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Ensemble bias-correction based state of charge estimation of lithium-Ion batteries

Yifei Li
Iowa State University

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Ensemble bias-correction based state of charge estimation of lithium-ion batteries

by

Yifei Li

A thesis submitted to the graduate faculty
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

Major: Mechanical Engineering

Program of Study Committee:
Chao Hu, Major Professor
Shan Hu
Chinmay Hegde

The student author, whose presentation of the scholarship herein was approved by the program of study committee, is solely responsible for the content of this thesis. The Graduate College will ensure this thesis is globally accessible and will not permit alterations after a degree is conferred.

Iowa State University
Ames, Iowa
2017

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TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>LIST OF FIGURES</th>
<th>iv</th>
</tr>
</thead>
<tbody>
<tr>
<td>LIST OF TABLES</td>
<td>vi</td>
</tr>
<tr>
<td>ACKNOWLEDGMENTS</td>
<td>vii</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>viii</td>
</tr>
<tr>
<td>CHAPTER 1 INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>1.1 Motivation and State of Art</td>
<td>1</td>
</tr>
<tr>
<td>1.2 Scope and Contribution of this Thesis</td>
<td>3</td>
</tr>
<tr>
<td>1.3 Thesis Outline</td>
<td>4</td>
</tr>
<tr>
<td>CHAPTER 2 LITHIUM ION BATTERY BASICS</td>
<td>5</td>
</tr>
<tr>
<td>2.1 Lithium Ion Cell Basics</td>
<td>5</td>
</tr>
<tr>
<td>2.2 Battery Management System</td>
<td>6</td>
</tr>
<tr>
<td>2.3 State of Charge Estimation Methods</td>
<td>7</td>
</tr>
<tr>
<td>CHAPTER 3 THE ENSEMBLE BIAS-CORRECTION BASED SOC ESTIMATION</td>
<td>13</td>
</tr>
<tr>
<td>3.1 The Ensemble BC with Adaptive Weights for Lithium-ion Battery Modeling</td>
<td>13</td>
</tr>
<tr>
<td>3.2 Performing Ensemble Prediction of Bias Correction</td>
<td>19</td>
</tr>
<tr>
<td>CHAPTER 4 EXPERIMENTAL DESIGN AND DATA ACQUISITION</td>
<td>22</td>
</tr>
<tr>
<td>4.1 The NCR18650 Cell and the Novonix HPC System</td>
<td>22</td>
</tr>
<tr>
<td>4.2 Experimental Design</td>
<td>23</td>
</tr>
<tr>
<td>4.3 Experiment Results</td>
<td>24</td>
</tr>
<tr>
<td>4.4 ECM Parameter Optimization</td>
<td>25</td>
</tr>
<tr>
<td>CHAPTER 5 VOLTAGE SIMULATION AND SOC ESTIMATION RESULTS</td>
<td>26</td>
</tr>
<tr>
<td>5.1 Cross Validation for Performance Evaluation</td>
<td>26</td>
</tr>
<tr>
<td>5.2 Voltage Simulation Results</td>
<td>27</td>
</tr>
<tr>
<td>5.3 SoC Estimation Results</td>
<td>31</td>
</tr>
<tr>
<td>Section</td>
<td>Page</td>
</tr>
<tr>
<td>-------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>CHAPTER 6 DISCUSSION AND CONCLUSIONS</td>
<td>38</td>
</tr>
<tr>
<td>6.1 The Effect of Inaccurate SoC</td>
<td>38</td>
</tr>
<tr>
<td>6.2 Summary of Experimental Validation</td>
<td>40</td>
</tr>
<tr>
<td>6.3 Limitations and Future Work</td>
<td>41</td>
</tr>
<tr>
<td>REFERENCES</td>
<td>42</td>
</tr>
</tbody>
</table>
**LIST OF FIGURES**

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Figure 1</td>
<td>Li-ion battery operating principle</td>
<td>5</td>
</tr>
<tr>
<td>Figure 2</td>
<td>Categorization of SoC Estimation Methods</td>
<td>7</td>
</tr>
<tr>
<td>Figure 3</td>
<td>Schematic of ECMs</td>
<td>9</td>
</tr>
<tr>
<td>Figure 4</td>
<td>Extended Kalman Filter Algorithm</td>
<td>12</td>
</tr>
<tr>
<td>Figure 5</td>
<td>A flowchart of the proposed ensemble bias-correction method</td>
<td>13</td>
</tr>
<tr>
<td>Figure 6</td>
<td>Flowchart of Ensemble BC Formulation in EKF based SoC Estimation</td>
<td>14</td>
</tr>
<tr>
<td>Figure 7</td>
<td>Experiment Setup – HPC Test System</td>
<td>21</td>
</tr>
<tr>
<td>Figure 8</td>
<td>Current and voltage measurements from SCPD and MCPD tests</td>
<td>24</td>
</tr>
<tr>
<td>Figure 9</td>
<td>Equivalent Circuit Model Parameters</td>
<td>25</td>
</tr>
<tr>
<td>Figure 10</td>
<td>Comparison of SECM-simulated voltage profiles without BC/with ensemble BC to measured voltage profile in SCPD test, CV#4</td>
<td>27</td>
</tr>
<tr>
<td>Figure 11</td>
<td>Comparison of SECM-simulated voltage profiles without BC/with ensemble BC to measured voltage profile in MCPD test, CV#6</td>
<td>28</td>
</tr>
<tr>
<td>Figure 12</td>
<td>Comparison of ESC-simulated voltage profiles without BC/with ensemble BC to measured voltage profile in SCPD test, CV#3</td>
<td>28</td>
</tr>
<tr>
<td>Figure 13</td>
<td>Comparison of ESC-simulated voltage profiles without BC/with ensemble BC to measured voltage profile in MCPD test, CV#5</td>
<td>29</td>
</tr>
<tr>
<td>Figure 14</td>
<td>CV#1, SECM based SoC estimation results in SCPD test</td>
<td>32</td>
</tr>
<tr>
<td>Figure 15</td>
<td>CV#5, SECM based SoC estimation results in MCPD test</td>
<td>33</td>
</tr>
<tr>
<td>Figure 16</td>
<td>CV#2, ESC based SoC estimation results in SCPD test</td>
<td>34</td>
</tr>
<tr>
<td>Figure</td>
<td>Description</td>
<td>Page</td>
</tr>
<tr>
<td>--------</td>
<td>-----------------------------------------------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>Figure 17</td>
<td>CV#7, ESC based SoC estimation results in MCPD test</td>
<td>35</td>
</tr>
<tr>
<td>Figure 18</td>
<td>Comparison of the difference in SoC and the change in simulated output voltage</td>
<td>39</td>
</tr>
<tr>
<td>Figure 19</td>
<td>Comparison schematic of the relationship between Ensemble BC Term, the difference in simulated output voltage and overall simulation error. (a) SECM; (b) ESC model</td>
<td>40</td>
</tr>
</tbody>
</table>
# LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table 1</td>
<td>Procedure of the proposed ensemble bias-correction method</td>
<td>20</td>
</tr>
<tr>
<td>Table 2</td>
<td>Basic Electrical Properties of Panasonic NCR18650 Cells</td>
<td>22</td>
</tr>
<tr>
<td>Table 3</td>
<td>Voltage simulation errors without/with ensemble BC of SECM</td>
<td>29</td>
</tr>
<tr>
<td>Table 4</td>
<td>Voltage simulation errors without/with ensemble BC of ESC model</td>
<td>30</td>
</tr>
<tr>
<td>Table 5</td>
<td>SoC estimation errors without/with ensemble BC of SECM</td>
<td>36</td>
</tr>
<tr>
<td>Table 6</td>
<td>SoC estimation errors without/with ensemble BC of ESC model</td>
<td>36</td>
</tr>
</tbody>
</table>
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To Those Who are so Generous

