Multi-physics, Multi-scale Models: Low and High Temperature Fuel Cells

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Objective
An objective of the Center for Energy Systems Research has been to develop comprehensive microscopic and macroscopic 2D and 3D models for the high temperature (Solid Oxide) and low temperature (Proton Exchange Membrane) fuel cells.

Macroscopic Modeling
Modeling efforts include a wide range of models for both PEMFC's and SOFC's PEMFC models include 1, 2, and 3D models ranging from single layer models (i.e. membrane and catalyst layer) to full cell models that include channel dynamics, water transport, reduced back-pressure due to water saturation, species diffusion through tortuous leading, and proton and electron transport throughout the fuel cell.  Usually macroscopic SOFC models have also been developed which account for mass, thermal, and charge transport in a planar SOFC.  The SOFC model also includes electrochemical effects and the chemistry of internal fuel reforming.

PEM Fuel Cell
Macroscopic models have been developed at the component and full PEMFC level:
- 1D models at the component level for the proton exchange membrane, and the cathode catalyst layer;
- 2D models developed for full PEMFC characterization based on agglomerate catalyst layers, which include the effects of water saturation on transport properties;
- 3D model designed to model all transport processes including gas species transport, water transport, proton transport, electron transport, and thermal transport.

Solid Oxide Fuel Cell
A detailed steady state 3D model of a planar anode supported SOFC is described which accounts for mass, thermal and charge transport as well as electrochemistry and the chemistry of internal fuel reforming.  Its main characteristics include the use of a continuous model for the electrochemical processes, allowing one to examine different three-phase boundaries.

Microscopic Modeling

Though the macroscopic approach to the fuel cell modeling eases the modeling efforts, it has certain disadvantages, i.e.
- The actual micro-structure of the porous layers constituting the fuel cell is not modeled.
- The effects of micromachining on cell operation and performance is only taken into account by considering homogeneous layers characterized by macroscopic, averaged parameters such as porosity and tortuosity.

Flooded Porous Agglomerate Model
This model assumes the active layer to have pores which are flooded with water.  Therefore, in the model there is an array of distributed anodes supported Pt particles surrounded by a flooded gas pore.

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Computational Facilities

The 3D model is an extension of the 2D model with a focus towards eliminating parameter adjustments along the channel and in the porous media.

Facilities at Virginia Tech

- Advanced software and facilities for data visualization, CFDvision® (note element software specifically modified for 3D modeling of SOFC and PEMFC behavior, in-house numerical modeling tools).
- Fuel Cell Fabrication and Testing Environment – microelectrode/nanocarbons fabrication including catalyst layer preparation equipment and process, test facilities for anode and cathode plates, including an in-house built test stand and a FTC test stand for fuel cells up to 300 W, AC impedance using on-site systems for conducting cyclic voltammetry to assess active catalyst area, SEM and TEM facilities, etc.

Collaborations

Virginia Tech