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Heat transfer in the dynamic cycling of lithium–titanate batteries

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ABSTRACT

Based on the coupled model of a three-dimensional thermal model and one-dimensional electrochemical model, the thermal behaviors of lithium–titanate battery under the discharge–charge cycling with various current are investigated. The temperature on the surface of battery increases with the increasing cycling rate. Two temperature peaks are observed during the constant-current discharge, constant-current and constant-voltage charge process based on the analysis of the heat generation. Additionally, the radiative heat transfer cannot be omitted when the battery is operated under natural convection at 0.5 C cycling rate, in this case, the radiative heat transfer is estimated to contribute 42% to the total heat transfer. The results can provide basic data for the thermal management of the battery pack during the discharging and charging processes.

1. Introduction

Batteries play a key role in the development of electric vehicles and hybrid electric vehicles [1]. Progress in the development of lithium-ion batteries with large capacity and high power has been advanced for application to electric vehicle. However, the thermal stability under various operation conditions is one of the most important safety considerations for large-scale lithium-ion batteries. Some thermal models of the lithium-ion battery were proposed in previous studies and the temperature distribution inside the battery was simulated. In general, the models can be classified into three types in dimension: one-dimensional, two-dimensional and three-dimensional models [2]. Bernardi et al. [3] developed a heat-generation model for battery systems concerning the heat contributions from electrochemical reactions, mixing enthalpies and phase changes. Chen et al. [4] embedded the basic equations of Bernardi's work into a three-dimensional thermal model for the heat source term.

As an effective tool, numerical simulation of heat transfer within batteries can be used to obtain the fundamental data on whether the generated heat can be easily dispersed out of batteries, and how to design a proper thermal management policy for the discharging and charging processes of batteries [5,6]. Jeon and Baek [7] provided the thermal behavior of lithium ion battery at several discharge rates. Based on the finite element method, Kim et al. [8] simulated the thermal behavior of a lithium-ion battery during galvanostatic discharge, constant-current (CC) and constant-voltage (CV) charge. Onda et al. [9] calculated the temperature rise of a small lithium-ion battery during rapid charging and discharging cycles. Most of these thermal models of lithium-ion batteries focused on the thermal behavior during galvanostatic discharging. Only few works reported the thermal behavior of lithium ion batteries during dynamic CC and CV charging. However, the lithium ion battery packs used for the electric vehicle application rarely cycle per these simple protocols. It is important to predict accurately the thermal behavior of lithium-ion batteries under various discharge and charge conditions to improve their performance and life, as well as ensuring the thermal safety. The objective of this paper is to provide deeper insight on the heat transfer inside the battery and heat exchange with the environment under various working conditions and boundary conditions. Additionally, the current distribution influence on the temperature distribution of the battery also was investigated by others. Tang et al. [10] used COMSOL Multiphysics to solve the 2D potential and current distribution during galvanostatic charge of lithium-ion batteries. Gerver and Meyers [11] developed a 2D electrochemical and 3D thermal model to simulate the current and temperature distributions. However, the novel work in this paper is on the effect of heat transfer not the influence of current distribution on the temperature. Therefore, the heat generation was treated as

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Nomenclature

a_s	specific interfacial area of the electrode
c	lithium ion concentration
C_p	heat capacity
D	diffusion coefficient of lithium ion
E	cell potential
$\partial E_{OC}/\partial T$	temperature derivative of equilibrium potential
f	mean molar activity coefficient of the electrolyte
F	Faraday's constant, 96,487 C mol^{-1}
h_c	convective heat transfer coefficient
h_r	the emissivity of the cell surface
i_0	exchange current density of an electrode reaction
J	transfer current resulted from the intercalation or deintercalation of lithium
k	electrochemical reaction rate constant
k	thermal conductivity
L	thickness of the different layers of the cell
R	the gas constant
r_s	radius of the spherical particle
T	absolute temperature
T_∞	the ambient temperature
t_+^0	transport number
α	charge transfer coefficients
κ	electric conductivity
ε	volume fraction of a phase
σ	the Stefan–Boltzmann constant, 5.670373×10^{-8} kg s^{-3} K^{-4}
η	activation over-potentials of an electrode reaction
ρ	effective density of the active battery material