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In addition, I would also like to thank my friends, colleagues, the department faculty and staff for making my time at Iowa State University a wonderful experience.
It is an essential task of battery management system (BMS) to online estimate the State of Charge (SoC) of a Lithium-ion (Li-ion) battery, an important indicator of the remaining charge in the battery. Accurate modeling of the electrical behavior of a Li-ion battery can provide an accurate approximation of the battery dynamic characteristics during charging/discharging and relaxation phases. This is essential to accurate online estimation of the battery SoC. Equivalent circuit models (ECMs) are widely used to assist with online SoC estimation because of their simplicity and high computational efficiency. This thesis proposes an ensemble bias-correction (BC) method with adaptive weights to improve the accuracy of an equivalent circuit model (ECM) in dynamic modeling of Li-ion batteries. The contribution of this thesis is threefold: (i) the introduction of the concept of time period; (ii) the development of a novel ensemble method based on BC learning to model the dynamic characteristics of Li-ion batteries; and (iii) the creation of an adaptive-weighting scheme to learn online the weights of offline member BC models for building an online ensemble BC model. Repeated pulsing discharge tests with single and multiple C-rates were conducted on seven Li-ion battery cells to evaluate the effectiveness of the proposed ensemble BC method.
CHAPTER 1 INTRODUCTION

1.1 Motivation and State of Art

The idea of powering the world with greener and smarter energy resources has attracted engineers and scientists for decades. Development in field of battery technology helps to move the steps faster. Battery, as a kind of energy storage system which enables the utilization of energy in form of electricity in a time delayed manner, has made its way through the market. With the rapid prevalence of the consumer electronics in the last several decades, battery has demonstrated its applicability as a stable and adaptive power source, from digital cameras to hybrid and electric vehicles. As the size and maximum energy of batteries increase with the ever increasing demand, new control and management approaches to monitoring and provide information about the performance, status and reliability of the batteries are in demand. The State of Charge (SoC) of a battery is one of the most important states in battery management [1]. SoC indicates how much energy is left to use in a battery and accurate knowledge of its value is of great importance. SoC is used by battery management system (BMS) to control the operation of batteries and accurate SoC estimation can help to improve the battery useful life [2]. However, unlike gasoline in the tank of vehicles, the remaining charge in a battery cannot be measured directly as, put it in a simple way, the remaining transferrable charges are ions stored in the electrode material [3-6]. Therefore, a large number of model-based estimators have been proposed to give estimates of this state using readily measurable quantities (e.g., voltage, current, and temperature) [5-12]. The resistor-capacitor (RC) network-based equivalent circuit models (ECMs) are the most
widely used in these SoC estimators owing to the low complexity and adequate accuracy of the ECMs [13-15]. In practical applications, one set of ECM parameters (e.g., resistances and capacitances) with constant values are often adopted for simplicity. However, the uncertainty in material properties and manufacturing tolerances lead to varying degrees of cell-to-cell variation. Therefore, the “best-fit” ECM parameters may differ significantly from one cell to another [13]. The SoC estimation accuracy on a cell may drop significantly if the adopted ECM parameters deviate largely from the “best-fit” parameters of the cell [6]. Furthermore, the electrical behavior of a battery cell is highly dependent on the operating conditions (e.g., SoC, temperature, C-rate) [16], and as a result, the “best-fit” ECM parameters of the cell may vary substantially with the operating conditions. Consequently, the “best-fit” ECM parameters are both cell- and condition-dependent, and it is obviously inappropriate to use one common set of ECM parameters to model different cells under different operating conditions. One way to address the above mentioned problem is to adopt an ECM with online-adjustable parameters [11, 12]. However, it can be difficult to achieve accurate estimation of the ECM parameters in cases where cells are operating in dynamic and unpredictable conditions, and the parameter-estimation process can be time-consuming when a large number of parameters need to be online calibrated. Alternatively, a bias-correction (BC) model can be introduced to compensate the modeling error of an ECM resulting from the cell- and condition-dependencies of the ECM parameters [6, 13, 17].

The assumptions underlying the BC method are that 1) the BC model can represent the systematic discrepancies of an ECM (i.e., the systematic differences between the ECM simulations and actual measurements from cells with varying dynamic characteristics); and 2) these discrepancies can be learned offline from extensive testing on a number of training
cells and adopted online to bias-correct the ECM for individual testing cells. Xi et al. [17] presented a systematic BC framework to characterize both the parameter uncertainty and the model uncertainty for an initially calibrated ECM of a battery cell. The cell-dependency of the ECM parameters (i.e., due to the cell-to-cell variability) was accounted for via statistical calibration of the ECM, and the condition-dependency of the model bias was characterized, in conjunction with statistical calibration, via design of experiments and response surface modeling. Sun et al. [6] developed a reference ECM of a battery pack, applied the reference model to the individual cells in the pack, and characterized and corrected the biases of the model for the individual cells. The radial basis function neural network technique was employed to construct response surfaces that constituted the BC models for the individual cells. Gong et al. [13] proposed a data-driven BC model to bias-correct a reference ECM. Features extracted from incremental capacity analysis were used in the BC model to account for the cell-dependency of the model bias. Although the concept of BC has been shown to be capable of improving the accuracy of voltage simulation in these previous studies, most of the existing BC methods mainly focus on the offline development of one or multiple BC models but lack the ability to consider cell-to-cell and condition-to-condition variabilities in the online adoption of the BC models. Thus, there is an important need to develop a generic BC method that accounts for the cell- and condition-dependencies in the offline development of BC models and facilitates online adoption of the cell- and condition-dependent BC models.

1.2 Scope and Contribution of this Thesis

Motivated by the aforementioned challenges, the objective of this thesis is to propose a novel generic framework that uses the model bias of a set of selected cells to form an ensemble BC term online for an individual cell. The ensemble BC term can be used to reduce
the battery dynamic behavior modeling error and help to improve battery SoC estimation accuracy. The contribution of this thesis consists three main aspects: (1) the introduction of the concept of ‘time period’ which facilitates the modeling of battery dynamic behavior when the battery is at rest, (2) the development of a novel ensemble method based on BC learning to model the dynamic characteristics of Lithium-ion (Li-ion) batteries, and (3) the creation of an adaptive-weighting scheme to learn online the weights of offline member BC models for building an online ensemble BC model. This thesis carries out experimental testing to verify the validity and effectiveness of the proposed ensemble BC method in battery modeling using commercial NCR18650 cells.

