Journal of Power Sources 286 (2015) 510–525

Contents lists available at ScienceDirect

Journal of Power Sources

journal homepage: www.elsevier.com/locate/jpowsour

Simplification of pseudo two dimensional battery model using dynamic profile of lithium concentration

Paulo Kemper [a], Shengbo Eben Li [b], Dongsuk Kum [a, *]

[a] The Cho Chun Shik Graduate School for Green Transportation, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 305-701, South Korea
[b] Department of Automotive Engineering, Tsinghua University, Beijing 100084, Peoples Republic of China

HIGHLIGHTS

- Developed a simplified P2D model that predicts the lithium concentration gradient.
- The dynamic lithium concentration profile is rigorously derived from the P2D model.
- The voltage and concentration RMS errors are reduced up to 74% compared to the SPM.
- The proposed model is utilized to predict the localized lithium plating.

ARTICLE INFO

Article history:
Received 22 October 2014
Received in revised form
2 February 2015
Accepted 22 March 2015
Available online 24 March 2015

Keywords:
Simplified pseudo-two dimensions
Pseudo-two dimensions model
Battery management systems
Electrochemistry battery model
Model order reduction

ABSTRACT

A sophisticated BMS often requires an accurate yet simple battery model. Simplified models such as the single particle model (SPM), however, provide limited insight because lithium concentration variations over the cell thickness dimension are often neglected. In this study, we propose a simplified electrochemical model that, by reviving the lithium concentration variation across the cell thickness, provides significantly improved prediction power over the SPM. The lithium concentration profiles are first derived according to the electrochemistry-based pseudo-two dimensions (P2D) model under the steady-state assumption, they are then relaxed into a dynamic model. By employing steady-state concentration profiles coupled with averaged dynamics, the proposed model predicts electrolyte and solid surface concentrations (c_e and c_{ss}, respectively) and potential variations across the cell during both transients and stead-state conditions. The proposed model is validated by comparing the cell voltage, c_e, and c_{ss} concentration RMS errors with respect to the P2D model under pulse and constant current inputs. The simulation shows that the proposed model achieves at least 74%, 77%, and 65% RMS error reductions for cell voltage, c_{ss} and c_e, respectively, when compared to SPM in constant current simulation. Finally, the presented model is used to predict and detect local lithium plating, which the SPM is not capable of doing; our method yields predictions similar to those of the original P2D model at computational loads comparable to SPM.

1. Introduction

Batteries are vital components for mobile electrical applications such as mobile phones and electric automobiles, which need to be unplugged from a power grid for long spans of time [1]. Lithium-ion batteries, in particular, sport an attractive compromise of power density, energy density, low self-discharge rate, battery life, and cost, which makes them one of the most popular chemistry choices for unplugged applications. However, electrochemical energy storage devices usually have safety boundaries that are impractical, if not impossible, to measure in real-world applications [2]. To ensure safe, prolonged, and reliable operations, significant research effort has been put into understanding, modeling, and predicting the key limiting phenomena, which has led to various battery models with different levels of complexity and prediction capabilities (Fig. 1).

Empirical models usually populate the lower computational complexity area [3]. Their performance is satisfactory within the range of experiments used to fit their parameters, but quickly

---

* Corresponding author.
E-mail addresses: p-k-f@kaist.ac.kr (P. Kemper), lishbo@tsinghua.edu.cn (S.E. Li), dskum@kaist.ac.kr (D. Kum).

http://dx.doi.org/10.1016/j.jpowsour.2015.03.134

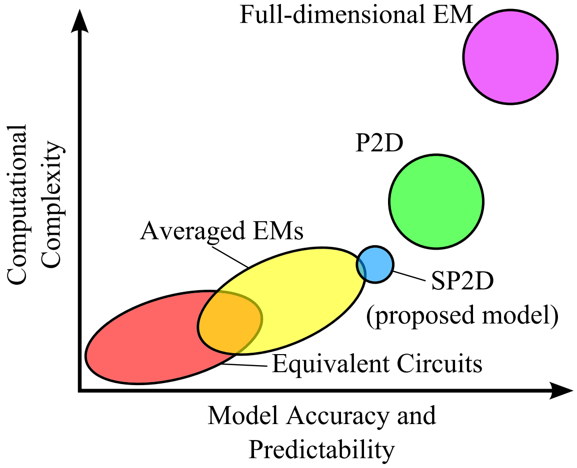

Fig. 1. Conceptual comparison of different models with respect to their complexity and prediction power.

