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A parameter estimation method for a simplified electrochemical model for Li-ion batteries

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ABSTRACT

Traditional electrochemical algorithms are too complex for use in real-time battery management systems (BMSs). Determination of parameters and implementation of algorithms are the key challenges for electrochemical models for Li-ion batteries. This paper develops a simplified electrochemical model that incorporates open-circuit voltage, liquid-phase diffusion, reaction polarization, and ohmic polarization, and uses a fast operating test to identify all the parameters to solve these challenges. The model is then implemented and compared against experimental measurements. Validations of parameter estimation and charge/discharge behaviors indicate that the developed parameter estimation method for the electrochemical model is effective. With this model and parameter estimation technique, electrochemical model-based state of charge (SOC) estimation can be realized online and can provide accurate results.

1. Introduction

Li-ion batteries are popular because of their high working voltage, large energy density, low self-discharge rate, and no memory effect [1]. Mobile phone explosions, a typical battery failure example caused by material design defects or non-standard usage of Li-ion batteries, have drawn much attention to the battery safety issue. The safe and reliable control of these batteries requires the use of battery management systems (BMSs) that incorporate models to aid in state estimation and further prevent batteries from overcharging/overdischarging. The models that have been mainly used in the past include equivalent circuit models (ECMs) [1,2], as well as pseudo 2-dimensional (P2D) models and their derivatives [3–5]. ECMs consist of a few electronic components (e.g., resistance, capacitance, and inductance) of which the parameters can be easily obtained by impedance analysis, least squares fitting, or intelligent algorithms such as genetic algorithm (GA) and particle swarm optimization (PSO) [6,7]. ECMs are widely used in BMSs [2,8] because of the high calculational efficiency, high identifiability of parameters, and accurate state-of-charge (SOC) estimation with absolute estimation errors less than 3.2% and low calculational cost.

Compared with ECMs, electrochemical models, such as the P2D model and its derivatives [9–12], which are based on theories of porous electrodes and concentrated solutions, can be used to more accurately simulate not only battery terminal voltage but also internal states (e.g., overpotential, liquid-phase Li-ion concentration). It is believed that with the above advantages, electrochemical models can play a greater role in BMSs in the near future. However, electrochemical models are more complicated due to their complex partial differential equations. And it is quite hard to accurately estimate all the parameters for individual cells. Consequently, electrochemical models are more often used in battery-material-aided and optimal designs, as well as thermal analysis [13–16].

Owing to the limits of electrochemical models in practical applications, much research was conducted to simplify these models [17–19] based on the P2D model with the purpose of enhancing the computational efficiency through mathematical transformation or approximate solution. The simplified ideas generally include:

1.1. Neglect of the partial processes of the P2D model

Sabatier et al. [20] neglected the effect of the liquid-phase

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diffusion process on battery behavior when solving partial differential equations (PDEs). Also, they assumed that the liquid-phase potential difference was zero at the two collectors, and its value was constant at any time and at any position in the thickness direction of the electrode plates. The simulation results showed that the simulation relative error of the terminal voltage was below 1.5% at room temperature or above, and larger than 5% at −10 °C.

1.2. Approximate solution of solid-phase or liquid-phase diffusion process of the P2D model

The single particle (SP) model assumes that the chemical reaction at any position in the electrode is completely uniform, and thus all the particles in each electrode can be represented by one single particle. The solid-phase diffusion concentration distribution can then be described by a parabolic equation. The SP model has a relatively simple formation and fast simulation speed [17], however, the simulation error at higher C rates is relatively larger than that at lower C rates [21,22]. The simulation accuracy at high C rates can be improved with the addition of the term of liquid-phase concentration overpotential to the battery model [17,22,23]. Kemper et al. [24] adopted the same idea to find the approximate solution of lithium-ion concentration distribution, and the accuracy of this simplified model was similar to that of the P2D model.

1.3. Mathematical transformation

By reconfiguring the P2D model using orthogonal transformation or orthogonal configuration, PDEs were transformed to be simple ordinary differential equations (ODEs) and algebraic equations, which enhanced the computational efficiency [25–27]. The simulation time was reduced from 10 s to 1.5 s [25]. However, the value of the characteristic root used for orthogonal transformation needs to be calculated according to the model parameters of individual cells. Consequently, how to accurately estimate them becomes a key issue for this method.

