



Reduced order model for a lithium ion cell with uniform reaction rate approximation

V. Senthil Kumar*

India Science Lab, General Motors Global R & D, Creator Building, International Technology Park, Whitefield Road, Bangalore 560066, India

HIGHLIGHTS

- ▶ Physics based reduced order model for lithium ion cells.
- ▶ Model reduction based on volume averaging and profile based approximations.
- ▶ Amenable for battery management system algorithms, detailed parameter estimation etc.

ARTICLE INFO

Article history:

Received 16 June 2012
 Received in revised form
 3 September 2012
 Accepted 5 September 2012
 Available online 10 September 2012

Keywords:

Lithium ion cell
 Reduced order model
 Battery management system
 Volume averaging
 Profile based approximations

ABSTRACT

The detailed isothermal electrochemical model for a lithium ion cell comprises of 10 coupled partial differential equations (PDEs). It is computationally intensive to use this model for detailed parameter estimation, battery packs, battery management system algorithms, calendar or cycle life predictions etc. This work describes a reduced order model framework, which reduces the detailed model PDEs, to a manageable set of ordinary differential equations (ODEs), which can be used for the above applications. Volume averaging PDEs yield ODEs. Hence volume averaging is the basic method used for model reduction. The gradient or profile information lost on volume averaging is recovered through profile based approximations. For the lowest order reduced order model (ROM), a uniform reaction rate, quadratic electrolyte concentrations and quartic solid phase concentrations are assumed. In this ROM only 5 linear ODEs are solved, and the rest are nonlinear algebraic evaluations. When compared with the detailed electrochemical model of a lithium ion cell, this ROM gives negligible error at nominal currents and a maximum error of about 3% at high currents, for a typical commercial cell.

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1. Introduction

Consider a lithium ion cell discharging current through a load, as in Fig. 1. Say the negative electrode is graphite. When the cell is in charged state lithium exists as the lithium carbide (LiC_6) in the negative electrode. During discharge LiC_6 breaks down releasing Li^+ ions into the electrolyte, and the electrons to the collector (through the solid conducting matrix of the negative electrode particles), which eventually flow into the external circuit. The electrons travel from the negative electrode to the positive electrode through the external circuit, while the Li^+ ions travel in the electrolyte from the negative electrode to the positive electrode. Say the positive electrode is some lithium metal oxide. The electrons (flowing through the external circuit) and Li^+ ions (diffusing through the electrolyte) combine on the surface of the positive

electrode particles to form neutral Li species, which then intercalate into lithium metal oxide. The intercalation reactions occurring during the discharge are reversible and the reverse reactions occur during charge.

Electrodes contain a solid phase comprising of active materials (and other additives), and a liquid electrolyte phase. Separator typically has some solid polymeric membrane and a liquid electrolyte phase. Neglecting the solid additives and inert polymeric membranes, there are totally five phases: active materials in the two electrodes and electrolyte phase in the three regions. For an isothermal operation of a single cell, drawing the mass and charge balances for these five phases, the detailed electrochemical model comprises of ten coupled partial differential equations (PDEs), Refs. [1,2]. It is computationally intensive (or often impossible) to use this detailed electrochemical model for

- *Battery packs*, since they have hundreds of single cells in series – parallel configurations.
- *Battery management system algorithms*, since on-board computational capabilities are nominal. Currently electrical

* Present address: Samsung Advanced Institute of Technology – India, SISO Private Ltd., Bangalore 560 093, India. Tel.: +91 80 4181 9999; fax: +91 80 4181 9000.

E-mail address: senthil.v.kumar@gmail.com.

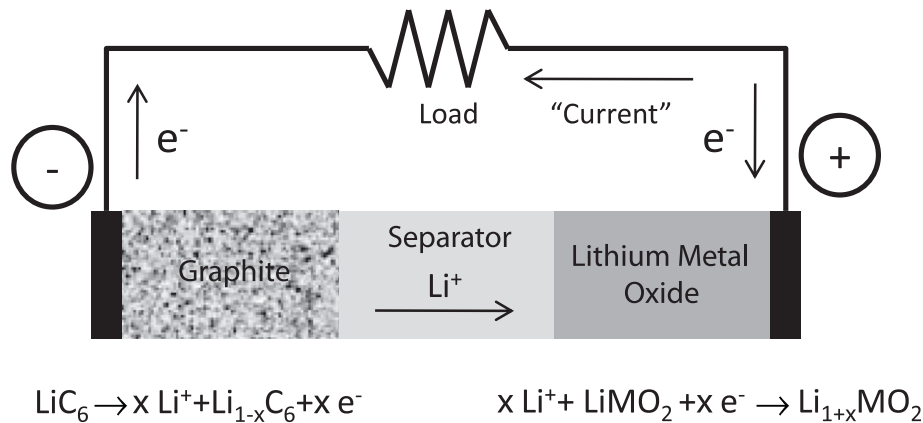


Fig. 1. Discharge of a lithium ion cell.

