Computers and Chemical Engineering 76 (2015) 87–97

Contents lists available at ScienceDirect

Computers and Chemical Engineering

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

Electrochemical model of a lithium-ion battery implemented into an automotive battery management system

Woosuk Sung, Chee Burm Shin*

Department of Chemical Engineering, Ajou University, Suwon 443-749, Republic of Korea

ARTICLE INFO

Article history:
Received 17 July 2014
Received in revised form 7 February 2015
Accepted 10 February 2015
Available online 24 February 2015

Keywords:
Lithium-ion battery
Battery model
Battery management system
Electric vehicle

ABSTRACT

This paper presents the development of an electrochemical model that can be implemented into automotive battery management systems (BMSs). Compared with empirical models, the electrochemical model features more accurate state estimates over a broader and longer use of the battery. In this work, model implementation schemes are devised to make the electrochemical model uncomplicated enough to be embedded into the BMS. A nonlinear system of partial differential equations in the model is discretized into a linearized system of algebraic equations (AEs). A solver selected to evaluate the resulting system of AEs is modified for its application to the BMS. As the BMS is preoccupied by its existing tasks, the reformulated equations and optimized solver are reorganized such that the limited computational resources of the BMS are appropriately exploited. The electrochemical model is consequently implemented into the BMS, predicting battery behaviors in 1 s intervals while occupying a 14 kB RAM.

1. Introduction

A battery management system (BMS) is an electronic control unit that is specifically designed to ensure that a battery is run within its safe operating area normally bound by the applied current, state-of-charge (SOC), and temperature. For this purpose, a BMS is required to fulfill the functions such as measurement, management, evaluation, communication, and logging. A BMS measures the current, voltage, and temperature from a battery. A BMS typically manages a battery by preventing the cells from the usage out of their safe operating area and balancing the cells by bringing all the cells to the same SOC. A BMS also calculates or estimates the internal states of a battery, which includes SOC, resistance, and state-of-health (SOH) (Andrea, 2010; Lu et al., 2012). To be more specific, SOC denotes the residual capacity with respect to the rated capacity, while SOH most often refers to the rated capacity with respect to the nominal capacity, despite it is usually defined differently. In addition, a BMS interfaces with other electronic control units running not only in-vehicle but also on-the-grid to provide the information about a battery.

Along with such diverse functions of a BMS, the evaluation of the internal states of a battery is particularly important in the electric vehicle (EV) applications. A lithium-ion battery (LIB) is typically used in EVs, because wider operating conditions with longer lifetime are required for the EV applications than the other applications. In practice, the automotive BMS is in service depending only on the direct measurements of the current, voltage, and temperature. These limited quantities about a battery hinder the automotive BMS from estimating the internal states of the battery such as the SOC and SOH. The automotive BMS is thus required to embed a battery model that can describe battery dynamics, for example, predicting the output voltage in response to the input current and temperature across diverse operating conditions, which is a basis for the state estimation. Due to these reasons, conventional BMSs favor empirical models which usually make use of an equivalent circuit built in combination with resistance and capacitance elements to mimic battery dynamics. An equivalent circuit model (ECM) is easy to handle and can match battery behaviors well particularly at near-equilibrium (Plett, 2004a,b; Liaw et al., 2004; Chen and Rincon-Mora, 2006; Hu et al., 2012). The ECM can also reasonably estimate the SOC of a battery at equilibrium (Plett, 2004a,b; Verbrugge and Koch, 2006). However, the ECM has limited applicability to the operating conditions far from equilibrium wherein EVs usually function with extensive and transient changes in the applied current, SOC, and temperature. To extend the usefulness of the ECM, resistance and capacitance elements should be further supplemented; however, this solution could rather undermine much of the ECM's own benefits.

Instead of the ECM, an advanced BMS tends to feature an electrochemical model which is physically justified, expecting possible advances in more accurate state estimates over a broader and longer use of a battery, for instance, when a battery is

* Corresponding author. Tel.: +82 31 219 2388; fax: +82 31 219 1612.
E-mail address: cbshin@ajou.ac.kr (C.B. Shin).

http://dx.doi.org/10.1016/j.compchemeng.2015.02.007
0098-1354/

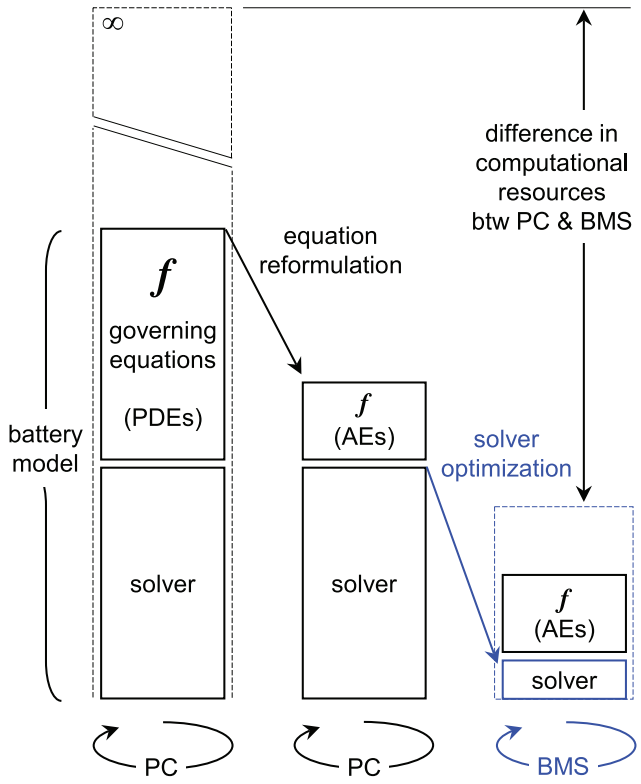

Fig. 1. A series of model implementation schemes. The equation reformulation in cooperation with the solver optimization is devised to embed the model into the BMS, despite its acute shortage of computational resources for the model simulation.

