



A simplified multi-particle model for lithium ion batteries via a predictor-corrector strategy and quasi-linearization



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ABSTRACT

The design of a simplified yet accurate physics-based battery model enables researchers to accelerate the processes of the battery design, aging analysis and remaining useful life prediction. In order to reduce the computational complexity of the Pseudo Two-Dimensional mathematical model without sacrificing the accuracy, this paper proposes a simplified multi-particle model via a predictor-corrector strategy and quasi-linearization. In this model, a predictor-corrector strategy is used for updating two internal states, especially used for solving the electrolyte concentration approximation to reduce the computational complexity and reserve a high accuracy of the approximation. Quasi-linearization is applied to the approximations of the Butler-Volmer kinetics equation and the pore wall flux distribution to predict the non-uniform electrochemical reaction effects without using any nonlinear iterative solver. Simulation and experimental results show that the isothermal model and the model coupled with thermal behavior are greatly improve the computational efficiency with almost no loss of accuracy.

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1. Introduction

Due to their high energy density, power density and long useful life, lithium ion batteries have been extensively used for energy storage devices in hybrid and electric vehicles (H/EVs), energy stations and mobile products. However, Lithium ion batteries must work within the safe and reliable operating conditions, which are restricted by temperature and voltage windows [1]. Advanced Battery Management Systems (BMSs) are therefore designed to monitor the states of the battery and regulate the energy storage device to work at an optimal mode [2]. The ability to simulate the dynamic behavior of lithium ion batteries using high-fidelity electrochemical-thermal models could provide very useful information for the design of BMS [3]. Electrochemical battery models based on first principles have shown the ability to accurately predict the internal concentration dynamics and the terminal voltage of the battery [4]. In particular, the Pseudo Two-Dimensional (P2D) model that follows the porous electrode theory [5] has been widely used

for modeling the dynamic response of lithium ion batteries at various operating conditions. The model is first proposed by Doyle et al. for predicting the performance of a lithium anode/solid polymer separator/insertion cathode cell [6]. Fuller et al. further applied the porous electrode theory to the modeling of a dual lithium ion insertion cell [7]. However, due to its significant computational complexity, the application of the rigorous P2D model is very limited especially for online applications [8].

In light of this, many mathematical order reduction methods have been proposed in literature to improve the computational efficiency of the P2D model. These methods include, but are not limited to, the Laplace transformation technique, the proper orthogonal decomposition, the polynomial approximation, the volume average technique, the Galerkin's method and the Padé approximation. The Laplace transformation technique has been applied to develop a low-order state variable battery model for hybrid electric vehicle applications [9]. The proper orthogonal decomposition technique has also been used to develop a simplified electrochemical-thermal model for a lithium ion battery [10]. Northrop et al. further developed a non-isothermal model for battery stacks based on orthogonal collocation and coordinate transformation [11]. The polynomial approximation combined with volume averaging method has been proposed by Subramanian to

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approximate the ion concentration distribution in the spherical particle [12]. In recent times, the Galerkin projection method has been applied as a model order reduction tool to approximate the diffusion partial differential equations (PDEs) describing the Lithium transport in the electrolyte solution. For instance, Dao et al. developed a simplified lithium ion battery model, and reduced the PDEs that describe the concentration and potential distributions in the liquid phase based on the Galerkin's method [13]. Fan et al. extended the Galerkin's method to nonlinear PDEs and incorporated concentration dependent properties in the electrolyte diffusion dynamics for predicting the behavior of a lithium ion cell at extreme conditions [14]. Padé approximation is another analytical model order reduction technique. The method was first applied by Forman to simplify the spherical diffusion equations in an electrochemical battery model [15]. Then, this method is also applied to approximate the diffusion PDEs in the electrolyte [16].

In addition to the mathematical order reduction methods, the physical structure simplification approaches are generally combined with the mathematical methods to obtain the simplified models. Such as the single particle (SP) model [17], the extended single particle (ESP) models, and the multi-particle (MP) models.

