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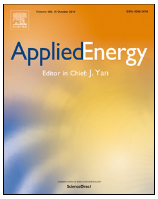

State estimation of lithium-ion cells using a physicochemical model based extended Kalman filter

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HIGHLIGHTS

- Two different recursive state-observer models using reduced p2D.
- Influence of reduction schemes analyzed for estimation process.
- Adjusted finite volume method for improved robustness.
- Modified EKF uses improved initialization and mass conservation.
- Estimation accuracy analyzed for both global and local states.

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ABSTRACT

Two time-varying linear state-space representations of the generally accepted physicochemical model (PCM) of a lithium-ion cell are used to estimate local and global states during different charging scenarios. In terms of computational speed and suitability towards recursive state observer models, the solid-phase diffusion in the PCM of an exemplaric MCMB/$LiCoO_2$ lithium-ion cell is derived with the aid of two different numerical reduction methods in the form of a Polynomial Profile and an Eigenfunction Method. As a benchmark, the PCM using the original Duhamel Superposition Integral approximation serves for the comparison of accuracy and computational speed. A modified spatial discretization via the finite volume method improves handling of boundary conditions and guarantees accurate simulation results of the PCM even at a low level of spatial discretization. The Polynomial Profile allows for a significant speed-up in computational time whilst showing a poor prediction accuracy during dynamic load profiles. The Eigenfunction Method shows a comparable accuracy as the benchmark for all load profiles whilst resulting in an even higher computational effort. The two derived observer models incorporate the state-space representation of the reduced PCM applying both the Polynomial and Eigenfunction approach combined with an Extended Kalman Filter algorithm based on a novel initialization algorithm and conservation of lithium mass. The estimation results of both models show robust and quick reduction of the residual errors for both local and global states when considering the applied current and the resulting cell voltage of the benchmark model, as the underlying measurement signal. The carried out state estimation for a 4C constant charge current showed a regression of the cell voltage error to 1 mV within 30 s with an initial SOC error of 42.4% under a standard deviation of 10 mV and including process noise.

1. Introduction and literature review

The high energy and power density compared to other battery chemistries [1] established the lithium-ion battery as the state of the art technology for electrical energy storage systems for a wide application field, ranging from small electronic devices up to large scale applications such as stationary storage systems or automotive battery packs [2]. However, the manufacturing costs are still challenging [3], which slows down a market penetration to an economically competitive energy storage system especially in the automotive sector [3].

To address this circumstance, current efforts [4] aim to push the price below US$200 per kW h or even lower for lithium-ion cells [2] within the next few years. Other estimations are cautiously optimistic and presume lower reduction of the production costs [5]. Besides the development of enhanced battery materials such as the active materials, the electrolyte, the metal collector foils and the separator [6] as well as the economical factors through increased production volumes [7], the size of lithium-ion cells [2] is regarded to be a substantial factor in

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order to decrease the production costs. The size of the cell is enlarged either by longer electrodes or by thicker coatings of composite material. Compared to small-sized cells, the application of large-sized (*i.e.* >10 Ah) [8] cells offers potential towards the reduction of cost per kW h [3]. This comes along with an influence on the cell performance based on dynamics [9] and inhomogeneity effects [10] within the cell. With increasing the cell's size, safety hazards may also rise as the convertable amount of energy during a failure scenario of a single cell correlates directly to the cell size. Maximizing the efficiency and minimizing safety threats [1] for a single cell or a whole battery pack consisting of larger sized cells, brings up new challenges for battery management systems (BMS). Battery monitoring algorithms mainly focus on an accurate prediction of the state of charge (SOC), the state of health (SOH), the capacity and impedance of a cell in order to ensure all operations within its safe operating area (SOA) by means of BMS control strategy [11]. Size effects must be considered for an accurate observing and controlling of cells such as increased inhomogeneities for the local current, concentration, potentials and temperature within the cell. Since state of the art model-based monitoring algorithms incorporate non-physicochemical models such as the equivalent circuit model (ECM), besides the cell's voltage, surface temperature and applied current, no information on the local scale can be incorporated for state estimation purposes. Falsely predicted SOC of a lithium-ion cell increases the threat of using the cell out of the SOA and local harming processes [12] may occur during operation. Considering electric vehicles, a more simple but very meaningful worst-case scenario would be a falsely predicted available range based on SOC and temperature estimation considering no local effects within large-sized cells, which would compound the issue of range anxiety of the customer. A more profound and mechanistic model for the lithium-ion cell which offers information on the local scale is the physicochemical model (PCM), commonly known as pseudo two-dimensional model [13]. The generally more complex and also more inaccurate model compared to the strictly empirical ECM offers great potential to ease the problems accompanied with inhomogeneities in large sized cells. By reformulating the underlying equations, state observer models can be derived, which are able to incorporate information on the local scale to enhance the accuracy of monitoring lithium-ion cell performance during challenging tasks such as fast charging.

