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Research Paper

Thermal-electrochemical coupled simulations for cell-to-cell imbalances in lithium-iron-phosphate based battery packs

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HIGHLIGHTS

- Electric circuit of the pack is incorporated to evaluate thermally-driven imbalance.
- Temperature and current deviation of a large complex battery pack are investigated.
- Deviation among the cell capacity is aggravated with larger temperature gradients.

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ABSTRACT

A thermal-electrochemical coupled model framework considering mass balance, charge balance, reaction kinetics, and energy balance is developed to evaluate thermally-driven imbalance among cells of a commercialized lithium-iron-phosphate battery pack consisting of a combination of series and parallel connections. Current distribution and joule heat generation of copper alloy sheets connecting several cells within a battery pack are also considered in the simulation. A running management built in MATLAB, R2010a (2010) is applied to deliver the coupling of the thermal-electrochemical model, among different modulus of COMSOL Multiphysics 5.0 (2014). Simulated voltage variation and temperature distribution of an individual cell during charge/discharge are validated with the corresponding experiments. The developed model is further applied to study the non-uniform temperature distribution and electrical imbalance among cells within the 4S6P LFP battery pack. Simulation results show that thermal imbalance could magnify the deviation of discharge current and capacity among individual cells and may accelerate the capacity losses of the cells within a battery pack. Our model can facilitate understanding of the impact of electrical imbalance on the battery pack and assist thermal management systems.

1. Introduction

The lithium-ion battery is a popular type of rechargeable batteries for portable electronics, with high energy density, no memory effect, and slow degradation. (Scrosati and Garche [3]) The lithium-iron-phosphate (LFP) battery with lithium iron phosphate as cathode material is of low cost, high power output, environmentally benign, and features intrinsic thermal safety. (Huang et al. [4]) This battery chemistry thus ranks among the most promising lithium-ion batteries that target hybrid electric vehicle (HEV) and electric vehicle (EV) markets, and rechargeable LFP battery packs are widely used as energy storage by automobile industries and in uninterruptible power supply (UPS) systems. However, one of the crucial limitations for the LFP battery pack is its operating temperature, which may strongly restrict the voltage, capacity, power, and cycle life. Overheating and non-uniform temperature distribution of the battery pack could lead to degradation and failure of cells. Thermal management of the battery pack is therefore essential for its long term performance and safety.

In order to analyze the thermal effects on the performance of batteries, Kumaresan et al. [5] developed thermal-electrochemical models coupling mass balance, charge balance, reaction kinetics, energy balance and heat transfer equations, and temperature dependences of transport and kinetic parameters are considered. In practice, the thermal-electrochemical coupled analysis can be used to obtain the optimal operating conditions such as pack temperature. Since thermal management needs to be carefully examined when new battery packs are developed,

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many studies proposed various cooling strategies to achieve more uniform temperature distribution. Xu and He [6] asserted that the heat dissipation of battery packs could be significantly enhanced with different arrangements of the cells and the air inlet/outlet. Wang et al. [7] and Chen et al. [8] investigated various cooling approaches to guarantee the batteries operated within the optimal temperature range as well as to provide effective solutions for the cooling system. Yang et al. [9] studied the thermal performances of battery pack to advise the appropriate arrangement of cylindrical cells for the efficient cooling system. Lan et al. [10] and Xu et al. [11] developed a novel cooling system based on aluminum minichannel tubes applied to the battery module and investigated its efficacy on the mitigation of thermal runaway.

Rather few studies investigate the influences of temperature deviations on the cell-to-cell current distribution of a battery pack. Bandhauer et al. [12] revealed that electrical imbalance could lead to serious battery failures if thermal runaway is induced. Guo and White [13] developed a thermal resistance model, coupling the so-called single particle model, energy balance equation, and basic circuit constraints, to simulate electrical and thermal behaviors among batteries connected in parallel configuration. Although the electrochemical behavior and heat generation among individual cells were considered, temperature of each cell was assumed to be uniform in the study. Moreover, even though the predicted temperature of the battery pack during charge/discharge cycles is consistent with experimental data, the individual cells show minute variations in electrical behaviors due to the relatively limited temperature deviation. Yang et al. [14] investigated the unbalanced cell discharging stemmed from a temperature difference between two parallel-connected cells via simulations and experiments, with an assumption of different initial temperatures at the beginning of the discharging process. A larger current is observed within the cell of higher temperature in the early discharging stage. On the contrary, the cooler cell experiences a smaller operating current. The unbalanced discharging current induced by the temperature difference between two parallel connected cells exacerbates the imbalance phenomenon. This imbalance discharge current may thus aggravate the capacity deviation between two parallel-connected cells and accelerate the capacity losses of the battery pack.

In the past, many researches overlooked the thermally-driven imbalance among the cells and its potential risk of thermal runaway and assumed the electrochemical behaviors and heat generation among individual cells of a battery pack to be identical. The thermal-electrochemical coupled analysis is thus applied in the present study to investigate effects of the non-uniform temperature distribution and thermally-driven electrical imbalance among cells on the performance of a commercialized battery pack consisting of a combination of series and parallel connections. The developed model framework enables us to examine the operating current, temperature distribution and heat generation among individual cells and the impact of thermally-driven imbalances on a large complex battery pack serving for practical applications.