### 1.3 Thesis Outline

The thesis is organized as follows: Chapter 2 first introduces the basic operating principles of Li-ion battery and BMS and then presents a summary of existing SoC estimation methods. Chapter 3 contains a detailed description of the proposed ensemble BC method. Chapter 4 introduces the process of experimental data acquisition and the result of ECM parameter determination. The voltage simulation and SoC estimation results are presented in Chapter 5 and an analysis and discussion of the results are given in Chapter 6. Chapter 7 concludes the thesis and points out directions for future work.
CHAPTER 2 LITHIUM-ION BATTERY BASICS

2.1 Lithium-Ion Cell Basics

Since Sony’s successful commercialization in the early 1990s, rechargeable Li-ion batteries have grown to be the major power source in many applications from handheld electronic devices to hybrid and electric vehicles [2]. With its competitive high energy density and relatively high electrochemical potential among rechargeable commercial cells, Li-ion batteries have become the most promising and fastest growing cell type on the market.

Similar to the widely used lead-acid battery, commonly-used Li-ion batteries consists of four basic components (see Fig. 1): a cathode (positive electrode), an anode (negative electrode), a separator, and the electrolyte as the medium for Li-ion transfer. The cathode typically consists of a type of metal oxide and the anode is often formed with porous carbon [1]. During discharge, the lithium ions de-intercalate from the anode, flow to the cathode through the electrolyte and separator, and intercalate into the cathode material.

![Figure 1. Li-ion battery operating principle [23]](image-url)
Numerous publications have discussed the operating principle of Li-ion batteries and interesting readers can find more detailed descriptions of Li-ion batteries in Ref. [23]. As inappropriate battery operations such as overcharging/over-discharging can expedite battery degradation by causing phenomena such as lithium plating, knowing accurately how much charge remains in a battery is of critical importance in rechargeable battery applications [1].

2.2 Battery Management System

In applications where battery cells serve as the major power source, accurate monitoring of battery states in real time and controlling of battery operation is critical to provide necessary knowledge of the status of battery cells and reducing the risk of unprecedented battery failure. BMS, typically a chip embedded in battery system, serves to control the battery operation and monitor the important battery states, such as SoC, state-of-health (SoH). Most BMS applications focus on monitoring the states of a single battery cell. The BMS in battery pack applications, where a battery pack consists of multiple cells, should be able to estimate the SoC of each individual cell in the battery system. Though small SoC estimation errors of the individual cells in a battery pack can be within tolerance on their own, for applications where a battery pack consists a large amount of cells, the small estimation errors in the cell level can add up to a large overall estimation error in the pack level which could lead to inappropriate control order. Thus, the task of further improving the states estimation accuracy becomes important in battery pack applications where the BC method which can capture the systematic discrepancies can be adopted to improve the SoC estimation accuracy.
2.3 State of Charge Estimation Methods

Existing SoC estimation methods include straightforward methods, such as coulomb counting and OCV mapping, and methods with more complexity, such as model-based estimators with sequential probabilistic inference and ECMs. In general, according to whether there is a feedback mechanism that corrects the SoC estimate directly derived from measureable quantities, the SoC estimation methods can be classified into two categories: the open-loop methods and the closed-loop methods.

2.3.1 Open-loop versus Closed-loop

The open-loop methods, such as coulomb counting and direct mapping from open-circuit voltage (OCV) are computational efficient and easy to implement. However, those methods typically lose accuracy in the presence of large noise in the measurements. The closed-loop methods, on the other hand, are often the combination of a sequential probabilistic inference technique (e.g., Kalman filter (KF) and extended Kalman filter (EKF)) and a battery model (e.g., the Thevenin ECM and an electrochemical model). Owing to the feedback mechanism, these closed-loop SoC estimators can often provide more accurate and robust estimation results. Fig. 2 shows some commonly used SoC estimation methods.

![Figure 2. Categorization of SoC Estimation Methods](image-url)
Throughout the years, researchers have proposed many SoC estimators. The SoC estimators can generally be classified as, the equivalent circuit model based estimator, the electrochemical model based estimator. Electrochemical models use partial differential equations to describe the behavior of the battery cells from the electrochemistry prospective. Carefully built electrochemical models can produce estimation results with very good accuracy and those models can serve as good SoC estimators. However, as solving high-order partial differential equations remains computational expensive task, implementing such models in computing power limited application like BMS is not appropriate. On the contrary, the ECM-based SoC estimators which uses a series of electrical circuit component to simulate the dynamic behavior of the battery, is computational efficient. As the ECM can produce voltage simulation result with good accuracy when with carefully tuned ECM parameters, ECM based SoC estimator is adopted in the research.

2.3.2 Equivalent Circuit Model Based SoC Estimator

Normally, a simple ECM includes: (1) an OCV term describes the cells characteristics when there is no charge/discharge; (2) a series resistance representing the ohmic resistance; (3) and a resistance-capacitance (RC) pair describes the dynamic behavior of a cell when the load changes. An example of such an ECM is shown in Fig. 3(a). The current variation in the RC pair and can be formulated as:

\[
    i_{RC,k+1} = F_{RC} \cdot i_{RC,k} + \left(1 - F_{RC}\right) \cdot i_k
\]

\[
    F_{RC} = \exp\left(-\frac{dt}{R_{1}C_{1}}\right) \tag{2}
\]
where $i_{RC,k}$ is the current through $R_i$ at the $k$th measurement time step, $i_k$ is the total current through the cell, $dt$ is the measurement time interval, $Q$ is the battery capacity and $R_i$ and $C_i$ are the resistance and capacitance values in the ECM, respectively.

In order to consider the hysteresis effect of the battery and improve the modeling accuracy, the ECM can be expanded to include a hysteresis voltage term. The enhanced self-correcting (ESC) model is a widely used model that considers the hysteresis effect. The hysteresis effect is represented by two states in the ESC model:

![Figure 3. Schematic of ECMs: (a) Simple ECM; (b) the Enhanced self-correcting model](image-url)
\[ h_{k+1} = \varphi_k \cdot h_k + (\varphi_k - 1) \cdot \text{sign}(i_k) \]  
\[ \varphi_k = \exp \left( - \eta \cdot i_k \cdot \gamma \cdot dt \right) \]  
\[ s_{k+1} = \begin{cases} 
 s_k, & i_k = 0 \\
 \text{sign}(i_k), & i_k \neq 0 
\end{cases} \]

where \( h_k \) the SoC-varying hysteresis voltage, \( \eta \) the coulombic efficiency and \( s_k \) the instantaneous hysteresis voltage. A schematic of the ESC model is shown in Fig. 3(b).

The ECM-simulated cell terminal voltage of the simple ECM (SECM) and the ESC model are formulated as in Eq. (6) and Eq. (7), respectively:

\[ V_{out} = OCV + i_k \cdot R_0 + i_{RC,k} \cdot R_1 \]  
\[ V_{out} = OCV + i_k \cdot R_0 + i_{RC,k} \cdot R_1 + M \cdot h_k + M_0 \cdot s_k \]

where \( M \) and \( M_0 \) are hysteresis factors.

