Comparison of Reduced Order Electrochemical Models and Multi-Physically coupled Models of a Lithium-Ion Cell during Fast Charging

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Present-day lithium-ion batteries can offer capacities of more than 3 Ah resulting in volumetric energy densities of 670 Wh/l or more. Such elevated energy densities can be achieved by applying highly capacitive active materials such as nickel-rich $Li(Ni_xCo_yMn_z)O_2$ cathodes and silicon-doped graphite anodes, which are highly compressed resulting in low porosities and high tortuosities of the composite electrodes. Consequently, these cells generally show a poor rate capability[1], which is based on comparably large gradients in concentration, potential and temperature formed during operation. These gradients pose a challenge for today's battery management systems (BMS) as significant spatial gradients are very likely to limit the cell's performance. Therefore, spatially resolved electrochemical models are gaining more attention nowadays forming a promising alternative to equivalent circuit model (ECM) based BMS-algorithms.

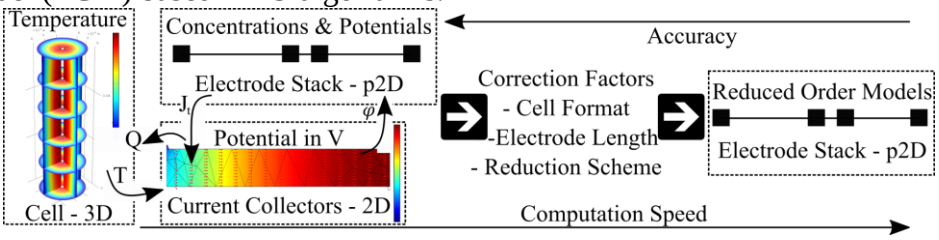

Figure 1 Schematic representation of deriving correction factors from simulation results gained from the applied MuDiMod framework (left) for an application in Reduced Order Models (ROM) (right)

In this work, we consider a commercial 18650–$Li(Ni_{0.82}Co_{0.12}Mn_{0.06})O_2$/silicon-doped graphite lithium-ion cell (LGChem) with a nominal capacity of 3.43 Ah (4.81 mAh/cm^2 at 1C). As standard pseudo-two-dimensional (p2D) newman-type[2] electrochemical models show low computational speed compared to ECMs, model order reduction is crucial to guarantee real-time suitability. The model order reduction is achieved by replacing the solid-phase diffusion equation with a Polynomial-approach[3], an Eigenfunction-method[4] as well as the reduction of all equations by using a Collocation-approach[5]. As the occurring electrochemical, electrical and thermal mechanisms can be assigned to different length scales, the previously discussed Multi-Dimensional Modeling (MuDiMod)[6] framework is used as a benchmark for our model order reduction, which includes a 3D-thermal, a 2D-electrical and 38 p2D-models. The MuDiMod framework is used to describe the temperature distribution, the current and potential gradients along the current collectors and the concentration and potential gradients through the electrodes at each location of the current collectors.

The study analyzes the inhomogeneous utilization during charging scenarios driven by polarization effects along the 61.5x5.9 cm sized electrodes and the temperature gradient from the core to the surface of the cell. Correction factors derived from this study are implemented in the ROMs depending on the reduction scheme, the length of the current collectors and the format of the cell, which allows to avoid hazardous scenarios such as localized lithium-plating during charging.

References:

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