Subscripts

e	the electrolyte phase
neg	negative electrode
pos	positive electrode
sep	electrolyte
neg_cc	negative current collector
pos_cc	positive current collector
i	different layer of active battery material, i.e. neg, pos, sep, neg_cc, pos_cc
s	the solid phase
eff	effective
oc	open circuit
rev	reversible
rxn	irreversible
j	X, Y, Z-direction

uniform throughout the core region of the system to improve the computation efficiency. As one new power cell for electric vehicles, the lithium–titanate battery was investigated in this work. For this type of battery, its positive electrode is nickel-cobalt-manganese-oxide lithium ($Li(Ni_{1/3}Co_{1/3}Mn_{1/3})O_2$, NCM), and its negative electrode is lithium titanate oxide ($Li_4Ti_5O_{12}$, LTO).

2. Model development

2.1. One-dimensional electrochemical model

Commercially available lithium-ion cells have three primary functional components, i.e. negative electrode, electrolyte, and positive electrode. Schematic of one-dimensional model of lithium-ion cell is shown in Fig. 1.

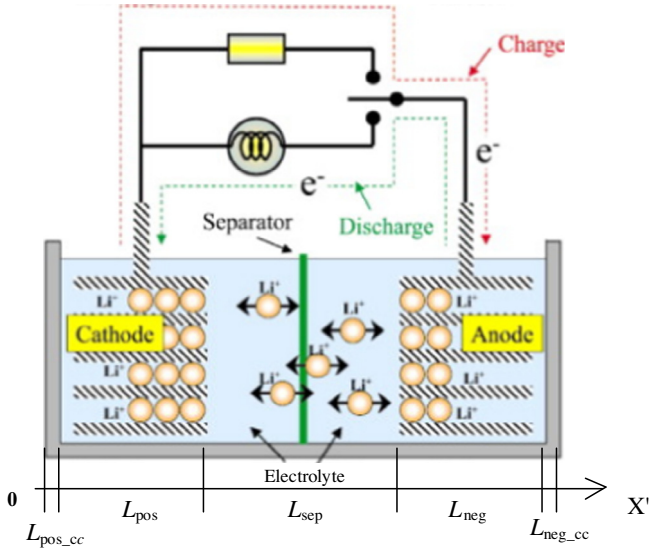

Fig. 1. Schematic of one-dimensional model of lithium-ion cell [12].

During charging, lithium-ions deintercalate from the positive electrode and intercalate into the negative electrode, and the reverse takes place during discharging. During charging and discharging, various chemical and electrochemical reactions occur as well as the transport processes of lithium ions. As limited knowledge on the multi-physics processes were obtained in the lithium-ion batteries, the following assumptions were proposed [4]: (1) positive and negative material are the spherical particles, the particle diffusion behavior follows Fick's second law of diffusion; (2) spherical particles uniformly distribute in the positive and negative electrodes; (3) the behavior of the electrolyte could be described by the theory of dilute solution; (4) the thermal physical properties in each layer are isotropic and their values equal to the average values within a certain temperature range.

The effects of current density, lithium-ion diffusion in solids, average radius on discharge capacity and temperature were studied through the electrochemical models of lithium-ion cells proposed by Cai and White [13]. Lu et al. [14] compared White's and Newman's models and found that Newman's model is more sensitive to current density, lithium-ion diffusion in solids, and average radius than that of White's model. According to the electrochemical models of Newman, the flux of material balance for the lithium-ions in an active solid material particle is governed by Fick's second law in spherical coordinates [15]:

$$\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_s}{\partial r}\right) \tag{1}$$

The material balance for the binary electrolyte in the liquid phase is given by:

$$\varepsilon_e\frac{\partial c_e}{\partial t} = \frac{\partial}{\partial x}\left(D_{eff,i}\frac{\partial c_e}{\partial x}\right) + (1-t_+^0)a_sJ \tag{2}$$

The charge balance for the solid and liquid phase is governed by Ohm's law:

$$-k_{s,eff}\frac{\partial^2\phi_s}{\partial x^2} = -a_sFJ \tag{3}$$