2. Mathematical model

Since highly conductive current collectors such as aluminum and copper foils are utilized to ensure homogeneous current distribution, the electrochemical behavior of the cylindrical cell can be reasonably assumed to be one dimension along the radial/thickness direction (Newman and Alyea [15]). The one-dimensional electrochemical model applying to the LFP battery here considers three components: the graphite negative electrode, separator, and lithium-iron-phosphate positive electrode. The chemical reactions in the LFP battery that our electrochemical model considered are as follows:

Positive electrode reaction

$$\mathrm{Li_{1-x}FePO_4 + xLi^+ + xe^- \leftrightarrow LiFePO_4} \tag{1}$$

Negative electrode reaction

$$\mathrm{Li_xC_6 \leftrightarrow 6C + xLi^+ + xe^-} \tag{2}$$

Total reaction

$$\mathrm{Li_{1-x}FePO_4 + Li_xC_6 \leftrightarrow LiFePO_4 + 6C} \tag{3}$$

During the charge process, the reactions proceed from the left-hand side to the right-hand side and lithium ions deintercalate from the positive electrode and intercalate into the negative electrode, while the reverse reaction takes place during the discharge process. The LFP battery domain that the one-dimensional electrochemical model considered includes the aforementioned three components and is described as three sequentially extended lines.

Since there are other physical phenomena in addition to the aforementioned electrochemical reactions, during charge and discharge processes an electrochemical model on the basis of coupled mass balance, charge balance, and reaction kinetics constitution laws is adapted here to simulate the electrochemical behavior of the LFP battery. This model consists of diffusion phenomena in the concentrated electrolyte and the solid phase electrodes, Ohm's law for the potential distribution, and the conservation of charge and mass. Moreover, the solid phase porous electrodes filled with the electrolyte and the diffusion mechanism in the electrodes are described by the porous electrode theory, which considers each electrode as a number of spherical particles with the surface area represents the porous electrode active surface area. Governing equations and boundary conditions illustrating the isothermal charge and discharge processes of a lithium-ion battery are listed in Table 1 to describe general dynamics of a battery system and are used to predict the behaviors of lithium-ion batteries during charge and discharge procedures (Doyle et al. [16]).

To describe the effect of heat generation from cell to pack level and formation of thermal hot spots within the battery pack, a three-dimensional thermal model is coupled to the electrochemical model. Performances of the LFP cell, such as the output voltage and storage capacity, are significantly influenced by its operating temperature. However, the heat generation of the LFP cell is in turn controlled by the electrochemical reactions occurring in the cell during charge and discharge processes and thus affects the

Table 1
Equations used in the thermal-electrochemical model.

Equations	Boundary conditions
Electrochemical model	
Separator	
$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - \frac{i_2}{z_+ v_+ F}\frac{\partial t_+}{\partial x}$ $\frac{\partial \eta}{\partial x} = \frac{I}{\kappa} + \frac{RT}{F}\left(\frac{s_+}{n v_+} + \frac{t_+}{z_+ v_+}\right)\frac{\partial c}{\partial x}$	$\nabla c = 0$ *at* $x = 0$ *and* $\delta_- + \delta_s + \delta_+$ $i_2 = I$ *at* $x = \delta_-$ *and* δ_s $\nabla \Phi_1 = \frac{I}{\sigma}$ *at* $x = 0$ *and* $\delta_- + \delta_s$
Electrodes	
$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - \frac{i_2}{z_+ v_+ F}\frac{\partial t_+}{\partial x} + \frac{aj_n(1-t_+)}{v_+}$ $\frac{\partial \eta}{\partial x} = \frac{I-i_2}{\sigma} + \frac{i_2}{\kappa} + \frac{RT}{F}\left(\frac{s_+}{n v_+} + \frac{t_+}{z_+ v_+}\right)\frac{\partial c}{\partial x}$ $aj_n = -\frac{s_1}{nF}\frac{\partial i_2}{\partial x}$ $I = F(k_a)^{\alpha_c}(k_c)^{\alpha_a}(c_{max} - c)^{\alpha_c} c^{\alpha_a}\left[exp\left(\frac{\alpha_a F}{RT}(\eta - U)\right)\right.$ $\left.-exp\left(-\frac{\alpha_a F}{RT}(\eta - U)\right)\right]$	
Thermal model	
$\rho C_p \frac{dT}{dt} = \nabla(\lambda \nabla T) + Q_{rxn} + Q_{rec} + Q_{ohm}$ $Q_{rxn} = FaJ(\Phi_1 - \Phi_2 - U)$ $Q_{rec} = FaJ\frac{\partial U}{\partial T}$ $Q_{rxn} = \sigma_{eff}(\nabla\Phi_1)^2 + \kappa_{eff}(\nabla\Phi_2)^2$ $+\frac{2\kappa_{eff}RT}{F}(1 - t_+)\nabla(lnc)\nabla\Phi_2$	$-\lambda\nabla T = h(T_\infty - T)$ *at* $t = Rz = 0$ *and* L