Electrochemical state and internal variables estimation using a reduced-order physics-based model of a lithium-ion cell and an extended Kalman filter

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HIGHLIGHTS

- Next-generation BMS will require estimates of cell electrochemical internal variables.
- Extended Kalman filter using physics-based reduced-order model finds these estimates.
- Method uses readily available measurements of voltage, current, and temperature only.
- Results agree closely to truth values and are robust to incorrect initialization.
- Automatic confidence intervals on estimates allow their use in follow-on application.

ARTICLE INFO

ABSTRACT

This paper addresses the problem of estimating the present value of electrochemical internal variables in a lithium-ion cell in real time, using readily available measurements of cell voltage, current, and temperature. The variables that can be estimated include any desired set of reaction flux and solid and electrolyte potentials and concentrations at any set of one-dimensional spatial locations, in addition to more standard quantities such as state of charge. The method uses an extended Kalman filter along with a one-dimensional physics-based reduced-order model of cell dynamics. Simulations show excellent and robust predictions having dependable error bounds for most internal variables.

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1. Introduction

This paper addresses the problem of estimating the present value of electrochemical internal variables in a lithium-ion cell in real time, using readily available measurements of cell voltage, current, and temperature. The variables that can be estimated include any desired set of reaction flux and solid and electrolyte potentials and lithium concentrations at any set of one-dimensional spatial locations, in addition to more standard quantities such as electrode or cell state of charge (SOC). The method uses an extended Kalman filter (EKF) along with a one-dimensional physics-based reduced-order model (ROM) of cell dynamics.

This work is motivated by the needs of next-generation battery-management systems (BMS). A BMS needs accurate cell state estimates to be able to manage the battery pack properly to ensure safe, robust, and reliable operation. Whereas state-of-the-art battery-control strategies address short-term objectives using voltage-based design limits, little has been done to improve battery performance and to extend lifetime using design limits based on internal electrochemical variables. Just as a present-generation BMS requires state-of-charge estimates to enforce voltage limits, next-generation BMS will require estimates of internal electrochemical variables to enforce the more advanced design limits.

It is quite common now to see articles proposing methodologies to estimate cell state of charge. Various approaches exist [1], but model-based methods seem to be dominant as the built-in feedback makes them robust, and a good model makes them accurate. In the estimation literature as a whole, the Kalman filter (KF) remains one of the most widely used model-based state estimators

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due to its simplicity, optimality, tractability and robustness [2]. Relying on an underlying linear model of system dynamics, the KF uses input—output measurements and probabilistic descriptions of uncertainty to generate a minimum-mean-squared optimal estimate of a system's internal state vector as it evolves in time. It is well known, however, that application of the KF to nonlinear systems can be difficult. A popular approach to overcome this difficulty is the implementation of an extended Kalman filter (EKF), which essentially linearizes the nonlinear system models in such a way that the linear KF steps can be used.

Model-based methods such as the KF and EKF require a mathematical description—that is, a *model*—of cell dynamics as part of the procedure for estimating internal states of the cell. In the electrochemical literature, these models tend to fall into one of two categories: those developed empirically by observing input—output behaviors and proposing equations to match those observations, and those developed from physics first principles.

Empirical models of cells are most commonly realized as *equivalent-circuit* models, since interconnected linear (and sometimes nonlinear) electric circuit elements are employed as analogs to observed behaviors [3]. These kinds of models are very commonly used in present-generation BMS implementations as they are relatively simple to develop and can predict cell input—output behaviors well so long as great care is taken in the selection of the model parameter values. Prior work shows good results for SOC-estimation using EKF with equivalent-circuit models [4—6], and indicates that model-based estimation using equivalent-circuit models may be adequate if the BMS requires estimates of SOC only and if cell aging can be captured sufficiently via slow adaptation of cell resistance and capacity parameter values.

Equivalent-circuit models can produce accurate predictions of cell voltage; however, they do not provide insight into the internal electrochemical variables of the cell. On the other hand, physics-based porous-electrode models do have this ability. Doyle, Fuller, and Newman [7,8] have developed such a physics-based model, which comprises coupled nonlinear partial-differential equations (PDEs). While physics-based models are far more challenging to derive, they offer two significant advantages over equivalent-circuit models: first, they predict cell operation outside the bounds of previously collected data (*i.e.*, they extrapolate well) and, second, they describe the electrochemical internal dynamics of the cell in addition to being able to predict cell voltage.

