Theoretical Analysis of Potential and Current Distributions in Planar Electrodes of Lithium-ion Batteries

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ARTICLE INFO

ABSTRACT

An analytical model is proposed to describe the two-dimensional distribution of potential and current in planar electrodes of pouch-type lithium-ion batteries. A concentration-independent polarization expression, obtained experimentally, is used to mimic the electrochemical performance of the battery. By numerically solving the charge balance equation on each electrode in conjugation with the polarization expression, the battery behavior during constant-current discharge processes is simulated. Our numerical simulations show that reaction current between the electrodes remains approximately uniform during most of the discharge process, in particular, when depth-of-discharge varies from 5% to 85%. This observation suggests to simplify the electrochemical behavior of the battery such that the charge balance equation on each electrode can be solved analytically to obtain closed-form solutions for potential and current density distributions. The analytical model shows fair agreement with numerical data at modest computational cost. The model is applicable for both charge and discharge processes, and its application is demonstrated for a prismatic 20 Ah nickel-manganese-cobalt lithium-ion battery during discharge processes.

1. Introduction

There is a growing interest in development of practical models to describe chemical, electrical and thermal processes in Lithium-ion (Li-ion) batteries with thin-layer cell (electrode) assemblies. From the macroscopic point of view, the multi-physics processes in Li-ion cells can locally be divided into two distinct parts: *i*) the processes in the electrolyte (solution phase), and *ii*) the processes in the electrodes (solid phase). These processes are strongly coupled; the former involves the transport (migration, diffusion, and convection) of mass and charge between the electrodes through an electrolyte solution accompanied by interfacial reactions at the surface of electrodes, while the latter deals with transport (mostly via conduction) of charges within the solid phase of the electrode assembly, i.e., current collectors and active material particles. Both categories of processes involve thermal effects, which are not the focus of this work.

To describe the processes within the electrolyte solution an electrochemical model with kinetic boundary conditions is required [1]. The most well-known physics-based electrochemical model for Li-ion batteries is the porous-electrode model, proposed by Newman and co-workers [2–4], and its variations for different lithium-based chemistries and applications; for examples see Refs. [5–13]. Such detailed electrochemical models are quite useful for cell design and optimization, however, they are typically of very high-order and complexity and are not suitable for real-time applications, in particular for multi-dimensional calculations and/or for thermally coupled models [14]. Also, for the case of Li-ion cells, due to simple treatment of active material in the porous-electrode model, numerous transport properties are needed to fit experimental data [15]. More recently, reduced-order electrochemical models for Li-ion cells are introduced [14,16–19]. The order reduction decreases the computational time and allows the model implementation into a real-time on-board electronic control unit, which is of particular interest in vehicle applications to estimate lithium ion concentrations and associated state-of-charge values. Nonetheless, the simplified models neglect some dynamics so that they cannot accurately predict the current-voltage behavior across different operating conditions.

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Nomenclature

a	width of electrode (m)
b	width of electrode tab (m)
c	height of electrode (m)
$\mathcal{C}_l$	interpolation coefficients for Y_{ec}
$\mathcal{C}_T$	temperature coefficient for Y_{ec}
$\mathcal{D}_m$	interpolation coefficients for V_{oc}
$\mathcal{D}_T$	temperature coefficient for V_{oc}
e	distance of tab centre from y-axis (m)
i	in-plane current density (A m^{-2})
I	applied current (A)
J	reaction current density (A m^{-2})
$\mathbf{n}$	unit normal vector on elctrode
N	number of cells in battery core
Q	capacity (Ah)
R_{ec}	electrochemical resistance (Ωm^2)
t	time (s)
T	temperature (K)
V	potential (V)
V_{oc}	open-circuit potential (V)
x	horizontal position in Cartesian coordinate (m)
y	vertical position in Cartesian coordinate (m)
Y_{ec}	electrochemical conductance per unit area (S m^{-2})

Greek

α_k	kth eigenvalue
δ	thickness (m)
ν	voltage transformation variable (V)
σ	electrical conductivity (S m^{-1})

