



# Simplification and order reduction of lithium-ion battery model based on porous-electrode theory

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## ABSTRACT

In this paper, effective and systematic steps in the mathematical simplification and reduction of physics-based lithium-ion (Li-ion) battery models to improve computational efficiency will be presented. The battery model used for simulations is an isothermal model proposed by Newman and Tiedemann [1] and Doyle et al. [2] which incorporates the concentrated solution theory, the porous electrode theory, and the variations in electronic/ionic conductivities and diffusivities. The simplified model is formulated by exploiting the nature of the model and the structure of the governing equations. Simulations show that the simplified model can reduce computational time significantly while still retaining the accuracy compared to the full-order rigorous model.

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## 1. Introduction

Due to its advantages such as light weight, low self-discharge rate, and high specific energy, Li-ion batteries have become one of the most popular types of battery in various applications such as portable electronics or electric vehicles. The charge–discharge rate for the lithium-ion battery can vary from 1 to 2C (1C is a discharge rate at nominal battery capacity) to a very fast pulse discharge up to 40–50C over a short time period on the order of 10–20s [3]. In the automotive field, Li-ion batteries are the core of the energy source and storage in new plug-in hybrid electric vehicles (PHEVs) as well as considered in many second generation hybrid electric vehicles (HEVs). The performances of Li-ion batteries play an important role in vehicle energy management. Hence, battery modeling is one of the most important tasks for electric and hybrid vehicle control. This requires a model that can simulate in real-time in order to make them compatible with estimation algorithms embedded in on-board electronic control units. For example, a battery management system in an HEV has to estimate the battery state of charge (SOC) [4–6] in real-time in order control the electrical power com-

ing in and out of the battery as well as to prevent the battery pack from excessive heating.

A full-order battery model, however, is not suitable for real-time applications as it usually takes hours to spatially discretize the system via a finite difference method and solve the system numerically as a collective of differential equations in terms of the field variables. Therefore, a fast and reliable approximate model is required. For automotive applications, a simplified battery model has to be carried out at a good accuracy while ensuring the maximum computational cost reduction to achieve an efficient system management. Subramanian et al. [7–9] developed a real-time simulation model using a combination of perturbation techniques, volume averaging, and intuition-based simplifications. Although they reported that the computational time for their real-time simulation model for a single process was around 100ms, to derive the lower-order model by using this method one needs to carry out preprocessing and have *a priori* knowledge of the behavior of the system under different conditions, which makes their method less flexible than desired. Other methods, including the Chebyshev polynomial method [10,11], residue grouping method [12], proper orthogonal decomposition method [13], and Padé approximation [14] have also been used to derive reduced-order models for Li-ion batteries.

In the methods using Chebyshev polynomials, the state variables are approximated by linear combinations of several Chebyshev polynomials, and then an approximate model is projected onto a subspace formed by these orthogonal Chebyshev polynomials to

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## Nomenclature

$a_k$	specific surface area of electrode $k$ ( $k = p, n$ ) ( $\text{m}^2 \text{m}^{-3}$ )
$\text{brugg}_k$	Bruggman coefficient of region $k$ ( $k = p, n$ )
$c_{e,\text{apprx}}$	assumed solution for electrolyte-phase concentration of $\text{Li}^+$ ( $\text{mol m}^{-3}$ )
$c_{e,k}$	electrolyte concentration in region $k$ ( $\text{mol m}^{-3}$ )
$c_{e,k,0}$	initial electrolyte concentration in region $k$ ( $\text{mol m}^{-3}$ )
$c_{s,k}$	concentration of $\text{Li}^+$ ions in the intercalation particle of electrode $k$ ( $\text{mol m}^{-3}$ )
$c_{s,k,0}$	initial concentration of $\text{Li}^+$ ions in the intercalation particle of electrode $k$ ( $\text{mol m}^{-3}$ )
$\bar{c}_{s,k}$	average concentration of $\text{Li}^+$ ions in the intercalation particle of electrode $k$ ( $\text{mol m}^{-3}$ )
$c_{s,k,\text{surf}}$	concentration of $\text{Li}^+$ ions on the surface of intercalation particle of electrode $k$ ( $\text{mol m}^{-3}$ )
$D$	electrolyte diffusion coefficient ( $\text{m}^2 \text{s}$ )
$D_{s,k}$	$\text{Li}^+$ ion diffusion coefficient in the intercalation particle of electrode $k$ ( $\text{m}^2 \text{s}$ )
$F$	Faraday's constant ( $\text{C mol}^{-1}$ )
$I$	applied current density ( $\text{A m}^{-2}$ )
$J_k$	wall-flux of $\text{Li}^+$ on the intercalation particle of electrode $k$ ( $\text{mol m}^{-2} \text{s}$ )
$K_k$	intercalation/deintercalation reaction-rate constant of electrode $k$ ( $\text{mol mol}^{-1} \text{m}^3$ )
$L$	total thickness of cathode-separator-anode (m)
$L_k$	thickness of region $k$ (m)
$n$	negative electrode
$N$	number of node points for Galerkin's approximation
$p$	positive electrode
$\bar{q}_{s,k}$	volume-averaged concentration flux of $\text{Li}^+$ ions in the intercalation particle of electrode $k$ ( $\text{mol m}^{-3} \text{s}^{-1}$ )
$r$	radial coordinate (m)
$R$	universal gas constant
$R_c$	residual function for concentration of $\text{Li}^+$ in electrolyte-phase
$R_{s,k}$	radius of intercalation of electrode $k$ (m)
$R_\Phi$	residual function for electrical potential in electrolyte-phase
$s$	separator
$t_+$	$\text{Li}^+$ transference number in the electrolyte
$T$	absolute temperature (K)
$U_k$	open-circuit potential of electrode $k$ (V)
$x$	spatial coordinate (m)

