Journal of Power Sources xxx (2017) 1–15

Contents lists available at ScienceDirect

Journal of Power Sources

journal homepage: www.elsevier.com/locate/jpowsour

A physics-based fractional order model and state of energy estimation for lithium ion batteries. Part I: Model development and observability analysis

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HIGHLIGHTS

- A novel fractional order electrochemical battery model with physical meaning is proposed.
- The number of model parameters is lumped from 30 to 9.
- Variable solid-state diffusivity effect is taken into consideration in the model.
- Observability analysis of the fractional order model is conducted on two lithium ion batteries.

ARTICLE INFO

Article history:
Received 24 May 2017
Received in revised form
12 August 2017
Accepted 12 September 2017
Available online xxx

Keywords:
Physics-based
Lumped parameter
Fractional order model
Variable solid-state diffusivity
Battery modeling

ABSTRACT

The design of a lumped parameter battery model preserving physical meaning is especially desired by the automotive researchers and engineers due to the strong demand for battery system control, estimation, diagnosis and prognostics. In light of this, a novel simplified fractional order electrochemical model is developed for electric vehicle (EV) applications in this paper. In the model, a general fractional order transfer function is designed for the solid phase lithium ion diffusion approximation. The dynamic characteristics of the electrolyte concentration overpotential are approximated by a first-order resistance-capacitor transfer function in the electrolyte phase. The Ohmic resistances and electrochemical reaction kinetics resistance are simplified to a lumped Ohmic resistance parameter. Overall, the number of model parameters is reduced from 30 to 9, yet the accuracy of the model is still guaranteed. In order to address the dynamics of phase-change phenomenon in the active particle during charging and discharging, variable solid-state diffusivity is taken into consideration in the model. Also, the observability of the model is analyzed on two types of lithium ion batteries subsequently. Results show the fractional order model with variable solid-state diffusivity agrees very well with experimental data at various current input conditions and is suitable for electric vehicle applications.

1. Introduction

Nowadays, lithium ion batteries have drawn a vast amount of attention on the electric vehicle applications attributed to their high energy density, power density, and long cycle life [1]. In order to guarantee the safety, efficiency, and durability during the operation, an intelligent battery management system (BMS) is definitely required. In the battery management techniques, battery modeling is a fundamental issue for almost all the functions, such as the state of energy (SOE) estimation, the state of health (SOH) estimation, and the state of power (SOP) capability prediction. A simple yet accurate battery model that can capture the dynamics of the time-varying, nonlinear electrochemical system is especially desired.

Among the existing battery models, physics-based electrochemical models based on the first principles have shown the abilities to not only capture the internal dynamics such as the lithium ion diffusion, Ohmic effect, and electrochemical kinetics,

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http://dx.doi.org/10.1016/j.jpowsour.2017.09.049
0378-7753/

but also predict the terminal voltage response against the performance changes combined with battery aging process [2]. Particularly, the pseudo two-dimensional (P2D) model developed by Doyle et al. [3] and the single particle (SP) model designed by Guo et al. [4] have drawn a lot of attentions in the fields of energy storage system design and management. However, due to the complexity of the P2D model, and limitations of the SP model, they are not suitable for the electric vehicle online applications. To trade-off the capabilities and the shortcomings of these models, many middle-level models with acceptable accuracy and high computational speed are proposed to simplify the structure of the rigorous P2D model, for instance, the simplified multi-particle (SMP) models [2,5–8] and the extended single particle (ESP) models [9–13]. Considering the fact that the charging current and the average discharge current during electric vehicle operation can be regarded as low C-rate (<1 C-rate), the ESP model incorporating the electrolyte dynamics is more appropriate for the electric vehicle online applications.

