Applied Energy 258 (2020) 113925

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

An adaptive sigma-point Kalman filter with state equality constraints for online state-of-charge estimation of a $Li(NiMnCo)O_2$/Carbon battery using a reduced-order electrochemical model

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HIGHLIGHTS

- A new SOC estimation algorithm based on a reduced-order model is proposed.
- An adaptive algorithm with state equality constraints is incorporated.
- A comparative study of nonlinear filters show the advantages of the proposed method.
- The proposed method is tested in real-time using a battery-in-the-loop test station.
- Significant improvements are achieved in reducing the voltage and SOC error.

ARTICLE INFO

Keywords:
Adaptive filtering
Equality state constraints
Lithium-ion battery
Reduced-order model
State-of-charge
Square-root sigma-point Kalman filter

ABSTRACT

A new SOC estimation method is proposed based on a reduced-order electrochemical model using an adaptive square-root sigma-point Kalman filter (ASR-SPKF) with equality state constraints. The constraints derived from the principle of charge conservation are introduced to improve the accuracy of both anode and cathode SOC estimations. Furthermore, the cathode SOC is estimated to represent the cell SOC for its fast convergence speed, which is due to the high magnitude of the cathode equilibrium potential. Approaches used to adaptively updating the covariance parameters of the filter based on the covariance matching method are also incorporated. As a result, the covariance matrix of process noise is adjusted automatically. Comparative studies of three nonlinear filters concerning estimation accuracy, error bounds, recovery time from an initial offset, and computational time revealed that the ASR-SPKF has the most outstanding performance. That is, 30% more accurate and 88% shorter the convergence time than the AEKF, and, computationally, 23% and 19% faster than the AEKF and ASPKF, respectively. Then, the proposed method was tested at different temperatures using a large-format lithium-ion battery with a nominal capacity of 42 Ah where the voltage and SOC error remained less than 22 mV and 2%, respectively. Finally, the proposed method was implemented in a battery-in-the-loop test station using a fast charging and a driving cycle profile, and the estimated voltage and SOC were compared with the experimental results.

1. Introduction

State-of-charge (SOC) represents the remaining capacity of a battery that can be released. It plays a crucial role in ensuring a safe and reliable battery operation by preventing under- or over-charge, and predicting available power and energy because of its close relationship to the lithium ion concentration, which is one of the core physical states of a lithium-ion battery. However, SOC cannot be directly measured. Many attempts have been made to find the best approach that enables an accurate estimation of SOC, and one of the most widely used methods is based on an equivalent circuit model (ECM) that uses electrical components–resistors, capacitors, and voltage sources–to mimic battery dynamics [1]. Then, parameters of the ECMs, as well as the SOC, are simultaneously updated by an estimator. However, the parameters of the ECMs do not provide physical information of the battery, such as ion concentrations, potentials, overpotentials, and current density, to name a few. The accurate estimation of such variables provides various benefits, such as the detection of ion

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https://doi.org/10.1016/j.apenergy.2019.113925
Received 3 June 2019; Received in revised form 6 September 2019; Accepted 18 September 2019
Available online 23 November 2019
0306-2619/

concentration depletion/saturation [2], degradation prediction that considers side reactions and lithium deposition reactions [3,4], and the optimization of ultra-fast charging protocols that considers concentration and potential limitations [5].

In fact, electrochemical models account for the transport of lithium ions, electrochemical kinetics, and material properties [6], which are ideal for the above-mentioned applications since they offer the advantages of providing information regarding internal physical variables, in addition to accurately predicting terminal voltage. The governing equations of the models are a set of coupled nonlinear partial differential equations (PDEs), and solving these equations demands considerable computational power. In order to use the electrochemical model in a real-time application while retaining its physical insights, the model order should be reduced, which results in a reduced-order model (ROM). The order reduction is performed by employing Padé approximation and residual grouping to simplify the equations of ion concentrations in both electrodes and electrolytes in conjunction with an analytical solution of cell potentials [7].

The estimator also plays a key role in accurately predicting the SOC. Despite the fact that the accuracy of a ROM can be improved by optimizing its parameters, there are still errors caused by model inaccuracy, uncertainties in initial conditions of the states in the model, and process and measurement noise. Therefore, to further reduce these errors, the nonlinear Kalman-based estimators are the potential candidates for the following reasons:

- The feedback loop can minimize the differences between predicted and measured terminal voltages so that uncertainties in the model and initial conditions are compensated.
- Recursive methods do not require the storage of all the past data but only the results of the last recursion. They are particularly suitable for estimating SOC online since the algorithm is usually embedded in a microprocessor with limited memory.
- Statistical methods are used to suppress unknown inputs (i.e., process noise) and uncertainties in the output (i.e., measurement noise). In particular, the process and measurement noises are assumed to be Gaussian distributed random variables. Although this assumption rarely holds true in practice, results reported in the research literature [1] and our results demonstrate that the method works well.
- Simple implementation with only several lines of code is even more suitable for a real-time application, such as SOC estimation, which is implemented in an onboard battery management system (BMS).