### 2.3.3 Extended Kalman Filter and State Space Model

The Kalman filter, as a special case of sequential probabilistic inference, gives the statistically optimal least mean-squared-error state estimator for linear time-invariant systems when all noises are assumed white and Gaussian. Extended Kalman filter (EKF) is an approximation solution for the non-linear time-varying systems such that the nonlinear behavior of the system is linearized at the current filter estimation trajectory. Since ECMs adopted in the experimental study of this thesis are nonlinear systems, the EKF is adopted during the implementation of SoC estimation.

As the EKF technique is widely used in many fields and has been discussed thoroughly in many research articles, interesting readers can refer to Ref. [8] for more detail.
Fig. 4 is a schematic of the essential EKF algorithm updating process. Consider a non-linear system with its filter designed as,

\[ x_{k+1} = f(x_k, u_k) + w_k \]  \hspace{1cm} (8)
\[ y_k = h(x_k, u_k) + v_k \]  \hspace{1cm} (9)

where \( x_k \) is a vector containing the system’s hidden states, \( u_k \) is the system input, \( y_k \) is the system output, and \( w_k \) and \( v_k \) are the process noise and measurement noise, respectively. In each time step, the EKF algorithm starts with predicting the prior state estimate at the present time step with the state estimate at the last time step and predict state covariance matrix is the same manner. After the measurement of the system output becomes available, the measurement error of output state prediction is first calculated. Then the Kalman gain is computed and used to generate the posterior state estimate and update the state covariance matrix. As shown in Fig. 4, the EKF uses the first-order derivative of the state transition equation \( F_k = \frac{\partial f(x, u)}{\partial x} \bigg|_{x = \hat{x}_{k-1}} \) and that of the measurement equation \( H_k = \frac{\partial h(x, u)}{\partial x} \bigg|_{x = \hat{x}_{k-1}, u} \) to update state estimates, replacing the original nonlinear model.
Time Update:
State Estimate
\[ \hat{\mathbf{x}}_{k|k-1} = f(\hat{\mathbf{x}}_{k-1|k-1}, u_{k-1}) \]
Predicted Covariance Estimate
\[ P_{k|k-1} = F_{k-1} P_{k-1|k-1} F_{k-1}^T + W_{k-1} \]

Measurement Update:
Measurement Residual
\[ E_k = y_k - h(\hat{\mathbf{x}}_{k|k-1}) \]
Kalman Gain
\[ K_k = P_{k|k-1} H_k^T (H_k P_{k|k-1} H_k^T + V_k)^{-1} \]
Update State Estimate
\[ \hat{\mathbf{x}}_{k|k} = \hat{\mathbf{x}}_{k|k-1} + K_k E_k \]
Update Covariance Estimate
\[ P_{k|k} = (I - K_k H_k) P_{k|k-1} \]

Figure 4. Extended Kalman Filter Algorithm
CHAPTER 3 THE ENSEMBLE BIAS-CORRECTION BASED BATTERY DYNAMIC BEHAVIOR MODELING

3.1 The Ensemble BC with Adaptive Weights for Lithium-ion Battery Modeling

The general procedure of the ensemble BC method is shown in Fig. 5. The objective of this method is to perform an online bias-correction of the ECM-simulated voltage profile for a testing cell with the knowledge of several representative cells of the same type. For the set of cells being involved in this research, a training set is formed with the representative cells (cell 1 to n-1) and the cell of interest is denoted as the testing cell (cell n). Before the bias-correction method can operate online, individual ECMs for both the training cells and the testing cells have to be established offline. The ECMs are built with data of each cell from a standard test which is designed to highly excite the battery cells. Provided the offline fitted ECMs, the online phase of the ensemble BC method works in a stepwise manner. As the testing cell operates, the current profile of it is first linearized and divided into discrete time periods. Here, a time period is defined as a segment of time in which the cell current holds steady. Knowing the current profile of the current time period \( s \), the method searches for the most recent time period that shares the same current profile with the time period \( s \) and such a time period is denoted as \( s' \) (see a current profile example at the bottom of Fig. 5). The BC term for the testing cell at time period \( s \) is then generated as the weighted sum of the member BC models. The member BC models are defined as the difference between the measured and the simulated voltage profiles of the training cells over time period \( s \). Experimental findings suggest that the similarities between cells in their electrical behavior are often consistent across different SoC levels. It thus follows that the observed similarities
between the testing cell and the training cells at a previous time period can be used to approximate the similarities at the current time period providing that the two time periods share the same current profile. The weights corresponding to the member BC models are then approximated by the difference between the measured voltage profile of the training cells and that of the testing cell in time period $s'$. An ensemble BC model that compensates the ECM simulation error for the testing cell can thus be calculated.

**Figure 5.** A flowchart of the proposed ensemble bias-correction method
The main procedure of the ensemble BC method is summarized as follows:

**Step 1:** Individual ECMs are established offline for all the training cells and the testing cell with measurements from a standard test;

**Step 2:** During online operation, the current profile of the testing cell is divided into discrete time periods and a time period s' most similar to the current time period s is found;

**Step 3:** During the current time period s, the measured and ECM-simulated voltage profiles of the n-1 training cells are utilized to generate the member BC models;

**Step 4:** Difference between the voltage measurements of the testing cell and that of the training cells in time period s' are utilized to approximate the weights of each member BC model in time period s.

**Step 5:** Predicted BC profile is generated as a weighted sum and used to correct the ECM-simulated voltage profile of the testing cell in time period s.

### 3.1.1 Building Individual ECMs (Offline Phase)

In the offline phase, ECMs individual to each cell needs to be established based on voltage and current measurements for all cells being involved. In this study, two ECMs are investigated: the SECM (as shown in Fig. 3(a)) and the ESC model (as shown in Fig. 3(b)).

In order to obtain the ‘best-fit’ ECM parameters, a cost function has to be defined to quantify the modeling error. The root-mean-square error of voltage simulation result is a widely used cost function in ECM parameter calibration for Li-ion batteries. The simplest cost function in this manner can be defined as,

\[
V_{\text{error}} = \frac{1}{N} \sum_k^N (V_{\text{mea},k} - V_{\text{sim},k})^2
\]

(10)
with $V_{\text{mea}}$ and $V_{\text{sim}}$ being the measured and simulated voltage of the battery cell, respectively.

While as sometimes the importance of part of a test may be above the other parts, weighted integration can be defined to enhance the ability of the ECM for simulation the behavior of a cell under certain condition,

$$V_{\text{error}} = \frac{1}{N} \sum_{k=1}^{N} \omega_k (V_{\text{mea},k} - V_{\text{sim},k})^2$$

(11)

After determining a cost function, model parameter calibration can be carried out. Since no analytical solution can be obtained in the task of finding the ‘best-fit’ ECM parameters, stochastic algorithms which search in parameter vector space is widely used to obtain an approximation of the ‘best-fit’ parameters. In the scope of this study, the particle swarm optimization is adopted as the stochastic algorithm to find the ‘best-fit’ ECM parameters.

