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Numerical simulation of thermal behavior of lithium-ion secondary batteries using the enhanced single particle model

Naoki Baba [a,*], Hiroaki Yoshida [a], Makoto Nagaoka [a], Chikaaki Okuda [b], Shigehiro Kawauchi [b]

[a] Thermodynamic System Research Div., Toyota Central R&D Labs., Inc., Nagakute, Aichi 480-1192, Japan
[b] Energy Creation & Storage Div., Toyota Central R&D Labs., Inc., Nagakute, Aichi 480-1192, Japan

HIGHLIGHTS

- We propose an enhanced single particle (ESP) model for lithium-ion batteries.
- The ESP model accounts for the solution phase limitation.
- The ESP model is available for the high rate charge–discharge analysis.
- We report the two-way electrochemical-thermal coupled simulation method.
- Temperature estimates during the charge–discharge cycle are calculated accurately.

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ABSTRACT

To understand the thermal behavior of lithium-ion secondary batteries, distributed information related to local heat generation across the entire electrode plane, which is caused by the electrochemical reaction that results from lithium-ion intercalation or deintercalation, is required. To accomplish this, we first developed an enhanced single particle (ESP) model for lithium-ion batteries that provides a cost effective, timely, and accurate method for estimating the local heat generation rates without excessive computation costs. This model accounts for all the physical processes, including the solution phase limitation. Next, a two-way electrochemical-thermal coupled simulation method was established. In this method, the three dimensional (3D) thermal solver is coupled with the quasi-3D porous electrode solver that is applied to the unrolled plane of spirally wound electrodes, which allows both thermal and electrochemical behaviors to be reproduced simultaneously at every computational time-step. The quasi-3D porous electrode solver implements the ESP model.

This two-way coupled simulation method was applied to a thermal behavior analysis of 18650-type lithium-ion cells where it was found that temperature estimates of the electrode interior and on the cell can wall obtained via the ESP model were in good agreement with actual experimental measurements.

1. Introduction

Lithium-ion batteries are attractive power sources for hybrid electric vehicles (HEVs) and electric vehicles (EVs) because they offer high cell voltages and energy densities. As a result, significant amounts of research have been focused on improving the power density, energy density, and life cycle performance of such batteries. However, because one of the primary issues in designing lithium-ion batteries is ensuring safety, ceaseless efforts have been expended towards overcoming thermal stability problems.

When evaluating thermal stability in the battery design phase, numerical simulation techniques provide useful information that is difficult or impossible to obtain experimentally. As a result, there have been numerous previous reports on thermal modeling of lithium-ion batteries over a wide range of exposed conditions. Many such reports go beyond normal use [1–11], with some focusing specifically on thermal abuse [12,13].

For example, Pals and Newman performed one-dimensional (1D) thermal modeling experiments to calculate temperature profiles in cell stacks [5,6]. This work was based on the 1D macroscopic model developed by Doyle and Newman [14] with the addition of a

* Corresponding author. Tel.: +81 561 71 7064; fax: +81 561 63 6920.
E-mail address: baba-n@mosk.tytlabs.co.jp (N. Baba).

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lumped heat generation term presented by Bernardi et al. [15] Chen and Evans [7–9] presented a multi-dimensional thermal model for lithium-ion batteries that focused on heat transport inside the cell stack without considering the electrochemistry of the cell. In their work, the heat generation rate was estimated using experimental discharged curves based on the lumped heat generation formulas given by Bernardi et al. Kim et al. [10,11] applied a two-dimensional (2D) model to parallel plate battery electrodes in order to simulate not only the potential and current density distribution, but also the temperature distribution. However, their modeling approach focused on ensuring current continuity on the electrodes and lumped heat generation terms in a fashion similar to the above-mentioned models.

In this study, we focus on the thermal behaviors of lithium-ion batteries under normal operating conditions. The objective of our work is the development of a multi-dimensional simulation method capable of evaluating both electrochemical and thermal behaviors inside lithium-ion batteries as accurately as possible, without the use of a lumped heat generation formula.

In order to achieve this, it was first necessary to develop a new variation of the commonly used single particle (SP) model for lithium-ion batteries. The previous simplified battery model [16–21] neglects the solution phase limitation. In contrast, the new and simplified battery model presented in this paper is capable of estimating heat generation rates using a detailed theoretical formula [1–3], since it accounts for all the physical processes, including the solution phase limitation.

