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A new extension of physics-based single particle model for higher charge–discharge rates

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HIGHLIGHTS

- The non-uniform reaction distribution effect is extended into single particle model.
- New model can accurately predict the pore wall flux distribution inside the electrode.
- New model can be used for higher charge–discharge rates up to 4C with a good accuracy.
- New model can be applied to the dynamic loads in EV and HEV applications.
- New model is a lumped-parameter analytical model with a good computational efficiency.

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ABSTRACT

A new approximate physics-based Lithium-ion cell model is developed by extending the descriptions of the non-uniform reaction distribution effect and the electrolyte concentration/potential distribution effect into single particle model, namely the extended single particle model. In this model, the simplification of the solid-phase diffusion is based on the existing approximate solution where a polynomial is used to approximate the concentration profile inside the particle. Diffusion in the electrolyte and the concentration polarization effect are simplified using the approximate solution based on parabolic profile approximation for the electrolyte concentration distribution. Especially, this model analyzes the mathematical description of the non-uniform reaction distribution effect inside the electrode, and an approximate solution of this effect is obtained by synthetically applying the volume average technique, approximated by the uniform reaction distribution situation, exponential profile approximation and the iterative calculation techniques. Thus the description of the non-uniform reaction distribution effect is successfully extended and the pore wall fluxes at the two current collector interfaces can be accurately predicted. Simulation results show that this model greatly improves the computational efficiency with little loss of accuracy.

1. Introduction

Lithium-ion batteries have been chosen as power suppliers for many systems due to their various advantages [1]. Obtaining an accurate mathematical model to describe the working and aging behaviors of the battery is the key to the research on battery reliability including issues such as battery health assessment, state of charge estimation, state of health estimation and remaining useful life prediction. Up to now, mathematical models of lithium-ion batteries' working dynamics have been investigated and used in the cell design, especially the pseudo 2D model (P2D), which is based on the theories of porous electrodes and concentrated solutions [2], and which describes the microcosmic behavior of the lithium ions inside the cell with the first principles-based derivation of the governing equations. These physics-based models have been used by various researchers to optimize the cell design and to study the effect of system parameters and thermal behavior [3]. Comparing to various experiential equivalent circuit models, the physics-based model can capture the electrochemical reaction dynamics and predict the batteries' behavior under any type of operating conditions with better accuracy.

Unfortunately, however, the rigorous physics-based model needs a high computational requirement due to its complex coupled nonlinear partial differential equations (PDEs). This characteristic limits its application such as real time control, on-line

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estimation and prediction embedded in a microprocessor. Therefore, it is important to simplify or reformulate the rigorous physics-based model, to explore analytical or approximate solutions for the model, and to seek the reduced order models to improve the computational efficiency. The goal of current work is to establish an approximate physics-based lithium-ion cell model which can be solvable real time with a normal computing requirement and can predict the behaviors of batteries with little loss of accuracy.

Many efforts have explored methodologies to update the original physics-based models in order to make them simpler and more computationally efficient like proper orthogonal decomposition (POD), Liapunov–Schmidt technique, the combination of coordinate transformation and orthogonal collocation, etc. [4–10]. These methods based on the mathematical techniques have their own limitations. For example POD-based techniques use the full numerical solution to fit a reduced set of eigen-values and nodes to get a meaningful solution with a reduced number of equations. However, this method requires rigorous numerical solutions to build the POD reduced-order models. Also, once the operating condition is changed, the boundary conditions are modified, or if the parameter values are adjusted significantly, the POD model needs to be reconstructed [8]. Subramanian et al. focus on the reformulation of the rigorous model toward real-time (milliseconds) simulation and parameter estimation, the reformulated model developed by them results in fewer differential algebraic equations (DAEs) which allows for easier and quicker computation compared with the traditional finite difference approach [7]. This method decreases the number of DAEs, but the complexity of each DAE increases, and the computational resources required for the system is still not ideal for the real-time simulation embedded in a microprocessor.

The single particle (SP) model is an existing approximate physics-based model. SP model considers all the reactions inside the electrode as distributed uniformly over all the particles, ignoring the variation of electrolyte concentration and potential with position and time. Due to this key assumption, SP model can be quickly simulated, but is only valid for limited conditions, such as low rates and thin electrodes [4]. As for dynamic operating conditions such as Federal Urban Driving Schedule and some conditions with high-rate charge–discharge pulses, SP model is no longer valid.

