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Bayesian calibration for electrochemical thermal model of lithium-ion cells

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HIGHLIGHTS

- Bayesian framework for calibration of the P2D-ECT model.
- Matrix-variate Gaussian process for computationally efficient implementation.
- P2D-ECT model parameter estimation and quantification of model uncertainty.
- Accurate model prediction across a range of temperatures.
- Novel insights into low temperature Li-ion cell operation.

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ABSTRACT

Pseudo-two dimensional electrochemical thermal (P2D-ECT) model contains many parameters that are difficult to evaluate experimentally. Estimation of these model parameters is challenging due to computational cost and the transient model. Due to lack of complete physical understanding, this issue gets aggravated at extreme conditions like low temperature (LT) operations. This paper presents a Bayesian calibration framework for estimation of the P2D-ECT model parameters. The framework uses a matrix variate Gaussian process representation to obtain a computationally tractable formulation for calibration of the transient model. Performance of the framework is investigated for calibration of the P2D-ECT model across a range of temperatures (333 K–263 K) and operating protocols. In the absence of complete physical understanding, the framework also quantifies structural uncertainty in the calibrated model. This information is used by the framework to test validity of the new physical phenomena before incorporation in the model. This capability is demonstrated by introducing temperature dependence on Bruggeman's coefficient and lithium plating formation at LT. With the incorporation of new physics, the calibrated P2D-ECT model accurately predicts the cell voltage with high confidence. The accurate predictions are used to obtain new insights into the low temperature lithium ion cell behavior.

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1. Introduction

Majority of the contemporary consumer electronic devices use rechargeable batteries as the primary energy source, while many other industrial applications employ rechargeable batteries as a secondary source of energy. Rechargeable batteries have also found a renewed interest in the automotive industry. Continuous improvement of the battery technology is essential for advancements of the electronic devices and other applications. Advancements in the battery technology are particularly important for the automotive industry, where novel electro-chemistries and cell designs can enable the development of cleaner electric (EVs) and hybrid-electric vehicles (HEVs) [1,2]. Accurate and credible physics-based battery models are required for investigation of these new electro-chemistries and subsequent optimized cell designs. The

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physics-based battery models (often after model order reduction [3]) can also be used on-board the next generation battery management systems for intelligent cell monitoring and control purposes. Reliable cell design and subsequent development of the model based battery management system require accurate model predictions. The designer or an on-board model based controller is expected to make safety critical decisions conditional on the model credibility [4]. Here, the model credibility reflects the user confidence on the model predictions [5]. Thus, establishing accuracy and the credibility assessment [6,7] of the physics-based battery models is a critical prerequisite for the future advancements of the battery technologies, including the development of novel cell designs and the battery management systems.

Lithium ion batteries are currently the most widely used rechargeable energy source for consumer electronic devices. Due to their low weight, low self-discharge rate, high energy and high power density, lithium-ion batteries are particularly attractive for automotive applications [8,9]. With the ever-increasing applications, mathematical modeling of the lithium ion batteries has attracted a significant interest of research community. Different lithium ion battery models, varying from the low fidelity empirical equivalent circuit models to the high fidelity continuum scale electrochemical models are reported in the literature [10,11]. Several authors use equivalent circuit models for lithium ion battery design, optimization and control tasks [12–15]. Comparison of the most widely used equivalent circuit models is available in the literature [16]. Though computationally efficient, the equivalent circuit models do not have a capacity to capture internal electrochemistry of the battery, and have limited accuracy and predictive capabilities [10].

For high energy automotive applications like EVs and HEVs, internal electro-chemical information can be exploited to extend the driving range while ensuring a safe battery operation. Continuum scale pseudo-two dimensional electrochemical thermal models (P2D-ECT) provide this detailed internal battery information. The P2D-ECT models are based on the porous electrode theory developed by Newman et al. [17,18]. Governing equations for the P2D-ECT model consists of a set of five coupled PDEs; four PDEs that define charge and mass balance for solid and electrolyte phases, and a fifth PDE that models thermal balance for the battery [19,20]. Butler-Volmer kinetics is used to obtain closure for the governing equations [10,21]. In the P2D-ECT model, the solid and electrolyte phase charge balance, electrolyte phase mass balance and energy balance equations are solved along the length of the cell. The solid phase mass balance equation is solved for a spherical particle in a so called pseudo-second dimension [10]. Details of the P2D-ECT model can be found in Refs. [10,11] and its reformulations are discussed in Ref. [22] and references therein.

