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Enhanced Physics-Based Models for State Estimation of Li-Ion Batteries

Battery models and state estimation algorithms are a key components of todays advanced Battery Management Systems (BMS) used in Electric Vehicles (EV). These models are thereby used to estimate non-measurable states to ensure safety, availability and to prolong the battery's life. This project focuses on pseudo-2D physics-based battery models namely the Doyle-Fuller-Newman (DFN) model and Single Particle Model (SPM), which are capable to represent battery internal electrochemical states that are essential for: (i) high-precision battery state estimation (ii) degradation minimization algorithms and (iii) fast charging applications. A three-step DFN model parameter identification procedure including QR decomposition with column pivoting, microstructure analysis and model optimization is proposed and applied on a commercial 18650 lithium-ion battery resulting in an RMSE smaller than 18mV on average over the full SOC range.

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Introduction

Today, internal battery states are mostly estimated using Kalman filters and battery models based on equivalent circuits (ECM) [1]. Unfortunately, these models are not capable to represent electrochemical states that are necessary for degradation minimization strategies to prolong battery life and enable fast charging applications. In the 1990s, Doyle, Fuller and Newman developed the pseudo-2D physics-based (P2D) battery model that accurately describes the electrochemical process of a lithium-ion battery [2, 3]. This model relies on porous electrodes and concentrated solution theories and is governed by four coupled nonlinear Partial Differential Equations (PDE) describing the mass and charge conservation in the solid and liquid phase and the Butler-Volmer equation describing the lithium transference at the interface between solid particles and electrolyte. The main objectives of this project are the implementation of a PBM for state estimation on a BMS using parameters experimentally identified on a lithium-ion battery.

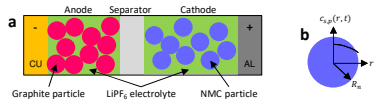

Figure 1: Pseudo-2D physics-based battery model **(a)** and detailed illustration of a single spherical particle **(b)**

Sensitivity Analysis

The model parameters are divided into three groups:

- Geometric parameters → geometry
- Thermodynamic parameters → equilibrium
- Kinetic parameters → dynamics

The most sensitive parameters are classified by QR decomposition with column pivoting, whereby each model parameter is varied independently according to scaled minimum and maximum values taken from literature.

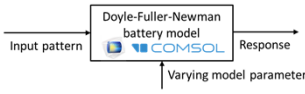

Figure 2: Sensitivity analysis by varying each model parameter

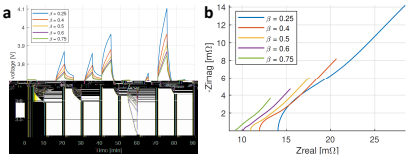

Figure 3: Time-domain voltage response during sensitivity analysis **(a)** and frequency-domain impedance during sensitivity analysis **(b)**

Parameter Identification

Microstructure analysis is used to determine the geometric parameters by optical and scanning electron microscopy (SEM) including energy dispersive X-ray spectroscopy (EDX) and subsequent image processing. The thermodynamic parameters are optimized with the Levenberg-Marquardt algorithm using Open Circuit Voltage (OCV) and Galvanostatic Intermittent Titration Technique (GITT) tests. The most sensitive kinetic parameters are identified with nonlinear least-square regression techniques based on trust region and multiple data sets with shared model parameters.

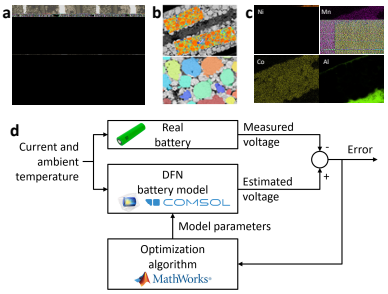

Figure 4: Optical microscopy to measure the layer thickness **(a)**, SEM and subsequent image processing to determine the porosity, active volume fraction and particle radius **(b)**, EDX to determine the coated electrode material composition **(c)** and model optimization **(d)**

Model Order Reduction

To implement the PBM on an embedded system, the DFN model is simplified to the Single Particle Model (SPM) that approximates the solid phase of each electrode with a single spherical particle. The PDEs of the SPM are reduced to Ordinary Differential Equations (ODE) assuming polynomial lithium concentration in the particle and applying volume-averaged methods to the solid and liquid phase to preserve the electrolyte dynamics [4]. Finally, the model is expressed in state-space and implemented on an embedded system.

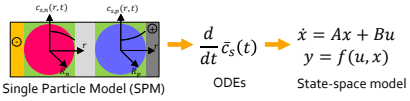

Figure 5: Simplification of the Single Particle Model (SPM) towards state-space representation for implementation on a BMS

Model Validation and Simulations

Dynamic drive cycles scaled consecutively to 2C and 5C peak discharge current highlight an average model estimation error lower than 18mV over the full SOC, an improvement of 5mV compared to traditional ECMs.
Cell internal variables such as the concentration of lithium and the potential in the solid and liquid phase are estimated in function of position and time.

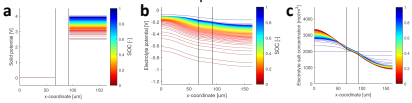

Figure 6: Simulation of solid phase potential **(a)**, liquid phase potential **(b)** and liquid phase salt concentration **(c)** for a complete 1C CC discharge cycle

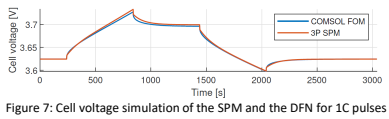

Figure 7: Cell voltage simulation of the SPM and the DFN for 1C pulses

Conclusions and Expected Impact

The DFN model parameters were successfully identified for a commercial lithium-ion battery using state-of-the-art testing and optimization methods. The validation showed excellent model performance for realistic driving cycles whereby the average RMSE is less than 18mV, which is an improvement of 5mV over traditional ECMs. The state-space model simplification matches the DFN and can be implemented on an embedded system. Physical battery models are therefore expected to become the key technology in advanced BMSs due to their ability to estimate electrochemical states. By combining physics-based models with degradation models, state estimation algorithms and optimal controls, battery life can be extended and fast charging can be enabled, accelerating the transition of mobile and stationary applications to sustainable energies.

References

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