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Numerical modeling of lithium ion battery for predicting thermal behavior in a cylindrical cell

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ABSTRACT

The thermal behavior of lithium ion battery during charge and discharge is investigated by a numerical simulation. The commercially available cylindrical 18650 battery is modeled in this study. Two different models are used. The porous electrode model is simulated to obtain the Li content inside the particles. The transient thermo-electric model is used to predict the temperature distribution inside the cell. The results suggest that the increase in temperature during discharge is higher than that during charge. The temperature difference between charge and discharge is decreased with increasing C-rates. At a rate of 1C, the discharge temperature increases with a waving region at the beginning, whereas the charge temperature increases until certain point and then decreases. The thermal behavior is closely related to the change in entropy and applied current.

1. Introduction

Temperature is one of the main factors that impacts on the battery performance and life. Proper thermal management can improve the battery performance and extend the cycle life as well as assure reliable safety. The thermal management of batteries has attracted attention recently due to the increasing interest in hybrid electric vehicle (HEV) and electric vehicle (EV) batteries. To define and optimize a thermal management system, it is inevitably necessary to understand the thermal behavior of batteries and its influence on the cycle life.

Early studies in the area of battery thermal management focused on a fundamental understanding of battery prototypes by numerical simulations. On the other hand, researchers have recently conducted numerical simulations and experiments on commercial lithium ion (Li-ion) batteries. Kwon et al. [1] and Kim et al. [2,3] simulated Li-ion polymer batteries to predict the temperature using a semi-empirical model. Duan and Naterer [4], Onda et al. [5,6], Inui et al. [7], Jeon and Baek [8] and Somasundaram et al. [9] examined the thermal behavior of Li-ion cylindrical batteries. They modeled the commercially available SONY-18650 battery. Nevertheless, a more systematic study based on thermodynamics and electrochemistry will be needed to understand how heat is generated and dissipated inside a cell.

In this study, the thermal behavior of cylindrical Li-ion battery is investigated numerically to identify ways of improving battery thermal management. The transient thermo-electric model incorporating a porous electrode model is simulated to predict the temperature distribution and profile inside a cell. The goal is to understand the thermal behavior of commercial Li-ion battery and provide realistic physical processes that occur during charge and discharge.

2. Model description

The Li-ion battery considered in this work is a cylindrical 18650 battery with 1.5 Ah capacity. Two different models are used: a porous electrode model to determine the Li content inside the particles; and the transient thermo-electrical model to evaluate the thermal behavior inside a cell. On the other hand, the coupling of electrochemistry and thermo-electricity is not made due to incompatibility of these two software packages. The detailed descriptions of each model are elaborated in this section.

2.1. Porous electrode model

The porous electrode model for the Li-ion battery has been described well in the literature [10–18]. In this study, the existing Li-ion battery model in COMSOL Inc. Multiphysics 3.5a with

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Chemical Engineering Module is used. This example is based on the work reported by Doyle et al. [19]. Fig. 1(a) shows a schematic diagram of a typical Li-ion battery. The unit cell consists of three regions: $LiCoO_2$ (LCO) cathode, LiC_6 anode and polypropylene (PP) separator. These porous components are filled with lithium hexafluorophosphate ($LiPF_6$) in ethylene carbonate (EC)/di-methyl carbonate (DMC) (1:2, vol%) electrolyte.

The porous electrode model is a multi-scale model consisting of two dimensionless geometries. In the first, a one-dimensional geometry consists of three sequentially connected lines, i.e., anode, separator and cathode, as shown in Fig. 1(b). This solves electronic and ionic potentials, and electrolyte concentration. In the second, a two-dimensional geometry consists of two rectangles to solve the Li-ion concentration inside the electrode particles as shown in Fig. 1(c). Each electrode is represented by a single spherical particle whose area is equivalent to that of the active area of the solid phase in the porous electrode. The following assumptions are made to establish this model: the particles are spherical and equal in size; the potentials and electrolyte concentration vary in the x-direction; in the particles, the diffusion of Li-ions to the x-direction is ignored; and the temperature variation and volume change during the cycle are not considered. The porous electrode model solves the cell performance according to the following equations:

$$V_{\text{cell}} = E_{\text{cell}}(x,y) - \eta_{\text{t}}, \tag{1}$$

$$E_{\text{cell}}(x,y) = E_{\text{ref}}(x) - E_{\text{ref}}(y), \tag{2}$$

where $E_{\text{ref}}(x)$ and $E_{\text{ref}}(y)$ are measured open circuit voltage (OCV) of LCO [20] and graphite [21], respectively.