Subsequently, a quasi-3D porous electrode solver was developed implementing the above new simplified battery model. This solver is basically applied to the 2D unrolled plane of spirally wound electrodes and provides distributed information on the potentials and lithium-ion concentrations, not only across the entire 2D electrode plane, but also across the thickness of the electrode itself, which can be obtained with the assistance of the new simplified battery model. As a result, the local heat generation rate resulting from the electrochemical reactions that occur during the charge–discharge process can be calculated in accordance with the detailed theoretical formula, and its 2D distribution data can be obtained across the entire electrode plane.

Finally, a two-way electrochemical-thermal coupled simulation method has also been established. Rising temperatures in a lithium-ion battery affect its performance because both the transport and physical properties strongly depend on temperature. In this method, the quasi-3D porous electrode solver transfers the information of the planer distribution of the heat generation rate to the 3D thermal solver. Following that, the 3D thermal solver simulates the temperature distribution of the spirally wound electrodes and returns the temperature information to the quasi-3D porous electrode solver. By executing the above-mentioned data exchange process, the temperature dependency of the transport and physical properties can be considered at every computational time-step.

This paper describes the abovementioned new charge–discharge SP model for lithium-ion batteries and the two-way electrochemical-thermal coupled simulation method in detail. In Sections 2 and 3, model development and validation of the new simplified battery model are shown in comparison with the conventional SP model. In Section 4, the two-way electrochemical-thermal coupled simulation method is described. In Section 6, simulated results of the electrochemical and thermal behaviors of a 18650-type lithium-ion cell during the charge–discharge cycle are expressed and discussed in detail with the aid of temperature measurements obtained from inside a real cell, which is shown in Section 5. Finally, conclusions of this paper are presented in Section 7.

2. Model development

In this section, the modeling approach for our new charge–discharge SP model for lithium-ion batteries is described in detail.

2.1. Conventional lithium-ion battery models

The literature on modeling approaches for lithium-ion batteries is quite extensive. However, conventional mathematical models can be classified roughly into two categories.

The first modeling approach was proposed by Doyle and Newman [14]. A schematic of this model, which consists of two composite electrodes and a separator, is shown in Fig. 1 and is referred to as the Newman model hereafter. A mathematical representation includes equations that describe: (1) mass transport of lithium in the solid phases, (2) mass transport of lithium-ions in the solution phase, (3) charge transport in the solid phases, and (4) charge transport in the solution phase. The Newman model is treated as a 1D macroscopic model across the thickness of the electrode in the local point on the electrode plane. To put it more precisely, the concentration of lithium within the solid phase is solved rigorously, using the extra pseudo second dimension along the radius of the particle. From the viewpoint of application to the 3D electrochemical-thermal coupled simulation for lithium-ion batteries, the advantage of the Newman model is its ability to accurately estimate heat generation rates, whereas its demerit is its high computational costs. The local heat generation rate is calculated from the detailed theoretical formula shown below [1–3].

$$q = \sigma^{\mathrm{eff}}\nabla\phi_s\cdot\nabla\phi_s + \left(\kappa^{\mathrm{eff}}\nabla\phi_e\cdot\nabla\phi_e + \kappa_D^{\mathrm{eff}}\nabla\ln c_e\cdot\nabla\phi_e\right) + a_{s,j}\bar{i}_{n,j}(\phi_s - \phi_e - U_j) + a_{s,j}\bar{i}_{n,j}T\frac{\partial U_j}{\partial T} \tag{1}$$

Eq. (1) requires the local point values and gradients of potentials and concentrations in the solid and electrolyte phase. Since the Newman model can be used to estimate these values at the each local point, the heat generation rate can be accurately estimated via Eq. (1). On the other hand, the Newman model requires the use of a μm-order mesh size to discretize a calculation domain across the thickness of each electrode in 1D. As a result, if the entire lithium-ion cell geometry of a 18650-type cell is discretized with the μm-order size, the number of computational meshes will be far in excess of ten million, which makes this methodology expensive and time consuming.

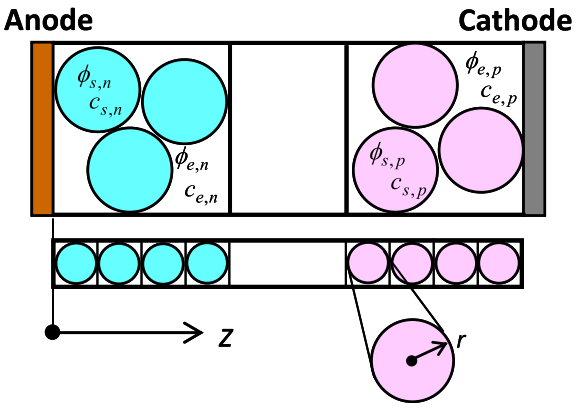

Fig. 1. Schematic of the lithium-ion battery model proposed by Doyle and Newman [12].