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Uncertainty Quantification Visualization Tool to Simulate Porous Lithium-Ion Batteries

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ABSTRACT

To maintain people's fast-paced lifestyles, a more powerful and reliable rechargeable battery is critical. During the manufacturing process, electrode parameters such as cathode thickness, the porosity of the positive electrode and radius of negative active materials are subject to uncertainty. Such uncertainty may have a dramatic impact on the performance of the battery. To optimize its performance, it is critical to quantify uncertainty due to variation in electrode parameters and measure the response of the system through multiscale computer simulation. To achieve this goal, a porous lithium-ion battery uncertainty quantification and visualization tool has been created. This tool consists of three components: 1) a generator of uncertainty input; 2) an electrochemical system simulator; 3) a statistical analysis and visualization module. This project focuses on the first and the third components. First, the uncertainty input generator provides the option of selecting one of two statistical models for the input parameter distributions: Gaussian and lognormal. For Gaussian and lognormal distributions, sample points and weights are generated based on Gauss-Hermite quadrature formula. Each module provides a GUI, built using an open source, class-oriented environment, the Virtual Kinetics of Materials Lab [1]. Ensemble simulations are performed using the electrochemical system simulator that in turn uses the data distributions obtained from the uncertainty input generator. In the statistics analysis and visualization component, the simulation results are quantified graphically through error bar plots that visualize the impact of the uncertainties that were introduced into the system. The variation of power and energy densities as a function of current density of the battery electrode is presented, enabling the user to visualize the uncertainty propagation from the three electrode uncertainty inputs and its impact on the battery performance.

[1] Alex Bartol; R. Edwin García; David R. Ely; Jon Guyer (2015), "The Virtual Kinetics of Materials Laboratory," https://nanohub.org/resources/vkmllive. (DOI: 10.4231/D3B853J85).

KEYWORDS

Uncertainty quantification, battery modeling, rechargeable batteries, distribution function, input generation