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A coupled nonlinear equivalent circuit – Thermal model for lithium ion cells

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HIGHLIGHTS

- ► Nonlinear equivalent circuit model with energy balance for lithium ion cells.
- ► Temperature-dependent variable resistors.
- ► The cell voltage and temperature represented by one pair RC model.
- ► Rate of heat generation steeply rises near the end of discharge.
- ► Coolant with higher heat transfer coefficient result in lower operating efficiency.

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ABSTRACT

A nonlinear equivalent circuit model is developed for lithium ion cells using variable resistors that are functions of the cell temperature. The voltage and thermal characteristics of a commercial cell with a $LiFePO_4$ positive and graphite negative electrode are modeled using a lumped energy balance coupled with the equivalent circuit representation. The cell voltage and temperature during full depth charge–discharge operations can be represented accurately by a one pair RC model. The model is able to represent cell voltage and temperature over a wide range of powers with a global set of parameters. The parameters established, model predictions of the heat generation rates under various conditions are examined. Due to the unique discharge behavior of $LiFePO_4$ positive electrode, the rate of heat generation is constant over most of the state of charge (*SOC*) window and steeply rises near the end of discharge. A higher heat transfer coefficient of the cooling medium, in addition to lowering the operating voltage, results in higher heat generation. Thus battery cooling systems should be designed to operate at an optimal rate of heat removal considering the operating efficiency, in addition to battery life.

1. Introduction

The lithium ion battery technology is established as the primary energy source in electric vehicle or hybrid electric vehicle applications due to its high energy density, light weight, low self-discharge and other features [1]. At present, a phospho-olivine compound, lithium iron phosphate ($LiFePO_4$) [2], has proven to be one of the leading candidates as the positive electrode material for hybrid and electric vehicle applications. $LiFePO_4$ is environmentally benign, highly stable, and inexpensive with a high capacity and operating voltage. A pertinent problem that has been observed in lithium based batteries is that of thermal runaway. Especially for large scale applications like automobiles, where a large array of cells are connected together, thermal management becomes critical and presently is one of the singular challenges for the industrial utilization of lithium based cells.

During battery discharge/charge, various electrical and electrochemical processes take place that release heat. Thermal modeling is an efficient way to calculate the temperature rise during operation and develop various cooling schemes for batteries. Thermal modeling gives insights into the contributions of the individual electrochemical processes. The general energy balance approach developed around two decades ago [3] has been incorporated in the macroscale continuous models [4] to calculate the temperature changes [5] during battery operations. Other developments in this area include two- and three-dimensional thermal models [6,7], finite element models [8] and models for EV batteries [9]. Electrochemical thermal [10] models that examine the interactions between electrochemical and thermal processes, approaches in modeling of $LiCoO_2$ based batteries [11] and recent developments on distributed thermal models [12] are worth

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mentioning in this context. Under normal conditions cell thermal response is modeled [13] using lumped parameters and heat generation rates as well.

Equivalent circuit models where the voltage response of the cell is represented as an electric circuit [14] has received much importance due to conceptual simplicity and applicability. These models can be integrated with control algorithms at a system level for on-board applications in an automobile. To develop an accurate model for battery performance, equivalent circuit models require less amount of data, must be robust, accurate over a wide range of operating conditions and easy to compute. The pertinent variables do not have spatial dependence and the model equations based on electrical circuit theory are solved as a set of ordinary differential equations. The equivalent circuit model is coupled with the energy balance models [15] to characterize the thermal behavior of NiMH battery packs with sufficient accuracy. The entropy of the $LiFePO_4$–graphite cell is measured [16] and the thermal characteristics are represented as a thermal equivalent circuit.

In a recent work [17], a nonlinear equivalent circuit model is developed using over-potential based variable resistors. The model is able to accurately represent the pulse voltage response of commercial lithium ion cells. This model, however, is developed for isothermal conditions. During cell operations, there is substantial amount of heat release and a non-isothermal model is essential to study the thermal response under these conditions. A non-isothermal model can be used to understand the dependence of the rate of heat generation on operating conditions and minimize thermal losses. In the present work a non-isothermal nonlinear equivalent circuit is developed using variable resistors that are functions of cell temperature. The equivalent circuit model is solved with the energy balance equation to obtain cell voltage and temperature simultaneously. The coupled model is used to study voltage and thermal characteristics of a commercial cell with $LiFePO_4$ positive and graphite negative electrode. In the previous work [17] the parameters are estimated from isothermal HPPC (Hybrid Pulse Power Characterization) data with minimal temperature variations during the pulse. As the aim of the present work is to develop a non-isothermal model, the parameters are estimated from a full depth discharge–charge data at various temperatures. As voltage and temperature are obtained simultaneously, the present approach can be potentially used as an on-board state estimator in battery management systems.