There are different types of nonlinear Kalman filters (KFs). One of the most widely used KFs is called the extended Kalman filter (EKF), which is based on the probability theory and a least-square minimization framework. The nonlinearity of a system is linearized by employing a first-order Taylor series expansion at each operating point to calculate the mean and covariance of the states. However, for a highly nonlinear system, such as an electrochemical model, the actual mean and covariance of the states may differ from the linearized results, which causes errors, and even divergence, in estimations. To overcome the drawbacks of the EKF, another nonlinear KF, a sigma-point Kalman filter (SPKF), takes a set of sample points and propagates them through the nonlinear system, from which the mean and covariance are calculated. The set of sample points, called the sigma points, is formed by calculating the matrix square-root of the state covariance. The SPKF performs better on a highly nonlinear system, such as the ROM, but the calculation of matrix square-root becomes one of the most costly operations. To further improve the computational efficiency of the SPKF, a square-root sigma-point Kalman filter (SR-SPKF) was developed [8] that propagates the square-root of covariance directly.

Some recent studies have focused specifically on utilizing an EKF with a ROM. For example, Santhanagopalan et al. applied an EKF to a ROM that simplifies a porous electrode into a single spherical particle and ignores the gradients of concentration and potential in the electrolyte [9], where the average concentration in the solid is used as the state for calculating the cell SOC. However, only the results for the anode were presented. A "three-sigma" error bound is used that indicates where the true state should remain 99% of the time. However, the results showed that the actual error was outside the error bounds 30% of the time, which implies that the error bounds provided by the EKF were not reliable. Domenico et al. applied an EKF to a ROM by averaging the input current as the cell kinetic current density [10]. The cell SOC and surface concentrations were estimated and compared with a full-order model. However, neither of these studies addressed the problem of initial SOC offset, and the SOC errors were primarily determined by the accuracy of the time update using the model. Therefore, it is difficult to evaluate the performance of the model and estimator separately. Similarly, Stetzel et al. estimated the SOC and internal variables, including ion concentrations, cell potentials, and current density, using an EKF in conjunction with a one-dimensional ROM and provided the bounds for errors [11]. Despite their detailed analysis of each state, the used simulation profile used was only a driving condition of approximately 60% SOC.

Alternatively, despite the fact that the SPKF was reported more suitable for nonlinear systems [12,13], it has not been fully explored with the ROMs. For example, the authors in Ref. [9] implemented the SPKF with few details. On the other hand, recent studies have more focused on using the SPKF in conjunction with the ECMs. Particularly, the authors in Ref. [14] proposed a co-estimator utilizes the recursive least square for parameters identification, the EKF for online parameter updating, and the SPKF for SOC estimation. It is reported that the RMSE of the latter was less than 2.5% with high robustness. Moreover, Yang et al. conducted a comparative study of the EKF, SPKF, and particle filter in conjunction with an empirical model where the RMSE of SOC estimation was less than 3% with computational efficiency that is comparable to the EKF [15].

In summary, most of the aforementioned studies employed the EKFs to the ROMs, while the SPKF was primarily applied to the ECM and the empirical models. We realized that there is a lack of a thorough analysis of the performance of different nonlinear KFs, other than the EKF, in conjunction with an electrochemical model. Therefore, the goal of this work is to answer questions including which nonlinear Kalman filter–among EKF, SPKF, and SR-SPKF–has the best performance when employed to the ROM; as well as how to modify the filters to achieve higher robustness. Specifically, we chose to investigate three enhanced nonlinear KFs that include a modified EKF, SPKF, and SR-SPKF in conjunction with a developed ROM [7,16] that entails a similar computational cost to that of an ECM. We investigated how state equality constraints affect SOC estimation results and how process and measurement noise can be automatically compensated for without manually tuning of filter parameters. Performance of the nonlinear KFs was compared with respect to the accuracy, computational time, and ability to reject the initial errors, which demonstrates that an adaptive sigma-point Kalman filter outperforms others that are validated in real-time using a battery-in-the-loop (BIL) test station. This paper provides three main contributions: (1) the proposed method incorporates additional equality constraints systematically without revisiting the structure of the original model, which addresses the problem of weak observability from the terminal voltage [10]; (2) estimation of SOC from the cathode results in a faster convergence speed when an initial offset of SOC is present; and (3) comparative studies as well as systematic analysis on several modified nonlinear Kalman filters are conducted to assess the best SOC estimator based on the ROM.

The remainder of the paper is organized as follows. In Section 2, the ROM is described and validated. Section 3 formulates SOC estimation state and output equations, describes the EKF, SPKF and SR-SPKF, as well as introduces modifications including state equality constrains and covariance adaption algorithms. Section 4 presents a comparison of SOC estimation results using the modified nonlinear filters, and the BIL results using the proposed method. Finally, Section 5 concludes this paper.