For the multi-particle models, Smith et al. developed a simplified electrochemical model based on the Laplace transformation under the assumptions of linear behaviors and the reaction current decoupled from the electrolyte concentration [9]. However, due to the approximate Butler-Volmer kinetics equation only valid for low reaction overpotential, the robustness of the model cannot be guaranteed. Northrop et al. proposed an electrochemical-thermal coupled multi-particle model based on the orthogonal collocation technique [11]. Lithium ion concentrations and potentials in the solid and liquid phases are approximated by a combination of polynomials and cosine trial functions. However, due to the fact that the method still relies on the nonlinear iterative solvers, the model is relatively complex and unsuitable for online applications. Luo et al. developed a three-particle model without using any nonlinear iterative solver [18]. In this model, the liquid phase concentration distribution is approximated by quadratic polynomials, the non-uniform distribution of electrochemical reaction pore wall flux is addressed under the assumptions that the current density distribution can be linearized, and the distributed pore wall fluxes in the Butler-Volmer equations can be partly replaced by the average value. As a result, model's solving complexity is seriously reduced. Later, Han et al. improved the model by applying a new solid phase diffusion approximate method [19]. Then, they developed a multi-particle model using four representative particles to obtain higher simulation accuracy [20].

In order to reduce the computational complexity of the Pseudo Two-Dimensional mathematical model, improve the approximate accuracy of the electrolyte concentration by quadratic polynomials, and calculate the non-uniform reaction behavior in an efficient and accurate way without using nonlinear iterative solver, a simplified multi-particle (SMP) model via a predictor-corrector strategy and quasi-linearization is proposed. In this model, the predictor-corrector strategy is used to simplify the computation complexity of differential algebraic equations by predicted the two internal states in advance and updated the value afterward. Quasi-linearization is applied to the approximations of the Butler-Volmer kinetics equation and the electrochemical reaction pore wall flux distribution. As a result, the computational time consumption of the SMP model is reduced by two orders of magnitude with almost no loss of accuracy. The SMP model is then coupled with a two-state thermal model by incorporating the temperature dependence of some electrochemical variables, and further validated against experimental data using various current input profiles at a wide range of temperature conditions.

The remainder of this paper is organized as follows. In the next section, the model simplification methods are introduced. In Section 3, the details about the model development, including the approximated solutions of the distribution of the electrolyte concentration across the cell length, the non-uniform electrochemical reaction and the solid phase diffusion are described, and followed by the description of solutions of the terminal voltage and the thermal behavior. Section 4 introduces the details about simulations and experiments. Finally, in Section 5, the efficiency and accuracy of the isothermal SMP model and the thermal SMP model are verified exhaustively.

2. Method description

In this section, the rigorous P2D model which is the background of this work is described firstly, and the physical structure of the SMP model is presented subsequently. Then, the details about the predictor-corrector strategy and the quasi-linearization method are discussed.

2.1. The rigorous P2D model

Newman's physics-based P2D model describes the porous electrode electrochemical system with pseudo two dimensions named x dimension and r dimension. The x dimension is defined along the thickness of the electrodes and the separator, where the mass transfer and charge transfer processes occur in the liquid phase and the electrochemical reactions take place at the interfaces between the active particles and the electrolyte. The r dimension is the second pseudo dimension, which refers to the radial direction of active particles in each electrode. Mass transfer takes place along the r dimension inside each active particle. Mass transfer, charge transfer, and electrochemical kinetics are described by a set of coupled PDEs and boundary conditions according to Fick's law and Ohm's law and Butler-Volmer kinetics, respectively. A schematic of the rigorous isothermal P2D model is illustrated in Fig. 1 and the equations used in the model are listed Table 1.

The relationship of the main governing equations is shown in Fig. 2. It can be observed that the Butler-Volmer kinetics equation and potential balance equation are the bridges to connect the various kinds of internal states and variables. Besides, most of the internal potentials, concentrations are related to the pore wall flux j .

2.2. Physical structure of the SMP model

The physical structure of the SMP model is presented in Fig. 3. Four representative particles are used in each electrode, and all the spacing distances between adjacent particles are the same. To mark the representative particle exclusively, subscripts i and m are used to denote the particle in the electrode i ($i = n$ or p), and the position m is $x_i = m$. In order to simplify the expression of equations in the following discussion, the abscissa along the thickness of the electrodes and the separator is normalized for each region:

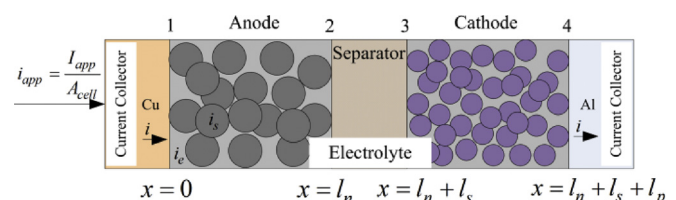


Fig. 1. Schematic of the P2D model.

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