Analyzing current researches on this issue, the authors believe that various mathematical techniques can be applied here, but the ultimate cause of the complexity roots in the nature of the model. Based on this notion, this paper focuses on exploiting the essential chemical and physical processes which characterize the behavior of the cell, the dominating essential process being found to be non-uniform reaction distribution effect inside the porous electrode. In addition, this effect is discovered to be the key reason why SP model is not valid for higher charge–discharge rates. Then, this paper presents the mathematical description of the non-uniform reaction distribution effect and develops an approximate solution to compute this effect. Based on this approximate solution for the non-uniform reaction distribution effect and the approximate solution for the electrolyte concentration distribution proposed by the authors before [11], SP model is extended. This new approximate physics-based model is named as extended single particle (ESP) model. Compared with SP model, ESP model extends the descriptions of the non-uniform reaction distribution effect and the electrolyte concentration/potential distribution effect; therefore, it improves the model prediction quality. Meanwhile, ESP model is derived from the analysis of the essential physical processes, which guarantees the accuracy and the availability under various operating conditions. In addition, ESP model describes the dynamics with analytical functions, decreases the computational requirement fundamentally, and, therefore, it can provide higher computational efficiency.

The remainder of this paper is organized as follows. In Section 2, the rigorous physics-based model (i.e. the P2D model) and the SP model are analyzed. In Section 3, the non-uniform reaction distribution effect and its mathematical description are presented. Then, the approximate solution of the non-uniform reaction distribution effect is derived. Lastly, the computation of the overpotentials and the terminal voltage are presented. ESP model is established. The validation of ESP model and its comparison with SP and P2D models are discussed in Section 4, followed by conclusions presented in Section 5.

2. State-of-the-art physics-based modeling

2.1. The rigorous physics-based model

As illustrated in Fig. 1, the lithium-ion cell consists of a negative electrode, a micro porous separator, a positive electrode and two current collectors at the ends of the two electrodes. Typically, both electrodes consist of a grain structure of quasi-spheric active particles in a μm scale. The lithium ions are transported by diffusion inside the active particles along the r-axis, which is called solid-phase diffusion process. The concentrations of ions at the surface of the active particles determine the potentials at different positions of the electrodes, and the difference in the potentials at the two interfaces between the current collectors and the electrodes determines the terminal voltage of the cell. The interspaces between the particles are filled with electrolyte. The electrochemical reactions take place at the interfaces between the particles and the electrolyte according to the Butler–Volmer kinetics. The electrons are transported to the current collectors, and the lithium ions carrying the charge travel via diffusion and migration in the electrolyte through the separator to the other electrode along the x-axis, as shown in Fig. 1. A detailed discussion on the principle of lithium-ion cell can be found in Ref. [12] for instance.

The rigorous physics-based full order Li-ion cell model is proposed by Newman and Doyle et al. [13], which is named as P2D model. Based on the theories of porous electrodes and concentrated solutions, P2D model mainly consists of ten coupled nonlinear PDEs, which describe the solid-phase diffusion within the particles, the diffusion in the electrolyte, the balance of the solid-phase potential and the electrolyte potential occurring in the three regions in a lithium-ion cell. The model typically gives solutions to the electrolyte concentration, electrolyte potential, solid-phase potential, and solid-phase concentration in the negative and positive electrodes and the electrolyte concentration and electrolyte potential in the separator [14]. The details of P2D model are given in Tables 1 and 2, and the parameters used in this study are given in Table 3.

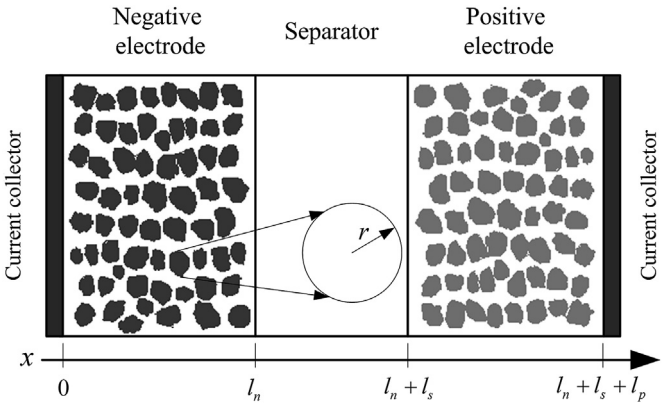

Fig. 1. Schematic representation of a lithium-ion dual intercalation cell [2].