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Improving temperature predictions for Li-ion batteries: data assimilation with a stochastic extension of a physically-based, thermo-electrochemical model

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ABSTRACT

Prediction and estimation of internal battery states are important tasks for safe operation of batteries. However, due to inherent uncertainties like parameter, model structural and measurement uncertainties, it is especially challenging to make accurate predictions. We present a novel method for handling the structural error of a thermo-electrochemical battery model. With structural error, we refer to the errors caused by simplifications taken during modeling. We extend the battery model of a $LiFePO_4$-graphite lithium-ion cell with an internal, stochastic error model in a minimally-intrusive way. We find the optimal error model parameters with Approximate Bayesian Computation and compare two error models of different complexity: an auto-regressive and a white-noise multiplier for the heat source term. Both extended models are then used together with a particle filter for data assimilation to determine adequate uncertainty bounds for predictions of the surface temperature at a 1 C discharge rate. We show that the auto-regressive extended model can use the assimilated data more effectively to increase the predictive performance of the model on average when compared to the white-noise extended model. Our main conclusion is that accounting for the time-correlated character of model errors helps improve data assimilation and predictive performance of physically-based thermo-electrochemical battery models.

1. Introduction

In recent years, secondary lithium-ion batteries have become one of the most important parts of vehicles and consumer electronic devices due to the increasing importance and number of electric vehicles [1] and mobile electronic applications. In all these applications, the safe operation of the included batteries is of particular interest [2]. Among other safety strategies, safe operation requires the prediction and estimation of battery states such as the temperature distribution inside the battery. Unfortunately, any prediction task is challenged by inherent uncertainties that lead to prediction errors. Common error sources are measurement uncertainty, parameter uncertainty and model structural errors. With model structural errors, we refer to the uncertainties arising from simplifications, closures or other assumptions made during modeling. This paper addresses the handling of model structural errors for the estimation of physical battery states. Our specific focus is on the time-correlated character of model structural errors that violate the assumptions usually taken in uncertainty analysis and data assimilation. Our state of interest is the battery surface temperature.

Selected battery states like the surface temperature [3,4] or the state of charge and state of health are commonly estimated for prognostic and health monitoring purposes [5]. The focus lies on estimation techniques that allow quick evaluation with low computational effort. For this task, the most widely used techniques are equivalent-circuit models and, more recently, data-driven black-box techniques like neural networks or support vector machines. An overview can be found in recent review papers (e.g., [6,7]). Especially equivalent-circuit models are commonly combined with data assimilation techniques like Kalman filters [8] and their derivatives (e.g., [9]). In their definition of the system equations, most authors usually implement an error term as additive, random white noise [5]. One exception is Fridholm et al. [10] who recently applied an additive correlated error (instead of white noise) within an adaptive Kalman filter.

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Another option for battery state estimation is to use physically motivated models formulated as (partial) differential equations (PDEs). These models are referred to as physically-based models in the following. They are based on fundamental physical principles and therefore attributed with a certain credibility. In contrast to equivalent-circuit models and data-driven methods, physically-based models naturally allow the estimation of a whole range of physical battery states, including the temperature distribution within the cell.

Because of the higher computational demands of physically-based models, there exist far fewer studies that use physically-based models of different complexity for battery state estimation (e.g., [11,3,12]). Recently, Tagade et al. [13] developed a general Bayesian framework for the estimation of cell states and used a reduced-order model that was derived from a physical model but chose not to investigate model structural errors in their study. In an earlier publication, Tagade et al. [14] formulated the structural model uncertainty of a thermo-electrochemical model in a Bayesian calibration framework by means of a white noise discrepancy function that was added to the model equation.

To the best of our knowledge, there has not been any study that tries to improve the temperature prediction performance of a physically-based battery model by addressing the model structural error with an *internal error model* in combination with data assimilation. By *internal error model*, we refer to an error model that acts on the level of the PDEs, in contrast to an additive error model that is added to the model response without affecting the PDE solution in subsequent time steps.