In this work, the PCM is used for implementation of two different recursive state observer models to show the suitability for accurate state monitoring of lithium-ion batteries under varying load scenarios. To the author's best knowledge, the presented work is the first attempt to estimate local states of a fully-spatially-resolved PCM solved via the finite volume method (FVM) using a modified extended Kalman filter (EKF) which conserves lithium mass and the states' physical interpretation along with their spatial distribution.

1.1. Models for monitoring lithium-ion batteries

The literature review reveals plenty of models to describe and predict the behaviour of lithium-ion batteries. In the following part, the decision for the PCM model is outlined in comparison to other, widely used models of lithium-ion batteries in the application field of battery monitoring algorithm.

Artificial neural networks (ANN) models incorporate mathematical models which reduce the error between input and output signal using weighting and cost functions, which are adjusted by training data. To parameterize an ANN, all battery operation areas need to be covered and the training process becomes a time and cost-intensive task. The work of Cai et al. [14] deals with a model for a nickel-metal hydride battery and uses the applied current and the cell voltage as input signals. Since a trial of different functions of these input signals is needed, a dramatical increase of the computational costs is seen. The authors aspire to a more computationally efficient model incorporating a mechanistic description of the electrochemical behaviour of a lithium-ion cell and thus neglect this type of model for this work.

Besides ANN models, the equivalent circuit model (ECM) is widely used in research and application field of the BMS for monitoring the global states of a lithium-ion battery. The work of Hu et al. [15] presents a variety of different ECMs and the reader is referred to this publication for more profound information. In short, the ECM is an empirical, mathematical approach which requests little computational power [11], therefore less simulation time and can be easily parameterized via experimental data of the cell [9]. The main drawback of this approach is its limited validity beyond the chosen parameterization window as the model parameters are fitted to experimental data under specific operating conditions [9] and the model itself is not based on general physical or chemical principles governing the performance of electrochemical cells. In automotive applications, the extending operating window in terms of temperature, voltage and applied current may lead to false predictions and subsequent reduction of lifetime, safety and performance. Since the efforts of Plett et al. which firstly used a non-linear Kalman filter (*i.e.* EKF) [16] to estimate the cell's SOC and subsequently a Sigma-Point Kalman Filter [17] to further increase the accuracy of the estimated global states of the cell, the application of filter and observer techniques is widely used in order to gain accurate monitoring of lithium-ion batteries via the ECM. Other works focussing on the same problem such as Zhang et al. [18] fitted the ECM parameters based on electrochemical properties and showed a distinct improvement compared to commonly used parameterization methods.

Most recent work of Wei et al. [19] seem to further ease the inaccuracy as well via data-driven, online adapted ECM parameterization. Nevertheless, since the ECM still lacks of a mechanistic description of the cell's electrochemical behaviour and no local states in the lithium-ion battery can be estimated, this model is not suitable for this work.

The newman-type PCM [13] – often referenced as pseudo two-dimensional model – correlates the fundamental principles of transport phenomena, thermodynamics and electrochemistry on a macroscopic (*i.e.* electrolyte domain) and microscopic (*i.e.* particle domain) scale for a lithium-ion battery [9]. Compared to the strictly empirical ECM, the mechanistic PCM not only consumes more computational time based on its complexity but also requires vast parameterization effort due to the amount of more than 30 parameters and the nature of the parameters such as transport properties, electrode's morphology or reaction rate constants. The comparably high computational demand and parameterization effort results in a model which then shows superior validity over a wider range of applications and offers the incorporation of further physics-based processes such as aging phenomena [20], volume expansion [21] and safety related effects [22]. Large-sized cells and increased coating thicknesses of the electrodes inevitably promote gradients in potential and concentration, which can be simulated by the PCM. Based on the growing importance of localized cell utilization, the PCM is the model of choice in order to describe the performance of future cell generations accurately enough.

1.2. Recursive state observer models using PCM

The complexity of the parameterization for a PCM recommends an application of filter techniques to iteratively reduce the deviance between simulated and measured states of a lithium-ion battery. Only a few research efforts [23–25] are dealing with recursive state observer models using the PCM [26], which shows the necessity of our work.

Smith et al. [23] reduced the PCM to a single input multiple output model, which is linearized at 50% SOC. Based on this model, a linear Kalman filter was implemented for the estimation of local potentials, concentration gradients and the SOC from the applied current and cell voltage measurements. The estimation for a 6 Ah lithium-ion cell shows good performance within a SOC range from 30% to 70% by using 2 A and 25 mV process noise for the applied current and the cell voltage. The computational efficiency is comparable to the performance of ECMs [23], however, the filter performance beyond 70% SOC could be