In the reduced order models, some mathematical order reduction techniques have been proposed to further reduce the complexity of the PDE-based model. Subramanian et al. developed an efficient approximate approach for the lithium ion diffusion inside porous electrode using polynomial functions [14]. This technique is further used in the electrolyte concentration approximation inside electrodes and separator to reduce the computational complexity in many ESP models [5,9,15,16]. Forman et al. developed a reduced order model by deriving a family of Padé approximations technique from the partial differential equations (PDEs) that describe the spherical diffusion [17]. Result shows the simulation efficiency is significantly improved. Afterward, Marcicki et al. proposed a simplified extended single particle model based on this technique [18]. In the model, lithium ion diffusion dynamics in the solid phase and electrolyte are both approximated by the Padé approximations. Dao et al. developed a simplified lithium ion battery model based on the Galerkin projection method [19]. The number of equations that describe the concentration and potential distributions in the liquid phase is considerably reduced. Fan et al. extended the Galerkin's method to nonlinear PDEs and incorporated concentration dependent properties in the electrolyte diffusion dynamics in the extended single particle model for predicting the behavior of a lithium ion cell at the extreme conditions [12]. Sabatier et al. proposed a fractional order extended single particle model with a continuous form for the electric vehicle applications [13]. The paper describes that the fractional differentiation is able to describe the solid phase ion diffusion process with a small number of parameters and states, while the electrochemical variables can still describe the characteristics of the batteries with a simple structure and good accuracy.

However, there are several limitations of these methods. For example, there are always a large number of parameters to characterize the electrochemical and thermal properties of the battery in the integer order models. As a result, the parameter identification procedure becomes extremely challenging. Besides, in order to reach the desired accuracy, high order truncations and more states are usually necessary to characterize the lithium ion diffusion dynamics in the solid and liquid phases, which make the models not suitable for the control and estimation applications. For the fractional order model has been mentioned, it is difficult to convert the continuous form to a discrete form. As a result, the applications of the model are limited. Moreover, the phase change effect [20] is not taken into consideration in these models, which will produce significant errors in the varying operating conditions.

To this extent, an electrochemical model with fewer parameters and acceptable accuracy for the electric vehicle applications is still desired. In order to achieve this target, a physics-based fractional-order battery model with lumped parameters is proposed. The model is developed under the framework of an extended single particle model. Fractional-order differential and Laplace transformation method are applied to approximate the diffusion kinetics in the solid phase. Electrolyte diffusion overpotential is predicted by a first-order resistance-capacity equivalent circuit with only two lumped physical parameters. In order to fit the experimental data with different C-rates and charging/discharging profiles, phase change phenomenon represented by the variable solid-state diffusivity (VSSD) [21] is taken into account in the model. As a result, the proposed model is under a simple structure, yet with complete physical meanings. For the purpose of online state estimation, the observability of the model is analyzed with two chemistry lithium ion batteries. In order to verify the accuracy of the model, simulations and experiments are conducted on a $LiFePO_4$/graphite (LFP) battery and a $LiNiMnCoO_2$/graphite (NMC) battery. Results indicate that the proposed model shows almost no loss of accuracy compared with the original extended single-particle model. By taking the VSSD effect into consideration, the model describes the battery dynamics with high accuracy and robust. The model has the capability to be applied to the battery state online estimation applications.

The outline of this paper is as follows: Section 2 describes the development of the physics-based fractional-order model for lithium ion batteries. Section 3 presents the details about the model observability analysis. Subsequently, the simulation and experimental details are presented in Section 4. In Section 5, the accuracy of the new model is extensively verified based on the analysis of the simulation and the experimental results. Finally, some conclusions and the concluding remarks are provided in Section 6.

2. The physics-based model design

2.1. The extended single particle model

The extended single particle (ESP) model [10,12,22] is the starting point of the new physics-based fractional-order model. It follows the assumption that has already been used in the conventional single particle models that the electrochemical reaction along the x-dimension in each electrode is considered uniform. However, in order to improve the accuracy and expand the applicability of the model, the Ohmic effect and concentration distribution in the electrolyte phase are taken into consideration in the ESP model. This model can be characterized by a set of PDEs. The physical structure is described in Fig. 1, and the governing equations of the ESP model are listed in Table 1.

In the governing equations of the original extended single particle model, V_{cell} is the battery terminal voltage, and is expressed by the potential difference between the two current collectors. I_L is the applied load current on the cell with the current being defined to be positive for discharging and negative for charging. By substituting

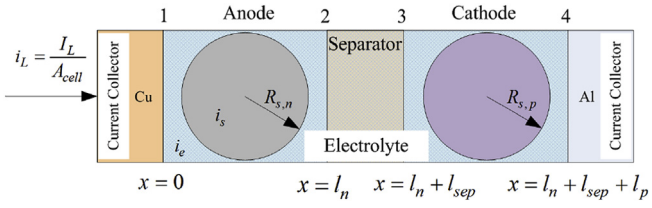

Fig. 1. Physical structure of the extended single particle model.