Lehrstuhl für Energiesysteme
TUM School of Engineering and Design
Technische Universität München

Master's Thesis

(Simulative)

Comparison of Model Parameters in Impedance-based Equivalent Circuit Fitting with Measurement Noise for Solid Oxide Cells

Description

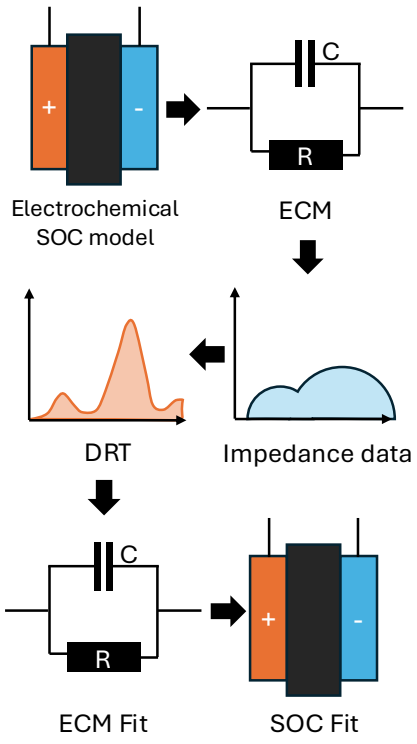
Electrochemical impedance spectroscopy (EIS) is a widely used technique for characterizing physico-chemical processes in electrochemical systems such as solid oxide cells (SOCs). Deconvoluting the impedance spectrum via the distribution of relaxation times (DRT) yields characteristic time constants and effective equivalent circuit model (ECM) parameters (resistances, capacitances, and inductances) which serve as the basis for back-calculating the mechanistic parameters of interest, such as activation energies and exchange current densities. This thesis aims to simulate synthetic EIS spectra from a physically-based SOC model and its corresponding ECM, including realistic measurement noise. The mechanistic parameters are then recovered from the noisy impedance data via DRT-based fitting. The resulting ECM and physico-chemical parameters are compared against the ground truth to assess fit quality, and an uncertainty quantification is implemented to report each parameter's mean and standard deviation. The work will be implemented in Python using the nonlinear optimization package CasADi.

Requirements

- High interest in electrochemistry / reaction engineering
- Good Python programming skills
- Helpful: Mathematical understanding of optimization / machine learning / signal processing

Tasks

1. Research SOCs, EIS, ECM, DRT, Python CasADi
2. Implementation & validation of a 0D electrochemical SOC model & the according ECM
3. Simulation of EIS data (with & without measurement noise)
4. Transformation into frequency domain using DRT
5. Fitting of ECM parameters
6. Calculation/fitting of mechanistic cell parameters from ECM
7. Implementation of uncertainty quantification (e.g. Bayesian DRT)
8. Final parameter comparison & assessment of uncertainty intervals



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