driven far from equilibrium during its entire lifetime (Smith, 2010; Chaturvedi et al., 2010; Rahimian et al., 2011; Moura et al., 2012). The electrochemical model is derived from the porous electrode and concentrated solution theories fundamentally based on thermodynamics, kinetics, and transport phenomena. The electrochemical model is represented by coupled nonlinear partial differential equations (PDEs) in spatiotemporal coordinates, concerning the conservations of mass and charge in the solid and liquid-phases, respectively, and by Butler–Volmer kinetic expression (Newman and Thomas-Aleya, 2004; Thomas et al., 2002; Newman and Tiedemann, 1975; De Vidts and White, 1997; Wang et al., 1998). The electrochemical model is typically solved numerically (Botte et al., 2000). However, this computation should be extremely prohibitive, particularly considering its implementation into a computationally inexpensive BMS (Subramanian et al., 2007, 2009). Similar to typical embedded systems (Barr and Massa, 2006), the computational resources of the BMS used in this work only include a 16-bit processor with an on-chip 50 kB run-time memory with no floating-point unit (FPU), which should be vastly insufficient for running a numerical solver to evaluate the coupled nonlinear PDEs of the model in a timely fashion even with a high degree of accuracy.

In order to overcome such difficulties, as illustrated in Fig. 1, the governing PDEs in the model are required to be efficiently reformulated, while a solver is expected to be highly optimized, both for implementing the model into the BMS. This study aims at developing and demonstrating the electrochemical model that can be embedded into the automotive BMS, with a specific emphasis on devising the model implementation schemes primarily including solver optimization. To achieve this goal, an original system of ten PDEs in the model is spatiotemporally discretized into a linearized system of 41 algebraic equations (AEs), seeking for reducing the model complexity while almost uncompromising the model accuracy. For this model reformulation, the spatiotemporal discretization methods suggested by Ramadesigan et al. (2010) and Northrop et al. (2011) are generally adopted. To solve the resulting system of AEs, CSparse, a free library implementing a number of direct methods for sparse linear systems (Davis, 2006), is duly selected and then extensively modified, aiming at maximizing execution speed while minimizing memory footprint. For this solver optimization, preprocessing as well as dynamic memory allocation is effectively performed along with the other schemes. Afterwards, for embedding the model into the BMS which is already consumed by the existing BMS tasks, the reformulated equations as well as the optimized solver are again partly altered such that the limited computational resources of the BMS can be shared with many existing BMS tasks.

In this work, the implementation schemes of the electrochemical model into the BMS are developed to realize the benefits of the electrochemical model. The complex electrochemical model provides more precise and various state estimates than the other simple models. The electrochemical model can be utilized for a broader and longer operation of the battery for the EV applications. The model implementation schemes include the equation reformulation along with a solver optimization to make it possible for this heavy model to be implemented into the computationally light BMS. This work is closely related to the previous papers (Ramadesigan et al., 2010; Northrop et al., 2011) which provide a rich background specifically in terms of reformulating the equations in the electrochemical model. In contrast to these papers, this work is novel in the optimization of the solver to compute the reformulated equations by using the limited computational resources of the BMS. Based on the literature reports, this work is the first that gives a detailed account of the model implementation schemes proven to be applicable to the automotive BMS.

2. Model formulation

2.1. Electrochemical model

The electrochemical model of an LIB is described separately in Appendix for the sake of brevity. Instead, as shown in Fig. 2, the general feature of the electrochemical model is schematically depicted, underlining its variables: the dependent variables such as electric potential φ, Li(-ion) concentration c, and the molar flux of Li at the surface of the spherical active material particle j, which are partially differentiated by the independent variables such as spatial macroscale x coupled with microscale r, and temporal t.

2.2. Model reformulation

The electrochemical model, in the form of a coupled nonlinear system of PDEs, is to be solved numerically. As part of numerical solutions, spatial discretization can be performed using the finite difference or weighted residual methods, thereby reducing the model order from a system of PDEs down to a system of differential algebraic equations (DAEs).

For the first independent variable, spatial x, on which most of the dependent variables c_e, φ_s, and φ_e depend, the orthogonal collocation method is chosen (Northrop et al., 2011). Prior to discretizing the governing equations for c_e, φ_s, and φ_e, their coordinate is transformed, as described in Fig. 3. The original coordinate in the model has three regions defined in terms of x; positive electrode, separator, and negative electrode span $[0, l_p]$, $[l_p, l_p + l_s]$, and $[l_p + l_s, l_p + l_s + l_n]$, respectively. Through the coordinate transformation, each region is normalized to $[0, 1]$ and commonly defined with respect to a dummy variable X. For example, the governing equation for the liquid-phase Li-ion concentration (Eq. (A.12)) in the positive electrode is transformed as: