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Tutorial

Multiscale Modeling Methods for the Simulation of Electrochemical Devices for Energy Conversion and Storage

by
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Multiscale modeling approaches are emerging as practical tools in design and optimization of materials and devices for electrochemical energy conversion and storage. As researchers in applied science and industry are increasingly drawn towards adopting such methodologies, it remains crucial to develop a profound grasp of their underlying principles, capabilities and limitations. The tutorial will cover various facets in development and application of multiscale modeling methods, from theoretical foundations to practical implementation. As the central theme of presentations and discussions we will focus on theory and modeling of porous electrodes, which are of pivotal importance for a wide range of electrochemical technologies. Moreover, this topic embodies the full hierarchy of phenomena, from molecular electrocatalysis to effective properties of materials and to processes at the device level, that must be incorporated in order to understand, analyze and optimize the operation of electrochemical power generators. Participants are expected to have solid knowledge of electrochemistry and basic experience in physical-mathematical modeling.
The tutorial will consist of the following modules:

1. **Background on Porous Electrode Theory (30 min)**
   - Basic principles of porous electrodes
   - Porous electrodes for electrochemical energy conversion and storage(supercapacitors, photoelectrochemical cells, batteries, polymer electrolyte fuel cells); overview of materials, structure, function, and operation; generic aspects and specific requirements;
   - Challenges for electrode design and operation.
2. **Hierarchy of Structural Effects in Catalyst Layers of PEM Fuel Cells (60 min)**
   - How to evaluate the electrochemical performance of catalyst layers?
   - Overview of the hierarchy of scales involved in catalyst layer operation.
   - Ptelectrocatalysis at the (sub-)nanoscale: oxygen reduction reaction, Pt nanoparticle stability and Pt dissolution; first principles calculations and analytical modeling.
   - Structure and processes at the mesoscale: coarse-grained MD studies of structure formation; local reaction conditions at and in agglomerates of Pt/carbon; nanopore model of oxygen reduction reaction (with application to ultrathin catalyst layers).
   - Modeling catalyst layer operation at the macroscale: coupling scheme of meso- and macroscale processes; fitting of experimental performance data and evaluation of CL effectiveness factor; electrochemical transmission line model as a diagnostic tool; catalyst layer as a watershed: transitions in water balance and electrochemical performance.
3. **Multiscale modeling techniques and (45 min)**
   - Multiphysics and multiscale models: concepts, definitions, hierarchical vs. direct multiscale models (with literature examples for electrochemical power generators), modular models within non-equilibrium thermodynamics and bond graphs.
   - Numerical methods for direct multiscale models; use of Matlab and C programming, data-flow platforms for communication between discrete and continuum models.
4. **Case study: Multiscale models for batteries(45 min)**
   - Modeling of intercalation and conversion reactions in lithium ion, lithium sulfur and metal air batteries.
   - Electrochemical modeling in batteries: phase field approach, concepts, mathematical formulation, numerical techniques, examples.
   - Charge transport and thermal modeling in batteries: finite element methods, mathematical formulation, numerical techniques, examples.

PRACTICE (60 minutes)

In the practice session, participants will be divided up into two groups. In each groups, we will form teams of 2-3 participants. The assignment will be similar or identical for both groups: they will analyze electrochemical impedance data of porous electrodes for batteries, fuel cells or supercapacitors. However, one group will develop and apply an analytical electrode model whereas the other group will develop and apply a computational model. In the concluding discussion, we will compare results and evaluate the different approaches applied.

Group 1: Application of analytical electrode models to impedance data of electrochemical devices. Develop and solve a simple transmission line model of porous electrodes; apply analytical expressions obtained to experimental data of porous electrodes; extract parameters of fuel cells catalyst layer and battery intercalation electrode ; use extracted data for further analysis (calculate Pt effectiveness factor, calculate reaction penetration depth).

Group 2: Develop and implement a mathematical electrode model in Matlab: apply to same data as in (1) and perform similar tasks.

For a better participation in the practice session is recommended a personal computer for each participant, ideally with Matlab installed in it, or alternatively, Scilab and Octave which are totally free:

http://www.scilab.org/en; http://www.gnu.org/software/octave/