



## Extension of physics-based single particle model for higher charge–discharge rates

Saeed Khaleghi Rahimian, Sean Rayman, Ralph E. White\*

Department of Chemical Engineering, University of South Carolina, Swearingen Engineering Center, 301 Main Street, Columbia, SC 29208, USA

### HIGHLIGHTS

- We extended the physics-based single particle model for higher charge–discharge rates up to 5C.
- The improved single particle (ISP) model was compared with full-order pseudo two dimensional (P2D) model.
- The ISP model could predict the P2D model results up to 5C while the simulation time was reduced by a factor about 5.

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### ABSTRACT

An isothermal reduced order physics-based Li ion battery model is developed by incorporating solution phase charge and material balances into single particle (SP) model. Li ion concentration and potential profiles in electrolyte phase are approximated by polynomial functions. A cubic polynomial is used for electrolyte concentration and potential inside electrodes, while separator liquid phase potential and concentration are estimated by parabolas. Diffusion inside solid particles is also simplified using an approximate solution based on analytical solution for the solid concentration. Applying the aforementioned reduction techniques decreases the degree of freedom of full order model by more than 100, while the cell voltage relative error of proposed model is less than 1% at different charge–discharge rates up to 5C.

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### 1. Introduction

Due to high energy density of Li ion cells with respect to other kind of batteries (three to four times of Lead acid and Nickel cadmium and twice of Nickel metal hydride) rechargeable Li ion batteries are used extensively in different markets and applications ranging from consumer electronics (e.g. laptops, cell phones) to automotive (e.g. Hybrid Electrical Vehicles) and aerospace (e.g. satellite power sources) [1]. However, Li ion cells are unforgiving if operated outside of tight safe operating area [2]. In order to guarantee safe charge–discharge operations of a Li ion cell, most battery systems consist of a battery management system (BMS) to control charging–discharging [2]. The core of a BMS is a battery model that finds the relationship between currents and voltages measured at terminals [3].

Li ion cell models are categorized into two main groups. The first type is empirical approaches that rely on capacitor–resistor networks such as equivalent circuit model (ECM) [4]. Due to

simplicity and low computational burden, empirical models have been used widely in online implementations [4]. However, physical insight of the cell is neglected, resulting in prediction errors when used over a broad operating region [3]. The second type includes physics-based models like Pseudo Two Dimensional (P2D) [5,6] where distribution of essential states inside the cell (e.g. solid and liquid phase Li ion concentrations and potentials) along cell sandwich is obtained by solving material and charge balances. Thus, physics-based models can be applied in different operation modes and also capacity fade phenomena are included in the model without any difficulty [7]. Nevertheless, the complexity and computational cost restricts the use of these models for onboard applications.

In order to make rigorous physics-based models more computationally efficient, various reduced models have been proposed [8,9,11–16]. The most simplified model developed by Atlung et al. [8] and later extended by Haran et al. [9] is single particle (SP) model where each electrode is represented by a single spherical particle and Li ion concentration and potential inside electrolyte phase are neglected. Although the SP model computation time is comparable with empirical ECM [10], it is limited for low rate operations (e.g.  $\leq 1.0C$ ) [11]. V.R. Subramanian et al. approximated

\* Corresponding author. Tel.: +1 803 777 3270; fax: +1 803 777 0973.  
 E-mail address: [white@cec.sc.edu](mailto:white@cec.sc.edu) (R.E. White).

microscale diffusion equation in a spherical electrode particle based on polynomial profile [12]. They coupled the approximated solution with governing equations for the macroscale to predict the cell voltage as well as electrolyte concentration. Although it was shown that the number of differential algebraic equations (DAEs) reduced by order of 10, the resulting DAE is still large. In the next work by V.R. Subramanian et al., the full order DAE system was reduced further by approximating electrolyte concentrations inside electrodes and separator using polynomial functions [13]. They showed that approximated solutions for different quantities such as electrolyte concentrations and potential agreed well with full order profiles under 1C discharge rate. However, uniform electrolyte current densities were assumed in each electrode. As we will show later in this paper, this assumption is true only for low charge–discharge rates.

A physics-based reduced-order model was proposed by L. Cai and R.E. White based on proper orthogonal decomposition [14]. There were 50 equations in the reduced model (compared to 14,580 equations in high-order dimensional discrete model) that saved the computational time of the rigorous model by a factor about 7. Smith et al. developed a low order electrochemical model under assumptions of quasi-linear behavior (i.e., constant electrolyte properties and linearized Butler Volmer (BV) kinetics) and reaction current decoupled from electrolyte concentration [15]. They reduced a full order impedance transfer matrix to a 12th order state variable model that predicted the cell voltage to within 1% for pulse and constant current profiles at rates up to 50 C. However, the validity of the reduced model was lost when the electrolyte became depleted ( $C_e < 0.15 C_{e,0}$ ). Smith et al.'s model was further simplified by D. Di Domenico et al. assuming a constant electrolyte concentration and neglecting the solid concentration distribution along each electrode (resulting in constant current density in BV kinetics) [16]. Their reduced model is similar but higher order than SP model. Recently, T.-S. Dao et al. presented a simplified model using a volume average technique for solid phase concentration and Galerkin's approximation for electrolyte phase concentration and potential [17]. The current density was also assumed to be constant along each electrode. They obtained a set of  $2N + 10$  ( $N$  is number of node points for Galerkin's approximation) DAEs where  $N = 4$  resulted a reduced model in good agreement with rigorous model for 1 C discharge rate.