3.1.2 Formulating Ensemble BC Model (Online Phase)

During the time period $s$, the member BC model for each cell in the training set can be expressed as

$$MBC_{TR[i]}(t) = V_{TR[i],\text{mea}}(t) - V_{TR[i],\text{sim}}(t), \quad c_{TR[i]} \in \mathbb{C}$$

(12)

where $V_{TR[i],\text{mea}}$ and $V_{TR[i],\text{sim}}$ are respectively the measured and simulated voltages of the $i$th training cell, $c_{TR[i]}$, $\mathbb{C}$ denotes the set of all cells including training (denoted with subscript $TR\{i\}$) and testing cells (denoted with subscript $TS$). Denoting the testing cell as $c_{TS}$, the ensemble BC model $EBC$ of the testing cell can be formulated as a weighted-sum of the member BC models of the training cells as

$$EBC_{TS}(t) = \sum_{i} \left( \omega_{TR[i]} \cdot MBC_{TR[i]}(t) \right)$$

(13)
where $\omega_{TR[i]}$ is the weight of the $i$th training cell which quantifies the similarity between training cell $c_{TR[i]}$ and testing cell $c_{TS}$. This study proposes a new optimization-based method for obtaining the BC weights (see Section 3.1.3). After obtaining the weights for all training cells and the corresponding $EBC_{TS}(t)$, the bias-corrected ECM-simulated voltage of the testing cell can be determined as:

$$V_{TS,CORR} = EBC_{TS}(t) + V_{TS,sim}(t)$$

(14)

### 3.1.3 Optimizing BC Weights (Online Phase)

As discussed in the previous part, the objective here is to optimize the BC weights which based on the observed similarity between the testing cell and the training cells. To this end, the difference between the ensemble bias-corrected ECM-simulated voltage profile ($V_{TS,CORR}$) for the testing cell $c_{TS}$ and the measured voltage profile ($V_{TS,mea}$) is minimized. The difference ($\Psi$) between these two voltage profiles can be defined as:

$$\Psi = V_{TS,mea} - V_{TS,CORR} = V_{TS,mea} - [EBC + V_{TS,sim}]$$

(15)

Using Eq. (13), Eq. (15) can be rewritten as:

$$\Psi = V_{TS,mea} - \sum_{i} \left( \omega_{TR[i]} \cdot (V_{TR,mea} - V_{TR,sim}) \right) + V_{TS,sim}$$

(16)

Let $\sum_{i} \omega_{TR[i]} = 1$, and Eq. (17) can be simplified as:

$$\Psi = \sum_{i} \left( \omega_{TR[i]} \cdot V_{TS,mea} \right) - \sum_{i} \left( \omega_{TR[i]} \cdot V_{TR,mea} \right) = \sum_{i} \left( \omega_{TR[i]} \cdot (V_{TS,mea} - V_{TR,mea}) \right)$$

(17)

The similarity between the testing cell and a training cell can be quantified as a parameter, $\nu_{TR[i]}$, that is defined as the mean absolute difference between the measured voltages of the training and testing cells over the entire time period $s$. 
\[ v_{TR[i]} = \frac{1}{\Delta T^s} \int_{t \in [0,\Delta T^s]} \left| V_{TR[i],mea}(t) - V_{TS,mea}(t) \right| dt \]  

(18)

where $\Delta T^s$ is the duration of the time period $s$. Training cells which share more similarity with the testing cell in their electrical behavior should be assigned with higher weights. A squared exponential kernel is employed to define the weights of member BC models.

\[ \omega_{TR[i]} = \frac{1}{\sigma^2} \exp \left( -\frac{v_{TR[i]}^2}{\theta^2} \right) \]  

(19)

where $\sigma$ and $\theta$ are two hyper-parameters that are estimated for each time period by minimizing the $\Psi$ function in Eq. (17):

\[ \text{minimize } \Psi(d) = \sum_i \left( \omega_{TR[i]}(d) \cdot v_{TR[i]} \right) \]  

(20)

subject to. \[ \sum_i \omega_{TR[i]}(d) = 1 \]  

(21)

where $d = [\sigma, \theta]^T$ is a vector of the two hyper-parameters. The weight of each member BC model can then be calculated using Eq. (19). With the optimized weights, the ensemble BC model for the testing cell in the time period $s$ can be formed using Eq. (13).
3.2 Performing Ensemble Prediction of Bias Correction

Table 1 shows the procedure of the proposed ensemble BC method. The objective of the method is to bias-correct the simulated voltage profile of the testing cell during a time period $s$ that has a constant current profile. The bias correction uses an ensemble BC model, in which the weights of the member BC models are determined based on relevant measurements in the past. The relevant measurements are acquired from the training and testing cells during the most recent time period $s'$ that has the same current profile as the current period $s$. The algorithm starts by defining the testing cell $c_{te}$ and the training cells $c_{tr}$ (line 1). In the weight optimization step, the method first identifies the last time period $s'$ which has the same current profile with that of $s$ (line 3). The parameter that quantifies the similarity between each training cell and the testing cell is calculated using Eq. (18) (line 5). The hyper-parameters of the squared exponential kernel are then optimized with Eq. (20) (line 6). Then the weights assigned to the member BC models are calculated using Eq. (19).

In the ensemble prediction step, the member BC models of all training cells are first determined (line 10). Then, the time period that has the same current profile is identified and the corresponding weights are extracted (lines 11 and 12). Finally, the ensemble BC model for the testing cell during the current time period $s$ is formed with Eq. (13) and applied to correct the simulated voltage profile (lines 13 and 14).

Fig. 6 shows the flowchart of the proposed ensemble BC method when it is incorporated with EKF to estimate SoC online. It is worthy to point out that one of the major differences between the implementation of the proposed method in voltage simulation and in SoC estimation lies in the simulated voltage output. The simulated output voltage in the
Table 1. Procedure of the proposed ensemble bias-correction method

Algorithm: Ensemble Bias-Correction

1. Define the testing cell \((C_{TS})\) and training cells \((c_{TR} \in \mathbb{C} \setminus \{c_{TS}\})\).

2. for \(s = 1: S\) do

3. Start weight optimization:

4. Identify the last time period \(s'\) in which the same current profile is observed

\[ \text{find } s' \mid I_{TS}^{s'}(t_{i}^{s'}) \approx I_{TS}^{s}(t_{i}^{s}) \]

5. Calculate the similarity measures for the training cells:

\[ \nu_{TR}^{s'}(d') = \frac{1}{\Delta T} \int_{t_{TR}^{s'}} |V_{TR_{i,mea}}^{s'}(t) - V_{TR_{i,mea}}^{s'}(t)| \, dt \quad c_{TR} \in \mathbb{C} \setminus \{c_{TS}\} \]

6. Optimize the hyper-parameters in BC weights, \(d = [\sigma, \theta]\).

\[ \text{minimize } \Psi(d) = \sum_{i} \omega_{TR_{i}}(d') \nu_{TR_{i}}^{s'}(d) \]

subject to: \(\sum_{i} \omega_{TR_{i}}(d) = 1\)

7. Calculate optimal BC weights:

\[ \omega_{TR_{i}}(d', \nu_{TR_{i}}^{s'}) = \frac{1}{\sigma} \exp \left( -\frac{(\nu_{TR_{i}}^{s'})^2}{\theta^2} \right) \]

