Parameterization of physics-based models in Li-ion batteries by using Bayesian methods

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Modeling physical processes inside a battery is an inevitable step in accelerating battery research. Physics-based models enhance our underlying understanding and thereby improve the lifetime of lithium-ion batteries (LIBs) and future battery design. The procedure of parameterizing and validating a specific model, is an intractable challenge due to the complicated coupling of many mechanisms. Depending on the model complexity, the parametrization task becomes unsolvable for standard local approaches and global optimization becomes essential.

In a first study, we investigate the parameterization of Solid-Electrolyte Interphase (SEI) growth models, as a simple case study for a global Bayesian algorithm. The ongoing growth of the SEI is considered the main degradation mechanism during battery storage, and it also makes a significant contribution during battery operation [1]. To distinguish the proposed SEI growth mechanisms, i.e., solvent diffusion, electron diffusion, and electron conduction, we perform inverse modeling of storage degradation data, to exclude other degradation effects, with an automated parameterization routine based on Bayesian methods [2].

We show that sample-efficient Bayesian methods [2,3] are outstanding tools to parametrize physics-based models within reasonable sample numbers, operate as a consistent model selection criterion, and give reliable uncertainties and correlations in the parametrization [4]. We show that suitable feature selection can further improve the algorithmic performance and ensure the correct identification of the physical features. As a result, we identify electron diffusion [5] as the dominant growth mechanism of the SEI during battery storage. For future studies this result can be used to analyze degradation data with more mechanisms included. In conclusion, our inverse model routine helps to identify and parametrize degradation mechanisms of LIBs. As this method is transferable to analyze battery data in general [6], we use this approach for the automated parameterization of full-cell battery models in a follow up study.

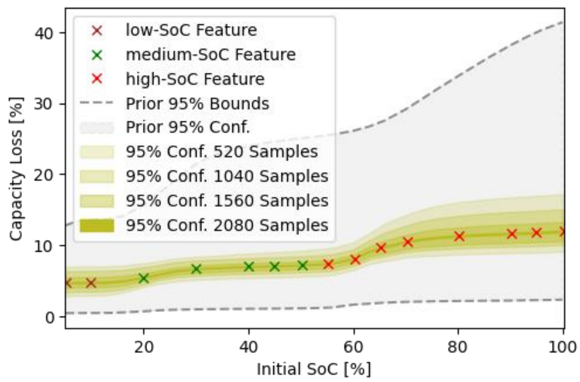

Fig. 1: Consecutive convergence of parameterization and uncertainty for storage data [5]

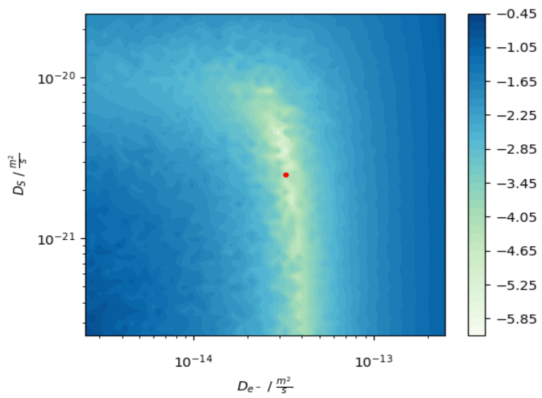

Fig. 2: Loss function of a specific feature choice in parameter space considering noisy data [5]

References:

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