### Greek letters

$\epsilon_k$	volume fraction of region $k$
$\epsilon_{f,k}$	volume fraction of fillers in region $k$
$\eta_i$	time-dependent variable of $i$ 'th basis function for electrolyte-phase concentration (s)
$\theta_k$	dimensionless concentration of $\text{Li}^+$ ions in the intercalation particle of electrode $k$ ( $\theta_k = c_{s,k}/c_{s,k,\text{max}}$ )
$\kappa$	ionic conductivity of electrolyte ( $\text{S m}^{-1}$ )
$\kappa_{\text{eff},k}$	effective ionic conductivity of the electrolyte in region $k$ ( $\text{S m}^{-1}$ )
$\rho_i$	time-dependent variable of $i$ 'th basis function for electrolyte-phase potential (s)
$\sigma_k$	electronic conductivity of solid phase of electrode $k$ ( $\text{S m}^{-1}$ )
$\sigma_{\text{eff},k}$	effective electronic conductivity of solid phase of electrode $k$ ( $\text{S m}^{-1}$ )

$\Phi_e$	electrolyte-phase potential (V)
$\Phi_{e,\text{apprx}}$	assumed solution for electrolyte-phase potential (V)
$\Phi_s$	solid-phase potential (V)

form a reduced-order model, which can then be solved for the unknown coefficients in the truncated expressions. Smith et al. [15] developed a control-oriented one-dimensional (1D) electrochemical model by using the method of residue grouping. Their transfer functions are represented by a truncated series of grouped residues with similar eigenvalues. Cai and White [13] proposed an approach based on proper orthogonal decomposition for tackling the problem by using two steps of approximation: partial differential equation (PDE) discretization and truncation of the number of orthogonal modes. Cai and White showed that the order-reduced model simulated seven times faster than the full-order model for a similar level of accuracy. The electrode-averaging method was used by Speltino et al. [16] who made several simplifications such as neglecting solid concentration distribution and assuming constant electrolyte concentration. As a result, their model simulated fast, but with a heavy loss of information.

In this paper, an efficient method for reducing the order of Li-ion battery models using  $\text{LiCoO}_2$  and  $\text{LiC}_6$  electrodes derived from the porous electrode theory will be discussed. The simplified model in this paper uses the volume-average integration proposed in Subramanian et al. [7], Wang et al. [17], and Gu et al. [18] for approximating the  $\text{Li}^+$  concentration in the solid phase in the electrode material. For modeling the  $\text{Li}^+$  concentration and electrical potential in the electrolyte phase, Galerkin's approximation will be used under the assumption of a galvanostatic discharge condition. Maple 14 was used to generate the mathematical model and perform many of the model reductions and simplifications. The paper begins with a brief overview of the intercalated Li-ion models and its mathematical governing equations, followed by a discussion on the use of the volume-average and Galerkin's method to simplify the model. Simulation results and a comparison between the simplified and full-order models will also be provided to demonstrate the effectiveness of the proposed battery model reduction method.

## 2. Lithium-ion battery model based on porous-electrode theory

### 2.1. Overview

Most of the current rigorous Li-ion battery models are derived from the porous electrode and concentrated solution theories proposed by Newman and Tiedemann [1] and Doyle et al. [2] which mathematically describe charge/discharge and species transport in the solid and electrolyte phases across a simplified 1D spatial cell structure. This 1D model of a Li-ion battery considers dynamics along only one axis (the horizontal  $x$ -axis) and neglects the dynamics along the remaining two axes ( $y$ -axis and  $z$ -axis) [1,2,19–23]. This approximation is applicable to most cell structures as the length scale of a typical Li-ion cell along the  $x$ -axis is on the order of 100  $\mu\text{m}$ , whereas the length scale for the remaining two axes is on the order of 100,000  $\mu\text{m}$  or more [24].

There are four main components in a typical Li-ion cell as shown in Fig. 1: the negative composite electrode connected to the negative terminal of the cell, the positive composite electrode connected to the positive terminal of the cell, the separator, and the electrolyte. The negative electrode contains lithium stored in the lattice sites made from graphite, usually in the form of  $\text{Li}_x\text{C}_6$ . The positive electrode can have various chemistries, usually a metal oxide or an inter-metallic oxide such as  $\text{Li}_x\text{Mn}_2\text{O}_4$  or  $\text{Li}_y\text{CoO}_2$ . During

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