8. End weight optimization

9. Start ensemble model formulation:

10. Determine the member BC models for all training cell at time period \(s\)

\[ MBC_{TR_{i}}^{s}(t) = V_{TR_{i,mea}}^{s}(t) - V_{TR_{i,mea}}^{s}(t) \quad c_{TR_{i}} \in \mathbb{C} \]

11. Find the time period \(s'\) that has the same current profile as \(s\).

12. Load the weights of the member BC models for all training cells from time period \(s'\)

13. Form the ensemble BC model for the testing cells

\[ EBC_{TS}(t) = \sum_{i} \omega_{TR_{i}}(d', MBC_{TR_{i}}^{s'}(t)) \quad c_{TR} \in \mathbb{C} \setminus \{c_{TS}\} \]

14. Correct ECM-simulated voltage profile

\[ V_{TS,corr}(t) = EBC_{TS}(t) + V_{TS,meas}(t) \]

15. End ensemble model formulation

16. End for

Voltage simulation implementation is computed based on knowledge of true SoC value. However, in SoC estimation, the output voltage prediction is based on the SoC estimate in EKF.
Figure 6. Flowchart of Ensemble BC Formulation in EKF based SoC Estimation
CHAPTER 4 EXPERIMENTAL DESIGN AND DATA ACQUISITION

Two experimental studies with single and multiple C-rate pulsing tests were conducted to demonstrate the effectiveness of the proposed ensemble BC method. This chapter presents the experimental design and testing results of two case studies.

4.1 The NCR18650 and the Novonix HPC System

Seven Panasonic NCR18650B cells from the same batch were used in the experimental studies. The basic parameters of these Panasonic cells are listed in the Table 2. The cells were individually tested under self-designed current profiles using the Novonix High Precision Charger (HPC) system. The measurement inaccuracy of the current and voltage sensors of the HPC system is less than 0.01%. The cells were placed inside the built-in thermal chamber of the HPC system. The effect of temperature is neglect in this experiment and the test temperature was set at 30 °C. Fig. 7 shows the experimental setup.

<table>
<thead>
<tr>
<th>Table 2. Basic Electrical Properties of Panasonic NCR18650 Cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal voltage</td>
</tr>
<tr>
<td>Maximum operating voltage</td>
</tr>
<tr>
<td>Minimum operating voltage</td>
</tr>
<tr>
<td>Number of cells</td>
</tr>
<tr>
<td>Mean of cell capacity</td>
</tr>
<tr>
<td>Standard deviation of cell capacity</td>
</tr>
</tbody>
</table>
4.2 Experimental Design

The cells used in this experimental study are first tested to calibrate their characteristic. A set of experiments, including static capacity test, OCV-SOC test, were conducted for cell properties calibration. After quantifying the basic characteristics of the cells, experiments with two self-designed pulsing discharge profiles were conducted and the results are presented in this section.

The seven cells were cycled with two self-designed pulsing profiles, namely single C-rate pulsing discharge (SCPD) test and multiple C-rate pulsing discharge (MCPD) test, as shown in Fig. 8(a) and (c). The SCPD test contained 20 repeated pulses, each consisting of a 30-minute C/10 discharge and a 6-hour relaxation (see Fig. 8(a)). The MCPD test also contained 20 repeated pulses, each consisting a series of discharge pulses with different C-rates (see Fig. 8(c)) and a 4-hour relaxation. Both pulsing profiles were designed to cycle cells on almost their entire SOC range (100-10%), so as to testify the applicability of the proposed method under different SOC levels.
4.3 Experiment Results

The partial voltage profile measured from cell #3 under the SCPD test is shown in Fig. 8(b), and that measured from cell #5 under the MCPD test in Fig. 8(d). The experimental data from both pulsing discharge tests were used to demonstrate the proposed ensemble BC method.

**Figure 8.** Current and voltage measurements from SCPD and MCPD tests: (a and b) current and voltage profiles of cell #3 in SCPD test; (c and d) current and voltage profiles of cell #5 in MCPD test.
4.4 ECM Parameter Optimization

With the experimental data of SCPD, individual ECMs are built for each cell in the experimental study. Two ECM topologies are investigated in the method validation process: the SECM, (Fig. 3(a)) which includes an OCV term, one Ohmic resistance and one RC pair; the ESC model (Fig. 3(b)) with all components of the SECM and two hysteresis voltage terms which quantifies the SoC-varying hysteresis and the instantaneous hysteresis. The weighted-sum cost function is adopted and the weights are defined as the inverse-proportion of the length of time of each pulsing \( C_{\text{rate}} \). The particle swarm optimization is used to optimize the model parameters. The ECM parameter optimization results are shown in Fig. 9.

![Figure 9. Equivalent Circuit Model Parameters: (a) SECM; (b) ESC](image)
CHAPTER 5. VOLTAGE SIMULATION AND SOC ESTIMATION RESULTS

5.1 Cross Validation for Performance Evaluation

A 7-fold leave-one-out cross validation (CV) was used in this experimental study to evaluate the generalization performance of the proposed ensemble BC method. In each CV trial, the seven cells were grouped into two sets: a training set, which comprised six cells whose data was used to construct member BC models, and a testing set, using the only other cell as the testing cell. Individual ECMs for each cell being tested were built with data from the SCPD tests and the parameters of the ESC models were optimized by minimizing the average root mean square error (RMSE) of voltage simulation, as in Eq. (11), Section 3.1. The member BC models, representing knowledge of the systematic discrepancies of the individual ECMs, were then extracted for each cell in the training set by subtracting the simulated voltage profile from the measured voltage profile. For each kind of ECM topology investigated, the testing cell was first used to evaluate the effectiveness of the ensemble BC model in bias-correcting the testing cell’s ECM for more accurate estimation of the voltage profile, then the applicability of the method for SoC estimation is studied. When studying the voltage estimation accuracy, the effect of adaptive weights is compared to that of equal weights. As the leave-one-out CV is adopted and seven cells are involved in the study, the CV process was performed seven times, with each of the seven cells left out as the testing cell at a time. The CV trials were marked as CV#i \( (i = 1, 2, \ldots, 7) \), where \( i \) is the index of the cell selected to be the testing cell.
5.2 Voltage Simulation Results

The voltage simulation results from the SECM without and with bias correction are shown in Fig. 10 (CV#4), Fig. 11 (CV#6), of the SCPD and the MCPD tests, respectively. Fig. 12 (CV#3) and Fig. 13 (CV#5) shows that from the ESC model, of the SCPD and the MCPD tests, respectively. Simulation results for the entire SOC range are shown in all the figures and two zoom-in plots showing details at some discharging pulses are included in each figure. For simplicity, the results of voltage simulation by ensemble BC with equal weights are not shown in the figures.