Electrochemical battery models contain numerous physics-based parameters and need electrochemical measurements, which often require the dismantling of the cell into components to obtain the corresponding electrochemical parameters, such as liquid-phase conductivity [28–30]. Even when the cells are of the same materials manufactured by the same company, their charging/discharging behaviors are not the same. In order to accurately simulate battery behaviors or estimate battery SOC based on a certain accurate model, it is necessary to obtain the parameters for individual cells. A general method of model parameter estimation is thus needed for practical applications.

Masoudi et al. [31] estimated two and four parameters that were difficult to measure experimentally or approximate theoretically by homotopy optimization scheme. The parameters of the battery model were successfully identified with very little experimental data. However, increasing the number of estimated parameters resulted in a higher final objective function value. Rahman et al. [32] used a gradient-free optimization technique, namely, PSO algorithm to estimate the parameters for an electrochemical model. Although the identified model parameters were within reasonable accuracy as evidenced by the experimental validation results, the developed method identified only four specific parameters, which failed to represent all the electrochemical characteristics for individual cells. The above methods are not applicable for estimation of all the parameters that are changing with battery aging states.

The most frequently used method for nondestructive parameter estimation is GA [33–35]. As for parameter estimation, it can be used to simulate the processes of natural selection and mutation and determine the optimal set of parameters to minimize the errors between simulated and experimental data. However, given that the individual number in the population of GA is 100 and 26 parameters for the P2D model can be found by the 100^{th} iterative calculation, the computing time of the algorithm will last about 28 h [36], which is a great limit. The determination of model parameters for individual cells was still a challenge.

Our previous research developed a method to obtain all the parameters, but the operating condition test for the first step of the parameter estimation procedure took too much time (>50 h) [37]. Based on the literature, there is no simple and fast method to obtain all the parameters for the electrochemical model. To solve the challenges mentioned above, a modified parameter estimation method has been developed. The main contributions of this paper are as follows: (1) an electrochemical battery model is developed with simplified parameter estimation processes, (2) a test is developed for identifying all parameters in less than 8 h, and (3) the accuracy of the model and parameter estimation method is maintained at 1 C rates or below for individual cells. The rest of this paper is organized as follows: Section 2 develops the simplified electrometrical model; Section 3 introduces the designed operating conditions and parameter estimation method in detail; Section 4 discusses the necessary validations; and Section 5 presents the conclusions.

2. Electrochemical model

Although the SP model can be quickly simulated, there are still a number of electrochemical parameters that need to be determined for individual cells. Based on the SP model [18,21] and our previous research [37], a simplified model with regrouped and reduced parameters is adopted in this paper. The electrochemical model is developed based on the following assumptions: (1) the non-uniform reaction distribution effect inside the electrode is neglected, and the pore-wall flux density is approximately calculated by the operating current density; (2) the physical property is approximated by a single particle, and the electrolyte and solid-phase concentration distribution can be considered to approximately obey the parabolic profile; (3) the degrees of reaction polarization of both electrodes are the same, as well as the solid-phase diffusion process; and (4) the effect of battery internal temperature on model parameters is neglected at room temperature.

2.1. Open-circuit voltage

The solid-phase surface concentration of the particle directly determines the open-circuit voltage (OCV). Assuming that the battery internal temperature and ambient temperature are constant, the OCV can be described as [37].

$$E_{ocv}(t) = U_p\left[y_{surf}(t)\right] - U_n\left[x_{surf}(t)\right] \tag{1}$$

where U_p and U_n are the OCV of electrodes, which are known functions that can be obtained directly from the references, and y_{surf} and x_{surf} are the surface Li-ion concentrations of the particle of each electrode. When the current is zero, y_{surf} and x_{surf} are equal to the average Li-ion concentration, which can be described as

$$y_{avg}(t) = y_0 + I(t)t/Q_p \tag{2}$$

$$x_{avg}(t) = x_0 - I(t)t/Q_n \tag{3}$$

where I and t are constant current load and time; y_0 and x_0 are initial values of y_{avg} and x_{avg}, respectively; and Q_p and Q_n theoretically represent the capacities of effective active materials.