circuit based models are used for battery management systems, due to their minimal mathematical complexity (first order ordinary differential equations based mathematical structure).

- *Calendar or cycle life predictions*, since the model needs to predict cell behavior for real time periods as long as a few months.
- *Detailed parameters estimation*, since systematic optimization of parameters embedded within ten coupled PDEs is formidable.
- *inclusion of complex degradation mechanisms*, since they add to the numerical stiffness.

The aim of this work is to develop a reduced order model framework, which reduces the detailed electrochemical model comprising of ten PDEs for the isothermal behavior of a single cell, to a manageable set of ordinary differential equations (ODEs), which can be used for the above applications. It is preferred that the reduced order model framework has the following mathematical properties:

- It has minimal computational requirements so that it can be implemented in on-board battery management systems. It is numerically stable and easily optimized during parameter estimations. These properties are ensured if the model equations are first order ODEs (linear or nonlinear, could be coupled). Volume averaging PDEs yield ODEs. Hence volume averaging is the basic methodology used in this work for physics based model reduction.
- The model predictions should be grid or system size independent. For example, one could discretize the governing PDEs, with say 10 or 20 nodes for each electrode or separator region, as in the Method of lines. Model predictions in such a scenario will often be grid size dependent, and will give higher errors if the electrode or separator regions get thicker. Thus, ODEs should be solved not for the discretized original PDEs, but for physically relevant internal variables, which parameterize the internal field profiles. For example, in profile based approximations, interfacial concentrations are solved, and the concentration profiles in the individual regions are expressed in terms of these interfacial concentrations. A brief literature review of profile based approximations is given below.
- It has systematic mathematical approximations rather than phenomenological approximations. For example, a single particle model Ref. [3] neglects electrolyte potential and electrolyte concentration variations. Hence, a single particle model

cannot work at high currents. If a reduced order model is, however, based on systematic mathematical approximations, relaxing those approximations one can derive higher order models, which work at all scenarios. For example, the current work approximates the local reaction rates in an electrode to be the volume average reaction rates. This approximation can be relaxed to allow spatial variation of reaction rates, will be reported in future.

Solution of partial differential equations through profile based approximations was developed by Pohlhausen (1921) for a problem in laminar boundary layer theory, Ref. [4, p. 41]. He used a quartic velocity profile to satisfy the momentum integral equation and the relevant boundary conditions. Gluckauf (1955) [5] used a parabolic concentration profile to describe the diffusion in a sphere, in the context of chromatography. Ref. [6] used the parabolic approximation for diffusion in a sphere to describe the kinetics of adsorption in a fixed bed of spheres. Refs. [7,8], for example, describe higher order polynomial approximations for diffusion in a sphere. Ref. [9] extended these methods to reaction and diffusion in spherical and slab geometries. Ref. [10] reports parabolic and quartic profile based approximations for diffusion in active material spheres in the electrodes of a lithium ion cell. This work extends the profile based approximation for the rectangular electrolyte concentration fields in electrode and separator regions as well.

Sections 2–5 present the detailed field equations and derive the reduced order equations for solid phase current balances, electrolyte phase mass balances, total current balances and solid phase mass balances, respectively. These equations are the core conservation equations governing the isothermal behavior of a single cell. The results from these sections feed into the Butler–Volmer kinetics, in Section 6, for the electrochemical reactions happening on the surface of the active material spheres in the electrode regions. The reduced order model is derived across Sections 2–6. Often the derivation sequence is different from the computational sequence. Hence, the reduced order model results are collated in an algorithmic order in Section 7. The cell voltage predictions by the reduced order model are compared with those from the detailed electrochemical model for constant current and pulse protocols in Section 8.

2. Solid phase current balance equations

2.1. Field equations

Ohm's law is typically written for a one-dimensional conductor as $I = V/R$, where I is the current in Amperes (A), V the voltage in

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