Figure 10. Comparison of SECM-simulated voltage profiles without BC/with ensemble BC (optimized weights) to measured voltage profile in SCPD test, CV#4
Figure 11. Comparison of SECM-simulated voltage profiles without BC/with ensemble BC (optimized weights) to measured voltage profile in MCPD test, CV#6

Figure 12. Comparison of ESC-simulated voltage profiles without BC/with ensemble BC (optimized weights) to measured voltage profile in SCPD test, CV#3
Figure 13. Comparison of ESC-simulated voltage profiles without BC/with ensemble BC (optimized weights) to measured voltage profile in MCPD test, CV#5

Table 3 and Table 4 summarize the voltage simulation errors, namely the root mean square error (RMSE), without BC and with ensemble BC of equal weights and of optimized weights, of the SECM and the ESC model, respectively.

Table 3. Voltage simulation errors without/with ensemble BC of SECM

<table>
<thead>
<tr>
<th>Voltage Simulation RMSE ($10^{-3}$ V)</th>
<th>CV#1</th>
<th>CV#2</th>
<th>CV#3</th>
<th>CV#4</th>
<th>CV#5</th>
<th>CV#6</th>
<th>CV#7</th>
<th>Overall</th>
<th>Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>SCPD, BC with equal weights</td>
<td>1.572</td>
<td>1.348</td>
<td>1.277</td>
<td>2.722</td>
<td>1.297</td>
<td>1.525</td>
<td>1.811</td>
<td>1.651</td>
<td>79.2%</td>
</tr>
<tr>
<td>SCPD, BC with optimized weights</td>
<td>1.290</td>
<td>1.198</td>
<td>1.226</td>
<td>2.287</td>
<td>1.355</td>
<td>1.280</td>
<td>1.939</td>
<td>1.511</td>
<td>80.9%</td>
</tr>
<tr>
<td>MCPD, BC with equal weights</td>
<td>2.195</td>
<td>1.545</td>
<td>1.983</td>
<td>2.165</td>
<td>1.697</td>
<td>1.616</td>
<td>2.374</td>
<td>1.939</td>
<td>72.3%</td>
</tr>
<tr>
<td>MCPD, BC with optimized weights</td>
<td>1.525</td>
<td>1.305</td>
<td>1.441</td>
<td>2.001</td>
<td>1.460</td>
<td>1.541</td>
<td>1.938</td>
<td>1.602</td>
<td>77.2%</td>
</tr>
</tbody>
</table>
Table 4. Voltage simulation errors without/with ensemble BC of ESC model

<table>
<thead>
<tr>
<th>Voltage Simulation RMSE (10^{-3}V)</th>
<th>CV#1</th>
<th>CV#2</th>
<th>CV#3</th>
<th>CV#4</th>
<th>CV#5</th>
<th>CV#6</th>
<th>CV#7</th>
<th>Overall</th>
<th>Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>SCPD, BC with equal weights</td>
<td>0.770</td>
<td>1.616</td>
<td>0.790</td>
<td>1.107</td>
<td>0.936</td>
<td>0.974</td>
<td>2.158</td>
<td>1.193</td>
<td>63.1%</td>
</tr>
<tr>
<td>SCPD, BC with optimized weights</td>
<td>1.070</td>
<td>1.246</td>
<td>0.609</td>
<td>1.793</td>
<td>1.184</td>
<td>0.643</td>
<td>1.705</td>
<td>1.178</td>
<td>63.5%</td>
</tr>
<tr>
<td>MCPD, BC with equal weights</td>
<td>1.476</td>
<td>1.427</td>
<td>0.982</td>
<td>2.045</td>
<td>1.052</td>
<td>2.236</td>
<td>1.903</td>
<td>1.589</td>
<td>61.4%</td>
</tr>
<tr>
<td>MCPD, BC with optimized weights</td>
<td>1.475</td>
<td>1.404</td>
<td>0.929</td>
<td>2.455</td>
<td>0.969</td>
<td>2.120</td>
<td>1.638</td>
<td>1.570</td>
<td>61.8%</td>
</tr>
</tbody>
</table>

Five important observations can be made from the results. Firstly, the ECMs with ensemble BC can improve the voltage simulation accuracy. It is observed that the voltage simulation errors with ensemble BC are consistently smaller than those without, regardless of the topology of the ECM. The ensemble BC (optimized weights) method achieved an overall error reduction of more than 60% for both SCPD and MCPD tests. Secondly, the ensemble BC term generated using optimized weights slightly outperforms that with equal weights in terms of voltage simulation and conclusion can be drawn that the adaptive weights can effectively improve the modeling accuracy. Thirdly, the improvement to accuracy of voltage simulation is achieved regardless of the SOC level. Zoom-in plots of different cells show that the ensemble BC produces improve accuracy of voltage simulation at different SoC levels. Fourthly, the efficiency of improvement in voltage simulation is affected by the ‘dynamic level’ of the pulsing test profiles. Comparing the improvements in the SCPD test and the MCPD test, under same condition other than the current profile, the ensemble BC method can better improve the simulation accuracy of a ‘simpler’ current profile (i.e., SCPD). Finally, the remaining voltage simulation errors of SECM and those of ESC have the same magnitude.
These results suggest that the proposed method is capable of capturing the cell- and condition-dependencies of the ECM bias and improving the ECM modeling accuracy through ensemble BC.

5.3 SoC Estimation Results

As the proposed BC framework is found to be capable of reducing the voltage modeling error, it is implemented to estimate SoC with EKF. The ensemble BC with optimized weights is adopted. Fig. 14 (CV#1) and Fig. 15 (CV#5) show the SoC estimation results with the use of SECM on the SCPD test and the MCPD test, respectively. The estimation results with the use of the ESC model are shown in Fig. 16 (CV#2) and Fig. 17 (CV#7). Each figure has two subplots: the first subplot shows a comparison between the true SoC and the estimated SoC, without and with ensemble BC; the second subplot shows the SoC estimation error without and with ensemble BC. Similar to the presentation in Section 5.2, results from one trial is presented for each combination of testing current profile and ECM topology for simplicity of illustration.

Table 5 and Table 6 present the RMSEs of SoC estimation with the use of the SECM and the ESC model, respectively. Three important observations can be made from the results. Firstly, the ensemble BC can consistently improve the SoC estimation accuracy with EKF when the SECM is adopted. Secondly, the SoC estimation accuracy of the proposed ensemble BC method with the ESC model is not improved consistently: for the SCPD test, the proposed method fails to improve the SoC estimation accuracy. Finally, the remaining SoC estimation errors, i.e. the overall RMSE, with the two different ECM topologies are close in their values and having the same magnitude for both the SCPD case and the MCPD
Figure 14. CV#1, SECM based SoC estimation results in SCPD test: (a) Comparison of SoC estimation results without/with ensemble BC; (b) SoC estimation Error without/with ensemble BC.
Figure 15. CV#5, SECM based SoC estimation results in MCPD test: (a) Comparison of SoC estimation results without/with ensemble BC; (b) SoC estimation Error without/with ensemble BC.
Figure 16. CV#2, ESC based SoC estimation results in SCPD test: (a) Comparison of SoC estimation results without/with ensemble BC; (b) SoC estimation Error without/with ensemble BC.
Figure 17. CV#7, ESC based SoC estimation results in MCPD test: (a) Comparison of SoC estimation results without/with ensemble BC; (b) SoC estimation Error without/with ensemble BC
case, respectively. A discussion on the inconsistency in the improvement of SoC estimation accuracy is given in the next chapter.