This latter feature is of critical importance to next-generation BMS. The cell's internal dynamics are key to how it ages and degrades; thus, being able to estimate the present value of these internal electrochemical variables using a physics-based model is key to predicting and invoking controls to avoid degradation.

Control algorithms based on knowledge of the internal electrochemical state have the potential to expand the performance and extend the life of cells. They can predict power limits with respect to electrode surface depletion/saturation conditions and with respect to side reactions responsible for damage and sudden loss of power [9,10]. For example, some early "full-information" controls (*i.e.*, which assume perfect knowledge of cell internal variables, as precursor work to practical implementable methods which must estimate the values of these variables using only measurements of voltage, current, and temperature) [11] shows that electrochemically limited pulse charging a 6 A h cell to the same negative-electrode phase-potential $\phi_s - \phi_e$ at the negative-electrode/separator boundary as encountered at equilibrium at 100% SOC increases usable charge power by 22% and usable energy by 212% vs. voltage-limited charging.

A practical and implementable feedback control scheme particularly well suited to extending battery cell life while yielding

maximum performance is model-predictive control (MPC), which is gaining popularity throughout industry in other applications [12]. Employing a "look-ahead" strategy, MPC can foresee dynamic changes before they happen and efficiently compute stepwise-optimal control to achieve a quadratic performance objective. Most importantly however, MPC is able to handle hard (as well as soft) constraints on designated problem variables. The potential employment of MPC for improved cell-level battery control is directly dependent on the availability of certain electrochemical variables internal to the lithium ion cell. Since these variables are not easily (or at all) measurable, they must be estimated from easily obtained voltage—current—temperature information during cell operation. The estimates provided by EKF are highly compatible for use with MPC.

At this point in history, however, the computational complexity of porous-electrode PDE models precludes their use by EKF and real-time control systems. Instead, accurate reduced-order approximate models, which can predict both the cell voltage and internal electrochemical variables, are needed.

For example, Santhanagopalan et al. used single-particle models and simplified porous-electrode models in conjunction with extended and sigma-point Kalman filters to estimate cell SOC [13,14]. Di Domenico et al. used simplified averaged electrochemical models with both continuous-time linear Kalman filters and extended Kalman filters to estimate cell SOC and particle surface concentration at the current collectors [15,16]. Neither of these, however, addressed the problem of estimating general internal electrochemical variables at arbitrary points in the cell.

Other efforts similar to this present work include papers by Klein et al., which assumes constant electrolyte concentration and a polynomial approximation to solid concentration to arrive at a partial-differential algebraic model, sampled on a coarse grid across the cell, which is then used by an output error injection state observer [17,18]. This model is of higher computational complexity than the one we use in this work, and the output error injection observer does not provide confidence bounds on the estimated states. While the authors state that their observer can estimate the values of internal electrochemical variables, they show results of SOC estimation only.

Perhaps the most similar work is that of Smith et al. [10,19]. These authors simplify the electrochemical model using a transfer-function approach, as do we, which forgoes the necessity of solving PDEs on a spatial grid. However, they do not employ the nonlinear corrections and model blending that characterize the model that we use, and which significantly improve model predictions across a wide range of state-of-charge and temperature, and at high rates. Further, they used a linear Kalman filter on their fully linear model, as opposed to the nonlinear EKF used herein. And, while they state that their methodology can estimate internal electrochemical variables, they do not derive the extra steps needed to correctly estimate the variables and the confidence interval of the estimate from the *a posteriori* model state vector estimate and covariance, and they show results of cell and electrode SOC estimation only.

In this work, we use EKF with a one-dimensional physics-based reduced-order model of lithium-ion dynamics. This five-state discrete-time model is of similar computational complexity to an equivalent-circuit model, and gives very good predictions of cell voltage as well as the cell internal variables. We have presented this model elsewhere in a series of three papers: the first paper introduced the "discrete-time realization algorithm" (DRA) as a subspace projection method for converting a transcendental transfer function into a discrete-time state-space reduced-order model [20]. The second paper showed how to find transcendental transfer functions corresponding to lithium-ion internal cell dynamics [21], and invoked the DRA to create a ROM that is linearized to give