In this paper, the isothermal SP model without capacity fade [10] is improved to predict the cell voltage at higher charge–discharge rates up to 5C where the Li ion concentration in electrolyte phase (near to cathode/anode current collector during discharge/charge) depletes near to zero ( $C_e \sim 0.001 C_{e,0}$ ). Distribution of electrolyte concentration and potential along electrodes and separator are incorporated with the SP model equations by using polynomial approximations for the electrolyte concentrations and potentials. The new efficient reduced model consists of only 13 DAEs where cubic and quadratic polynomials are applied for solution phase transport and conduction in electrodes and separator respectively. As mentioned in Ref. [13] the proposed method is slightly different from standard collocation procedures because governing equations are also volume averaged to find polynomial coefficients. In order to enhance the accuracy of solid phase surface concentration, the volume average technique used in Ref. [10] is replaced by an approximated solution developed by M. Guo and R.E. White [18]. Comparison of constant current charge–discharge data obtained by full order P2D with improved single particle (ISP) model shows that there is a good agreement between the reduced and the rigorous models while the computation time of the new model is greatly less than the full model (a factor of 5).

## 2. Physics-based model

In this section, the assumptions and governing equations of full order P2D model for Li ion concentrations and potentials inside solid and solution phases are first presented. Then, the underlying assumptions and restrictions of simplified SP model are addressed. Finally, the SP model is extended to higher rates by coupling the electrolyte charge and material balances to solid phase diffusion. In all models, the BV expression is used to predict the rates of Li ions intercalation/deintercalation reactions.

### 2.1. Pseudo two dimensional model

Fig. 1 presents a schematic of a Li ion cell composing of two porous electrodes (solid matrix inside an electrolyte solution) and a separator (electrolyte solution). Most physics-based full order Li-ion cell models rely on the rigorous model of Doyle et al. [5] and T.F. Fuller et al. [6]. Transport of Li ions in the electrolyte phase is considered only in  $x$  direction (i.e. from the cathode through the separator into the anode during charge and vice versa during discharge) since the lengths of the cell in  $y$  and  $z$  directions are much greater than the cell thickness ( $>1000$ ). In the solid phase Li ions are assumed to react at the surface and move only in  $r$  direction. Thus, simulation of the cell can be regarded as a packed bed reactor model. In addition to material balances of Li ions inside liquid and solid phases, charge balances for each phase are required in order to obtain the potential distribution across the cell. Hence, there are four quantities describing the cell electrochemical behavior including solid and electrolyte Li ion concentration and potential. These variables are coupled by a charge-transfer kinetic resistance at the particle surface. In the following, governing equations and assumptions are presented.

#### 2.1.1. Solid concentration

Li ions travel inside spherical solid particles by diffusion process given by the Fick's second law:

$$\frac{\partial C_{s,i}}{\partial t} = \frac{D_{s,i}}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial C_{s,i}}{\partial r} \right) \quad i = p, n \quad (1a)$$

with the initial and boundary conditions:

$$\begin{aligned} C_{s,i}(r, t = 0) &= C_{s,i,0} \quad 0 \leq r \leq R_i \\ \frac{\partial C_{s,i}}{\partial r} \Big|_{r=0} &= 0 \quad t > 0 \\ -D_{s,i} \frac{\partial C_{s,i}}{\partial r} \Big|_{r=R_i} &= J_i(x, t) \end{aligned} \quad (1b)$$

where  $J_i$  is the pore wall flux at the interface between electrolyte and particles.  $D_{s,i}$ , the diffusion coefficient of Li ions inside solid particles, is a constant.

#### 2.1.2. Solid potential

The potential distribution in the solid phase of each electrode is obtained by Ohm's law together with the boundary conditions at two ends of the cell and the electrode/separator interfaces:

$$\begin{aligned} \sigma_{\text{eff},i} \frac{\partial^2 \phi_i}{\partial x^2} &= a_i F J_i(x, t) \quad i = p, n \\ \text{Cathode :} \quad -\sigma_{\text{eff},p} \frac{\partial \phi_p}{\partial x} \Big|_{x=0} &= I_{\text{app}} \quad \frac{\partial \phi_p}{\partial x} \Big|_{x=L_p} = 0 \\ \text{Anode :} \quad \frac{\partial \phi_n}{\partial x} \Big|_{x=L_p+L_s} &= 0 \quad \phi_n \Big|_{x=L} = 0 \end{aligned} \quad (2)$$

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