**Table 5.** SoC estimation errors without/with ensemble BC of SECM

<table>
<thead>
<tr>
<th>SoC Estimation RMSE: (10^{-3}%)</th>
<th>CV#1</th>
<th>CV#2</th>
<th>CV#3</th>
<th>CV#4</th>
<th>CV#5</th>
<th>CV#6</th>
<th>CV#7</th>
<th>Overall</th>
<th>Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>SCPD, BC with optimized weights</td>
<td>2.668</td>
<td>3.163</td>
<td>3.092</td>
<td>5.797</td>
<td>3.535</td>
<td>2.811</td>
<td>4.379</td>
<td>3.635</td>
<td>71.1%</td>
</tr>
<tr>
<td>MCPD, BC with optimized weights</td>
<td>0.906</td>
<td>0.982</td>
<td>0.843</td>
<td>1.263</td>
<td>1.334</td>
<td>1.255</td>
<td>3.932</td>
<td>1.502</td>
<td>83.0%</td>
</tr>
</tbody>
</table>

**Table 6.** SoC estimation errors without/with ensemble BC of ESC model

<table>
<thead>
<tr>
<th>SoC Estimation RMSE (10^{-3}%)</th>
<th>CV#1</th>
<th>CV#2</th>
<th>CV#3</th>
<th>CV#4</th>
<th>CV#5</th>
<th>CV#6</th>
<th>CV#7</th>
<th>Overall</th>
<th>Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>SCPD, no BC</td>
<td>1.478</td>
<td>2.329</td>
<td>1.853</td>
<td>2.027</td>
<td>1.545</td>
<td>1.894</td>
<td>2.826</td>
<td>1.993</td>
<td></td>
</tr>
<tr>
<td>SCPD, BC with optimized weights</td>
<td>1.825</td>
<td>4.160</td>
<td>2.860</td>
<td>4.840</td>
<td>1.896</td>
<td>3.068</td>
<td>4.058</td>
<td>3.244</td>
<td>-62.7%</td>
</tr>
<tr>
<td>MCPD, no BC</td>
<td>3.946</td>
<td>2.227</td>
<td>3.598</td>
<td>4.775</td>
<td>2.332</td>
<td>1.222</td>
<td>2.016</td>
<td>2.874</td>
<td></td>
</tr>
<tr>
<td>MCPD, BC with optimized weights</td>
<td>0.762</td>
<td>2.103</td>
<td>0.570</td>
<td>2.024</td>
<td>1.126</td>
<td>3.085</td>
<td>2.791</td>
<td>1.780</td>
<td>38.1%</td>
</tr>
</tbody>
</table>
CHAPTER 6 DISCUSSION AND CONCLUSIONS

6.1 The Effect of Inaccurate SoC

Although it is observed that the proposed method can consistently improve the voltage simulation accuracy, the SoC estimation results are not showing consistent improvement. To this end, a case study was conducted to unveil the fundamental reason of why the proposed ensemble BC method cannot consistently reduce the SoC estimation error.

In general, the effectiveness of the proposed method is under the influence of the modeling accuracy of the ECM. The two ECM topologies investigated are considered as two cases in the case study. To explain why the proposed method can succeed in improving the SoC estimation accuracy for the SECM but fail to do so for the ESC model. The two cases represent two different scenarios: (1) the overall simulation error, i.e., the difference between the ECM-simulated voltage and the measured voltage, is relatively large (SECM) and (2) the difference is relatively small. The explanation starts with how the ensemble BC terms were formed. The member BC models in the proposed method are defined as the difference between the training cells’ measured voltage and the ECM-simulated voltage (see Eq. (12)) and the simulated voltage is defined as the voltage simulation result from the adopted ECM with the current measurement as input into the ECM. Thus, at every time step in this process, the SoC value which is computed by coulomb counting is considered to be the true SoC. The member BC model value at each time step is, naturally associate with the true SoC value. However, during the process of estimating SoC with EKF, the SoC estimate which would be corrected with the knowledge of simulation error is different from the SoC value directly
calculated by coulomb counting. This difference in SoC value causes a difference in the ECM simulated output voltage (Fig. 18).

![Graph showing comparison of the difference in SoC and the change in simulated output voltage](image)

**Figure 18.** Comparison of the difference in SoC and the change in simulated output voltage

Although this difference is generally small as observed from experimental validation data, the direction and magnitude of this difference in the simulated output voltage is indefinite. In cases where the difference has the same magnitude and direction as the overall voltage simulation error, it can neutralize the effect of ensemble BC term (Fig. 19(b)). The overall simulation error is the difference between the ECM simulated voltage and the measured voltage. While, if the overall voltage simulation error is significantly larger than the difference, as in Fig. 19(a), the ensemble BC can still help to reduce the voltage simulation error as it can capture the systematical discrepancy.
Case I: SECM

Figure 19. Comparison schematic of the relationship between Ensemble BC Term, the difference in simulated output voltage and overall simulation error. (a). SECM; (b). ESC model

6.2 Summary of Experimental Validation

This thesis has proposed an ensemble bias-correction (BC) method with adaptive weights for improving the accuracy in dynamic modeling of Li-ion batteries. An adaptive-weighting scheme facilitates a systematic consideration of the cell- and condition-dependencies of the model bias when forming the ensemble BC model, and thus allows for optimally combining the member BC models to maximize the bias-correction capability of
the ensemble. Results from an experimental study suggest that (i) the proposed ensemble BC method is capable of reducing the modeling error of an ECM under both single and multiple C-rate pulsing tests; (ii) the ensemble BC model with online adaptive-weighting can capture cell-to-cell variabilities; (iii) the proposed method can achieve satisfactory generalization performance, as verified by the CV and (iv) the proposed method can improve the voltage modeling accuracy of ECMs with different topologies.

A EKF based SoC estimation approach is adopted to examine the practicableness of the proposed ensemble BC method in improving the SoC estimation accuracy. Two observations can be made: (i) the proposed ensemble BC method can improve the SoC estimation accuracy when the SECM is used and (ii) the proposed method cannot provide consistent SoC estimation improvement when the ESC model is adopted. Moreover, based on discussion in Section 6.1, the proposed method can be utilized to reduce the systematic modeling discrepancies when the overall modeling error is relatively large.

6.3 Limitations and Future Work

As have been indicated in previous chapters, the proposed ensemble BC method has several limitations. Firstly, the practical usefulness of the proposed method is highly constrained by its strong assumption that the current profile of each training cell should cover exactly that of a testing cell. Thus, constructing a training data set that meets this assumption in practical applications would require numerous offline tests on training cells and these tests may be too expensive to be tractable or the training data set may be too large to be deployable by BMS. Secondly, the addition of the ensemble BC term may have an adverse effect on SoC estimation, since the term is not adaptive to the inaccuracy in SoC estimation. Further research should be conducted to: (i) loosen the assumption on the current profile to
make ensemble BC practically useful and (ii) modify the model to make the ensemble BC generating scheme adaptive to the inaccuracy in SoC estimation.
REFERENCES


