

Measurement-Based Development of High-Fidelity Electrochemical Models for LFP Cells

Hasegawa Takatoshi ¹⁾ Miyazaki Ryotaro ¹⁾ Takahashi Kazunao ¹⁾ Araki Kengo ¹⁾
 Ejima Tomomi ¹⁾ Tsuji Hironobu ²⁾ Moriwaki Hirofumi ²⁾

1) IDAJ Co., LTD.

Yokohama Landmark Tower 37F, 2-2-1-1 Minato Mirai, Nishi-Ku, Yokohama City, Kanagawa, 220-8137, Japan

2) Toray Research Center, Inc.

3-2-11, Sonoyama, Otsu, Shiga, 520-8567, Japan

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Electrochemical battery models, represented by the pseudo-two-dimensional (P2D) model proposed by John Newman and co-workers, describe lithium-ion reactions and transport based on charge conservation, lithium-ion mass conservation, and the Butler–Volmer equation. Because battery characteristics can be calculated from cell design information and material properties, these models have the potential to predict the effects of changes in materials and cell structures. However, P2D models involve a large number of parameters and many of which cannot be uniquely determined without prior measurements. In recent years, the independent identification of individual physical parameters from a single terminal-voltage response has been recognized as challenging because of parameter non-identifiability.

In this study, the role of internal measurement data in achieving both accuracy and generalizability in battery performance prediction using an electrochemical P2D model was investigated. An LFP battery installed in a Chinese electric vehicle was analyzed by incorporating internal measurement data obtained through cell teardown into the model. The model predictions were validated against experimental results from constant-current (CC) charge/discharge tests conducted over a C-rate range of 0.2C–2.5C. The objectives of this study were to evaluate model accuracy through comparison with measured CC charge/discharge characteristics and to clarify the effects of internal measurement data on model accuracy and generalizability through comparison with models constructed by fitting only a single voltage response. In addition, the influence of the C-rate condition used for parameter identification on model generalizability was investigated.

For the LFP battery, cell teardown measurements were used to obtain geometric information. In addition, the areal loading, porosity, conductive additive-to-binder ratio, active material composition, and exchange current density of the positive and negative electrodes were determined. The porosity and thickness of the separator and the electrolyte salt concentration, solvent composition, transference number, self-diffusion coefficient, and ionic conductivity were also obtained. An electrochemical simulation tool, GT-AutoLion, was used to construct the battery models, and material properties that were not directly measured were supplemented using the material property database provided in the software. Model performance was evaluated by comparing the predicted voltage profiles with experimental CC charge/discharge data obtained over a C-rate range of 0.2C–2.5C. Three modeling conditions were considered: Case A, in which cell teardown measurement data were directly incorporated into the model; Case B, a model fitted only to the 0.2C characteristics to evaluate generalizability; and Case C, a model fitted only to the 2.5C characteristics for the same purpose. Parameter optimization was performed using a genetic algorithm by minimizing the mean squared error between the simulated and measured voltage and capacity characteristics. The evaluation metric was the relative error of the identified design parameters with respect to the cell teardown measurements.

For the Case A model, the overall trends of the voltage response, including the end points of both charge and discharge, were reproduced with high accuracy over the entire C-rate range from 0.2C to 2.5C (Fig. 1). In contrast, although Case B, which was fitted only to the 0.2C characteristics, showed good agreement with the measured voltage–capacity curve, several of the identified design parameters exhibited errors exceeding $\pm 50\%$ relative to the teardown measurement results. In addition, limitations remained in the prediction accuracy of the capacity at higher C-rates, including 1C and 2.5C. Conversely, Case C, in which fitting prioritized the 2.5C characteristics, showed reduced voltage prediction accuracy under the low-C-rate condition of 0.2C.

The results obtained in this study, in which fitting only to the 0.2C characteristics resulted in errors exceeding $\pm 50\%$ in parameters such as electrode thickness and active material particle size, support the presence of this parameter non-identifiability. Under low-C-rate conditions, concentration gradients within the electrodes and diffusion-related overpotentials are relatively small. Consequently, the sensitivity of the voltage response to diffusion-related parameters, such as electrode thickness and active material particle size, is reduced. Therefore, different combinations of parameters that deviate substantially from the actual measured values may still reproduce similar voltage and capacity characteristics. These results suggest that achieving both high model accuracy and generalizability requires not only multi-condition parameter fitting across multiple C-rates and temperatures but also the direct incorporation of detailed internal measurement data, as demonstrated in this study.

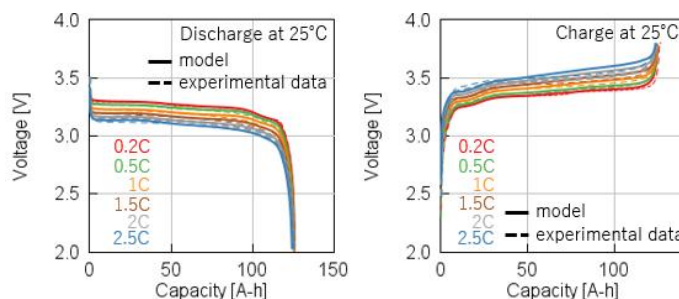


Fig.1 Case A model: charge-discharge at 25°C for each C-rate.