In the first part of study, parameters are estimated by minimizing the error between model outputs and experimental data. The global set of parameters thus estimated, model predictions of heat generation rates under various conditions are examined. In order to conceive appropriate cooling concepts when cells are used as energy source in automobiles, it is important to understand the dependence of heat generation on operating conditions. The interaction of the cell with the battery cooling system is through the heat transfer coefficient. Hence in the subsequent section, the effect of heat transfer coefficient on cell temperature and rate of heat generation is studied in detail. The results of this study provide key insights in the design of an efficient battery thermal management system.

2. Model development and experimental data

In the equivalent circuit approach various electrochemical processes in the cell are represented in terms of equivalent resistors, capacitors or other electric circuit elements. The general representation for a cell, with processes identified using electrochemical impedance spectroscopy (EIS) [18] is that of a sequence of RC (*R* is parallel to *C*) circuits with a Warburg element for diffusion. An equivalent representation amenable for time domain analysis is that of an *N* pair RC [17]. Output of an electric circuit model is the cell voltage represented in terms of cell current, equilibrium potential and the model parameters. Effect of temperature on individual electrochemical processes enters the equivalent circuit model through the temperature dependence of model parameters. Cell temperature is obtained using a lumped energy balance once cell voltage, entropy of charge transfer reaction and heat transfer coefficient of the cooling medium are known. By coupling the equivalent circuit and lumped energy balance models, cell voltage and temperature are obtained under any operating conditions. Details of the equivalent circuit model and the lumped energy balance are described in the next section. The subsequent section discusses the experimental data used in the model.

2.1. The equivalent circuit model and energy balance

In absence of degradation, important processes in a cell are ionic and electronic conduction, charge transfer reaction and lithium diffusion in the electrodes. In a recent work [17], it is shown that pulse response of a lithium ion cell is accurately represented by a 2 pair RC circuit. In the present work the interest is on modeling full depth charge–discharge processes and further simplifications to the model are sought. For example, it can be expected that faster transients, represented by one of the RC pairs are not significant. The resultant equivalent circuit is a 1 pair RC model (Fig. 1), and hence is considered in this study. The 1 pair RC model has a high frequency resistor *R* and a low frequency resistor R_{ct} parallel to a capacitor *C*. The high frequency resistor *R* represents ionic and electronic conduction, capacitor *C* represents the double layer and all the transients and resistor R_{ct} represents resistance due to all transport processes – diffusion in the electrodes and charge transfer reaction. It should be noted that in this level of representation, distinction between the electrodes is not made. The 1 pair RC model, though simplistic, has been successful in representing [14] the charge–discharge characteristics of lithium ion cells. The principal equation governing the cell behavior is the voltage balance across the cell:

$$V = V_0 + IR + V_1 \tag{1}$$

In Eq. (1), cell voltage *V* is related to equilibrium potential V_0, voltage drop across the resistance *R* due to current *I*, and voltage drop across the RC pair (R_{ct} parallel to *C*), V_1. The current balance across the RC pair is:

$$I = I_C + I_{R_{ct}}, \tag{2}$$

Eq. (2) can be rewritten in terms of capacitance *C* and resistance R_{ct} as

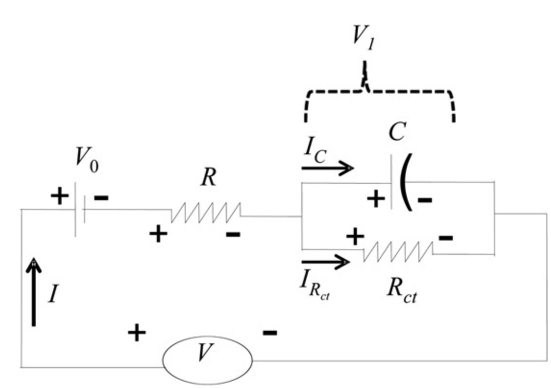

Fig. 1. The 1 pair RC equivalent circuit model.