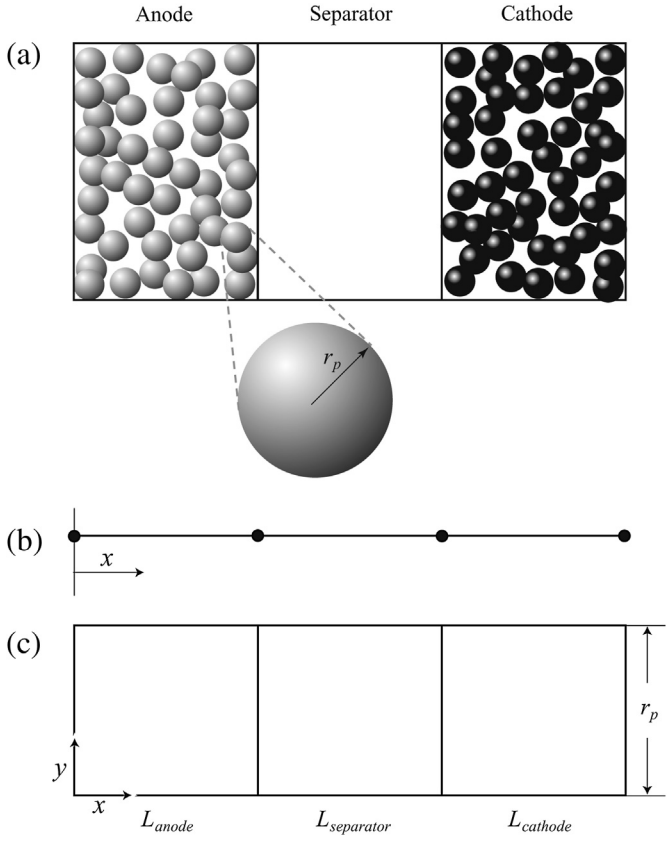

Fig. 1. Schematic of (a) a typical Li-ion cell and the porous electrode models: (b) one-dimensional model; (c) pseudo two-dimensional model.

Governing equations and constitutive equations used in this model described in Tables 1 and 2, and the parameters are listed in Table 3. The parameters of a cylindrical 18650 battery are collected from the literature [8,10,23–25]. More detailed description can be found in the literature [12–14], and COMSOL Multiphysics user's guide [22].

2.2. Transient thermo-electric model

A transient thermo-electric model is simulated to solve the energy equation using commercial finite element analysis (FEA) software, ABAQUS 6.7. The energy balance equation can be written as follows.

$$\rho C_{\text{P}} A \frac{\partial T}{\partial t} = \nabla(\kappa \nabla T) + \dot{q}. \tag{12}$$

The heat generation for battery systems can be expressed as,

$$\dot{q} = i\left(V^{\text{o}} - V - T\frac{\partial V^{\text{o}}}{\partial T}\right), \tag{13}$$

where $i(V^{\text{o}} - V)$ is the heat generation due to a joule heating and $-iT\partial V^{\text{o}}/\partial T$ is the heat generation due to an entropy change.

The heat generation due to a joule heating and an entropy change can be described by the following equations.

$$\dot{q}_{\text{joule}} = i(V^{\text{o}} - V) = \frac{i^2}{\sigma}, \tag{14}$$

$$\dot{q}_{\text{entropy}} = -iT\frac{\partial V^{\text{o}}}{\partial T} = -T\Delta S\frac{i}{nF}, \tag{15}$$

$$\Delta S = -\frac{\partial \Delta G}{\partial T} = -nF\frac{\partial V^{\text{o}}}{\partial T}, \tag{16}$$

where the Gibbs energy change is $\Delta G = -nFV^{\text{o}}$.

Fig. 2(a) shows the cylindrical Li-ion battery considered in this study. The cylindrical battery is composed of a spirally-wounded jelly-roll and can. The jelly-roll consists of five layers: cathode (LCO), cathode current collector (Al foil), separator (pp), anode (LiC_6) and anode current collector (Cu foil). Table 4 lists the geometry details and properties which are collected from the literature [3,10,13,23–25]. The jelly-roll is assumed to have a round structure for simplicity and minor effect on thermal analysis.

Table 1
Governing equations and source terms.

Governing equations	Mathematical expressions	
Conservation of electrons and ions	$\nabla\cdot\left(-\frac{\sigma_1^{\text{eff}}}{L_{\text{i}}}\nabla\phi_1\right) = -i_{\text{loc}}S_{\text{a}}L_{\text{i}}$	(3)
	$\nabla\cdot\left[-\frac{\sigma_2^{\text{eff}}}{L_{\text{i}}}\left(\nabla\phi_2 - \frac{2\nu RT}{F}\frac{\nabla c_2}{c_2}\right)\right] = -i_{\text{loc}}S_{\text{a}}L_{\text{i}}$	(4)
Mass balance	$\varepsilon_2^{\text{i}}L_{\text{i}}\frac{\partial c_2}{\partial t} + \nabla\cdot\left(-\frac{D_2^{\text{eff}}}{L_{\text{i}}}\nabla c_2\right) = -\frac{i_{\text{loc}}^{\text{i}}S_{\text{a}}^{\text{i}}L_{\text{i}}}{F}(1-t_+)$	(5)
Fick's diffusion equation	$y^2 r_{\text{p}}\frac{\partial c_1}{\partial t} + \nabla\cdot(-\mathbf{D}_1\nabla c_1) = 0$	(6)
	where $y = r/r_{\text{p}}$, $\mathbf{D}_1 = \begin{bmatrix} \frac{y^2 D_1 \times 10^{-6}}{r_{\text{p}}} & 0 \\ 0 & \frac{y^2 D_1}{r_{\text{p}}} \end{bmatrix}$	