The goals of this paper are to

- extend a physically-based battery model with an internal, stochastic error model that intends to provide a statistical envelope to structural errors,
- achieve this extension in a way that does not unnecessarily harm the physical credibility of the battery model,
- choose the error model such that the structure of the resulting extended model is plausible and such that the time-correlated character of errors is accounted for, and to
- use this extended model in a data assimilation context for predicting the battery temperature better than with previously used uncorrelated error assumptions.

To achieve these goals, we will combine an existing physically-based battery model [15,16] with an internal, stochastic error model and use this extended model in combination with a particle filter (e.g., [17]) to enable straightforward data assimilation. This combination will create an extended model with decent physical credibility that accounts for the model structural error, quantifies the uncertainty inherent in its predictions and can be updated with real-time measurement data.

In summary, this paper contributes a stochastic method that extends a physically-based battery model with an error model on the level of the PDEs to improve the quality and predictive reliability of temperature predictions. This unique approach offers a new method to tackle model structural uncertainties which exist in any physically-based battery model and allows for the implementation of a correlated error model. Moreover, we compare the usefulness of an auto-correlated and an uncorrelated white noise error model to support the idea of addressing the partial temporal persistence of model errors. Fig. 1 gives an overview of the proposed workflow in this paper.

In the following, we first briefly outline the physically-based battery model in Section 2.1 and the available experimental data in Section 2.2. Afterward, we extend the physically-based model with an internal error model to create the extended model and explain our procedure to find the optimal error model parameters in Section 3. Here, we consider two extended models of different complexity, i.e., a white-noise model and an auto-correlated model. Subsequently, we apply both extended models to data assimilation with a particle filter in Section 4. Finally, we investigate and compare the performance of the two extended models for temperature predictions at a 1 C discharge rate at room temperature in Section 5 to demonstrate the advantages of the auto-correlated error model. Section 6 summarizes and concludes this paper.

2. Prerequisites: physically-based battery model and experimental data

2.1. Physically-based battery model

The foundation of the presented methodology is a physically-based, thermo-electrochemical battery model. In this study, we use a model that uses the well-established battery modeling framework presented in Hellwig et al. [15] and Hellwig [16].

This modeling framework has been continuously developed over the last years for numerous applications for different battery types. Regarding lithium-ion batteries, this includes for example thermal decomposition reactions during thermal runaway [18], and more recently the aging of $LiFePO_4$-graphite cells [19]. Yet, for the purpose of this study the model as presented in [16] is sufficient, because we are mostly interested in predicting operational temperatures (not aging or thermal decomposition), and we are specifically interested in a tuned model that exhibits a realistic portion of model structural error to showcase the methodology. Thus, we reproduce the most important facts and equations from the cited sources.

The model simulates a 26650 A123 $LiFePO_4$-graphite cylindrical cell as a 1D (pseudo-2D or P2D) radially symmetric system and models different phenomena on different scales. Numerically, it is based on the finite volume method.

The (de-)intercalation of lithium in the electrodes follows:

$$LiC_6 \rightleftharpoons Li^+ + e^- + C_6 \tag{1}$$

$$FePO_4 + Li^+ + e^- \rightleftharpoons LiFePO_4, \tag{2}$$

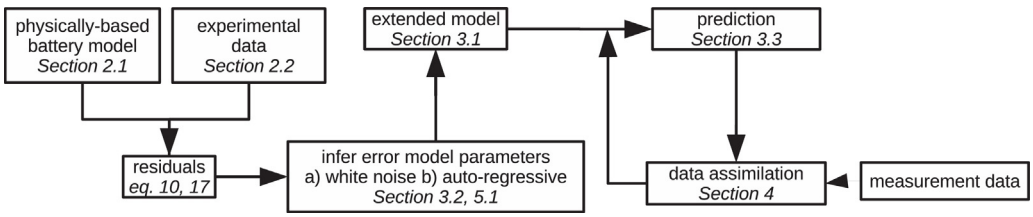

Fig. 1. Visualization of the overall workflow of the proposed method. We compare the prediction performance of two of these extended models (white noise and auto-regressive) against each other.