The P2D-ECT model contains many parameters that are unknown or poorly known. Moreover, some of the electrochemical behavior of the lithium ion battery, especially at low temperature and high current operations, is still poorly understood [23]. This poorly understood electro-chemistry either remains unaccounted, or heavily approximated, in the P2D-ECT model. The poorly known parameters and the unaccounted/approximated electro-chemistry induce uncertainty in the P2D-ECT model outputs. A detailed model calibration process is essential to reduce these uncertainties. The model calibration process is expected to achieve two key objectives [4]: a) parameter estimation to reduce uncertainty in the poorly known parameters; and b) quantification of the model uncertainty due to unaccounted/approximated electro-chemistry. The quantified model uncertainty assesses the credibility of the model. Current literature on calibration of lithium ion battery models, however, is limited to the parameter estimation.

In the context of lithium ion batteries, the parameter estimation methods are primarily focused on the equivalent-circuit models. Several authors use traditional least-square regression methods for equivalent circuit model parameter estimation [24–26]. Although limited, there are notable exceptions where parameter estimation of full P2D-ECT model is reported [27]. Forman et al. [28] use genetic algorithm (GA) for estimation of the P2D-ECT model parameters. Reimers et al. [29] use Levenberg-Marquardt (LM) algorithm in a least-square setting to estimate parameters that minimize the squared error between the predicted and measured cell voltage across a range of temperature and load current. The parameter estimation using methods like GA or MA, however, require several executions of the P2D-ECT model. The high computational cost of the P2D-ECT model, thus, renders these methods computationally very expensive. Several other authors use model order reduction to ensure computational tractability of the parameter estimation methods. Ramadesigan et al. [30,31] use the Gauss-Newton method with a reformulated model to estimate the parameters. Santhagopalan et al. [32] use the LM algorithm with a single particle model for parameter estimation. Masoudi et al. [27] use the homotopy optimization method with their reduced order model for parameter estimation that ensures convergence of the solution to the global optimum.

The optimization methods for parameter estimation are limited by two key deficiencies: 1) the optimization methods can not quantify uncertainty in the estimated parameters; and 2) the optimization methods can not take into account any prior information about the parameters, though, a physical interpretation can be obtained for the estimated parameters a-posteriory, as demonstrated in Ref. [33]. The Bayesian inference method effectively resolves both these deficiencies. Effectiveness of the Bayesian inference for lithium ion battery state estimation is demonstrated by Saha et al. [34]. In the context of P2D-ECT model, Ramadesigan et al. [30,31] compare the Bayesian inference method with the traditional Gauss-Newton optimizer for parameter estimation. Although Ramadesigan et al. [30,31] quantify model parametric uncertainty, they do not consider the effect of model structural uncertainty to asses credibility of the calibrated model.

In this paper, a Bayesian framework [4] is presented for calibration of the P2D-ECT model. The framework can simultaneously estimate the parameters and also assess the credibility of the model. The framework is based on a Bayesian inference method developed by Kennedy and O'Hagan [35] for calibration of a computer simulator. The Bayesian framework of Kennedy and O'Hagan [35] is widely used in the varied fields for calibration of simulators [36,37]. The implementation of the framework for calibration of the P2D-ECT model, however, is challenging due to the high computational cost and transient nature of the model output. In this paper, an extension of the Bayesian framework of Kennedy and O'Hagan [35] is proposed, which efficiently resolves both these challenges. Key innovation of the proposed Bayesian framework is a use of matrix variate Gaussian distribution [38–40], which makes calibration of the P2D-ECT model computationally tractable. The Markov Chain Monte Carlo (MCMC) sampling [41,42] is used for numerical implementation of the proposed framework.

Research work presented in this paper advances the current state of the art as follow: a) to the authors knowledge, this research work is a first reported full calibration of the spatially resolved P2D-ECT model; b) use of the matrix-variate Gaussian process priors is novel. The proposed algorithm for numerical implementation of the framework extends current state of the art of the Bayesian calibration methods; c) this paper introduces new physics to the existing P2D-ECT model and a method for efficiently testing the validity of the new physics. The paper also present new insights into the temperature dependence of the Bruggeman's relation.

As compared to the state of the art optimization based P2D-ECT

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