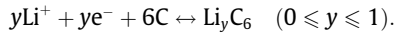
E-mail address: angel@mat.ucm.es

2. Mathematical model

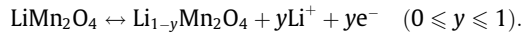
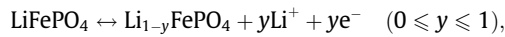
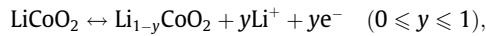
2.1. Generalities

A typical lithium-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, which is a concentrated solution containing charged species that can move along the cell in response to an electrochemical potential gradient.

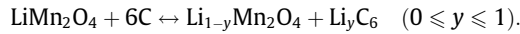
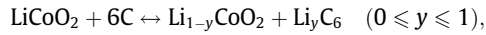
The negative electrode is an intercalated lithium compound usually made from carbon (typically graphite), with Li_yC_6 active material. Here $y \in [0, 1]$ is the stoichiometric value of the material, which changes during charging and discharging. For instance, during discharge, lithium ions inside solid Li_yC_6 particles diffuse to the surface, where they react and transfer from the solid phase into the electrolyte phase [6,7]. During charging, they move in the opposite way. Theoretically, in a fully charged lithium-ion battery this compound is LiC_6 (lithiated graphite; Li saturation; $y = 1$), in a semicharged/discharged battery it is Li_yC_6 , with $y \in (0, 1)$, and in a fully discharged battery it is just carbon (lithium depletion; $y = 0$). In practical operating cases, y never attains the extreme value of 0 and 1. The corresponding negative reaction equation is as follows:



The positive electrode is usually a metal oxide or a blend of multiple metal oxides [9] such as lithium cobalt oxide ($\text{Li}_{1-y}\text{CoO}_2$), lithium iron phosphate ($\text{Li}_{1-y}\text{FePO}_4$), or lithium manganese oxide ($\text{Li}_{1-y}\text{Mn}_2\text{O}_4$), with $y \in [0, 1]$. For instance, during discharging, the positively charged ions travel via diffusion and migration through the electrolyte solution to the positive electrode, where they react and are inserted into solid metal oxide particles [6,7]. During charging, they move in the opposite way. Theoretically, in a fully charged lithium-ion battery, $y = 1$ (lithium depletion), in a semicharged/discharged battery, $y \in (0, 1)$, and in a fully discharged battery, $y = 0$ (lithium saturation). Again, in practical operating cases, y never attains the extreme value of 0 and 1. The corresponding positive reaction equations for the examples described above are as follows:



Therefore, considering both the negative reaction and the positive reaction, we have the following corresponding total reaction equations:



A 1D electrochemical model is considered for the evolution of the lithium concentration $c_e(x, t)$ (mol m^{-3}) and the electric potential $\phi_e(x, t)$ (V) in the electrolyte and the electric potential $\phi_s(x, t)$ (V) in the solid electrodes, along the x -direction, with $x \in (0, L)$ and $L = L_1 + \delta + L_2$ being the cell width (m). We assume that $(0, L_1)$ corresponds to the negative electrode, $(L_1, L_1 + \delta)$ corresponds to the separator, and $(L_1 + \delta, L)$ corresponds to the positive electrode. This is coupled with a 1D microscopic solid diffusion model for the evolution of the lithium concentration $c_s(x; r, t)$ in a generic solid spherical electrode particle (situated at point $x \in (0, L_1) \cup (L_1 + \delta, L)$) along the radial r -direction, with $r \in [0, R_s]$ and R_s (m) the average radius of a generic solid active material particle. This 1D approximation is valid since the characteristic length scale of a typical lithium-ion cell along the x -axis is on the order of 100 μm , whereas the characteristic length scale for the remaining two axes is on the order of 100,000 μm or more [9]. R_s can be different at each electrode, and therefore we consider

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

The percentage of available local energy at time t (s) and radius r of a generic negative electrode particle situated at point $x \in (0, L_1)$ in the cell x -direction is the same as its stoichiometric value $y = y(x, r, t)$, which can be computed as

$$y(x, r, t) = \frac{c_s(x; r, t)}{c_{s,-,\max}},$$

where $c_{s,-,\max}$ (mol m^{-3}) is the maximum possible concentration in the solid negative electrode and $c_s(x; r, t)$ (mol m^{-3}) is the lithium concentration at time t , radius r , and point x . Therefore, the bulk state of charge (SOC) for the negative electrode (it can also be expressed for the positive electrode, but both are related and, therefore, it suffices to use only one of them) is

$$\text{SOC}(t) = \frac{3}{L_1(R_{s,-})^3} \int_0^{L_1} \int_0^{R_{s,-}} r^2 \frac{c_s(x; r, t)}{c_{s,-,\max}} dr dx. \quad (1)$$

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