Subscript

am	related to active material
cc	related to current collector
elec	related to electrode
eff	effective value of a property
batt	related to battery
cell	related to cell (electrode pair)
n	related to the negative domain
p	related to the positive domain
ref	reference value
tab	related to electrode tab
x	related to x direction
y	related to y direction

Superscript

–	averaged value of a property
$\sim$	shifted value of a property
max	maximum value of a property

When a battery exists and experimental data of the battery is available, empirical models which mimic the electrochemical performance of the battery can be generated. Empirical models are relatively fast and simple, thus are favored in control algorithms for battery management system [20]. Equivalent circuit models [21,22] and fitting function models [23,24] are common methodologies in this category.

In the present work, a simple concentration-independent polarization expression [23–25] is employed to describe the collective behavior of complex processes in the electrolyte solution between the electrodes. Standard constant-current discharge tests at a fixed environmental temperature are employed to determine the required coefficients in the polarization expression.

To model the overall battery performance, the processes in the electrolyte between the electrode must be linked to those which occur within the electrodes. For this, the governing equations, i.e., the charge balance equation coupled with the polarization expression, must be solved on each electrode. Based on this approach, several numerical analyses have been presented to describe the effects of electrode configuration on current and potential distributions inside the battery [26,27], and investigate the thermal effects in different operating conditions [28–32].

Similar to the above-mentioned studies, in the present work, the governing equations are solved numerically to obtain two-dimensional distributions of reaction current through the electrolyte, along with potential and current density distributions on the electrodes. However, the contribution of the authors to the subject is the development of a new "analytical" solution for this problem, which makes this work superior from the computational perspective. The key observation from our numerical simulations was that the processes in the electrolyte can be simplified such that the governing equations can be decoupled and an analytical solution for potential and current distribution on the electrodes can be derived. The proposed theoretical model and its implementation on an experimental pouch-type Li-ion battery are discussed in detail. The results are compared to numerical data with a fair agreement.

2. Formulation of the Problem

Figure 1a schematically shows the core of a pouch-type lithium-ion battery that is constructed of several cell assemblies, also known as electrode assemblies. In Fig. 1b, a single cell assembly is depicted. For better illustration, different layers in the cell assembly are shown separated. Each cell assembly includes a negative electrode, two separator sheets, and a positive electrode. The electrodes include active materials coated on both sides of current collector foils. Various active materials can be applied on electrodes depending on the chemistry of the Li-ion cell. In most Li-ion batteries, the current collector in positive and negative electrodes are foils of aluminum and copper, respectively. The separator sheet is an electrically inert membrane for transportation of cations (Li$^+$) between the electrodes. All layers, except current collectors, are porous and are soaked in a concentrated electrolyte liquid. The electrode tabs are the current collector foils extending outside the electrode plates for the purpose of electrical connection, and they are not covered by active materials.

Arrows in Fig. 1 present current streamlines during discharge processes. The through-plane straight arrows represent the transport of lithium ions (Li$^+$) between the electrodes, refereed to as "reaction current". The in-plane arrows in $x-y$ plane represent the transport of electric charges (e$^-$), i.e., the electrical current, on the electrode layers.

For convenience, the reaction current on both sides of each electrode in a single cell assembly can be considered to occur on one side of the electrode, as shown in Fig. 2. Consequently, the thicknesses of active material layers and the separator sheet in Fig. 2 are doubled.

A dimensional analysis can be performed to show that owing to the small thickness of layers in the cell assembly, compared to their dimensions in x and y directions, the distribution of potential in the electrodes is two-dimensional in $x-y$ plane [13]. Accordingly, the governing differential equation for the charge balance in each electrode reads

$$\sigma_{\text{eff},j}\left(\frac{\partial^2 V_j}{\partial x^2} + \frac{\partial^2 V_j}{\partial y^2}\right) + \frac{\mathbf{J}\cdot\mathbf{n}_j}{\delta_{\text{elec},j}} = 0 \quad (j = p, n) \tag{1}$$

where x and y indicate the Cartesian coordinate system (m), and $V_j = V_j(x, y)$ is the two-dimensional potential distribution in the