degrades as the cell is forced outside of the expected usage scenarios [4]. Equivalent Circuit Models (ECMs) are the most popular choice of empirical models. ECMs use lumped-parameter circuit elements, e.g. inductors, resistors, and capacitors, to represent battery dynamics, where these lumped-parameters are frequently described by empirical functions of SoC and temperature. This type of model is structurally simple and computationally efficient, and has been widely studied for SoC estimation, SoH prediction, etc. However, cumulative measurement errors, capacity degradation through usage life, environmental parameter variation, and device sensitivity to initial conditions heavily affect on-board performance [5–7]. Another issue is that, for a significant portion of empirical models, their states lack physical significance, i.e. they focus on abstractions towards lumped circuit elements based on perceived macroscopic behaviors rather than on the physical interactions among the elements on a microscopic scale. These models are then oblivious to potentially dangerous phenomena that can reduce battery life or even irreversibly damage it, such as when portions of the cell during charging could be undergoing lithium plating while the cell, in the average sense, is still respecting the suggested safety operation limits [2,4]. Lack of physical significance may also considerably limit their adaptiveness, and an exponentially-growing fitting space is often required to cope with more parameters [3,4].

At the opposite corner of the complexity/predictability plane there are electrochemical models (EM). These models usually account for lithium ion intercalation and diffusion in electrodes and electrolytes, various side-reactions, double-layer effects, and lithium concentration variations across the electrode layer, which are governed by first-principle physicals laws. One of the most widely known electrochemical models is the pseudo-two dimension (P2D) model, in which the solid diffusion is calculated inside virtual particles and the electrolyte diffusion is considered only across the cell thickness. Such models often lead to complex mathematics, which are comprised of partial differential equations (PDE) and algebraic equations. As a result, the electrolyte/solid potentials as well as the electrolyte/solid concentration can be calculated across the cell with significant accuracy. The unparalleled prediction abilities of the electrochemical models, however, are shadowed by the sheer number of states; this situation translates into significant computational resources needed to properly solve PDEs.

If the computational environment is limited but information is needed in real-time, which is usually the case for practical BMS applications, it is often necessary to tackle the computational overhead. Efforts to reduce the burden of solving the electrochemical equations have relied either on mathematical manipulation (e.g. polynomial approximation [8–11] and proper orthogonal decomposition [12]) or on simplifying assumptions (e.g. volume averaged models [13], averaged models [14–16], and a particularly popular subclass of averaged models called Single Particle Models – SPM [4,17]). These assumptions, however, are likely to hamper the prediction capabilities to the point that they offer no practical advantages over empirical models.

The loss of lithium concentration and potential gradient across the cell thickness dimension is a major drawback of the averaged models (SPM included). Recent efforts into obtaining gradients across the cell with simplified models do exist. Rahimian [10] and Han [11] used a polynomial approximation to calculate electrolyte concentration variation, but no attempt was made to address the solid concentration variation (Ref. [11] addresses only its effects through the open-circuit potential distribution). Both included polynomial coefficients arbitrarily and some of these need to be solved for each point in time, which incurs additional computational effort. Luo's contribution [18] addresses the potential variations across the cell, together with pore-wall flux variations. These ideas are insightful for some BMS functions (e.g. lithium plating prediction), but they offer no information about the concentration of lithium, which is necessary for ensuring cell safety. While [10] is an averaged model with an increased number of states, the contribution of [11], which provides some insight into concentration variations, requires multiple particles. That is also the case for [18], whose model actually requires three representative particles per electrode.

One critical problem arising from the lack of gradient knowledge is localized lithium plating, which is usually seen at boundaries and results in capacity losses as well as other safety concerns [19,20]. The lithium plating tends to occur during recharge at high SOC, and at low temperatures or high currents; without such gradient knowledge the BMS would have to employ a conservative control strategy in order to avoid localized lithium plating [3,4]. These problems are particularly important for large cells because they become more pronounced as the cell thickness increases [4], which in turn must be carefully considered during the cell design process. Therefore, a simplified EM that can predict concentration gradients with reduced computational load is necessary.

Aiming to provide a model with a computational burden equivalent to that of average models but with prediction capabilities similar to that of P2D, the Simplified P2D (SP2D) model was conceived. The main contribution of the SP2D is to provide a physics-based concentration profile, derived from the P2D model, coupled with electrolyte averaged dynamics, in order to recover the concentration gradients across the thickness dimension. The existence of these dynamic concentration profiles is the key difference between the SP2D and other averaged models. Knowing the concentration across the cell provides a basis for predicting much more accurate safety boundaries as well as other BMS functions and enables the design of studies with reduced computational burden.

The remainder of this paper is organized as follows: Section 2 introduces the first-principle model used as a base for the SP2D; the derivation of SP2D is presented in Section 3; Section 4 provides the model validation versus a higher-order EM, and also a comparison with SPM; Localized lithium plating prediction is presented in Section 5; and the concluding remarks and future work can be found in Section 6.

2. Electrochemical model – P2D

The pseudo-two dimensions (P2D) model is one of the most accurate and detailed electrochemical models that was developed