Integrated CFD Simulation Tool for Fuel Cell Performance Analysis

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Abstract

In order to continue improving the performance of fuel cell systems, increasingly complex cell designs and advanced materials are being incorporated into the cells. Detailed, physically based models can compliment the fabrication and testing of hardware prototypes to accelerate the improvement of cell design. In order for such modeling tools to be useful, they must be accurate, computationally efficient, and provide ease of use during both the model definition and analysis stages of the simulation.

We have developed a general capability for simulation of momentum, chemical species, energy, and electrical current transport with electrochemical reaction in fuel cells, which meets these criteria for an engineering analysis tool. The electrochemical analysis is integrated within the commercially available finite volume based multi-physics simulation package CFD-ACE+. As a result of this integration, the solution of momentum, heat, mass, and electrical current transfer in the porous media comprising fuel cell membrane and electrode assemblies is tightly coupled. The principal components of the model formulation are:

- solution of two electrical potentials, for both the membrane and solid phase, with coupling through the electrochemical kinetics;
- robust implementation of the general, non-linear Butler-Volmer rate expression for electrode kinetics;
- treatment of the catalyst layers as volumes, as opposed to the common approximation of the catalyst layers as surfaces;
- incorporation of catalyst loading and catalyst support pore size effects on the observed kinetics;
- full porous media effects on momentum, energy, and species transport including anisotropic permeability to flow and automatic calculation of effective transport properties as a function of the local solution;
- rigorous energy transport analysis including the conversion from chemical to electrical forms;
- two- and three-dimensional capability on both structured and unstructured grids;
- complete model definition through a graphical user interface; and
- printed summaries of key quantities for post-processing, in addition to graphical output of all solution variables and computed properties.

These capabilities were developed primarily for prediction of the performance of hydrogen PEM fuel cells. Due to the general nature of the model structure, analysis of other cell types should be possible with little or no additional development.

We will present validation of this integrated tool by comparison with published reports of hydrogen PEM fuel cell performance[1]. Sample results of such a validation study are shown in Figure 1, which compares predicted and experimentally measured cell performance as a function of operating temperature and pressure. A critical analysis of three-dimensional effects such as mass transfer to the portion of the active layers adjacent to current collectors and non-uniform current density distributions in membranes will also be presented. These results will clearly demonstrate the need for fully three-dimensional simulations to analyze the factors controlling performance of typical fuel cell designs.

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References

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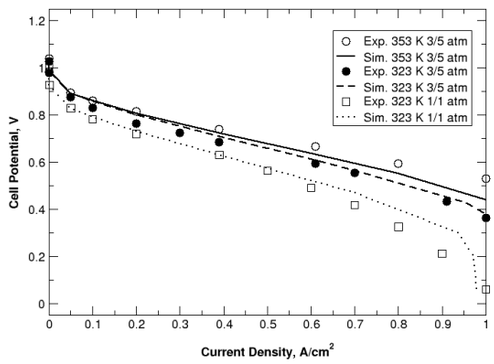

Figure 1. Comparison of experimentally measured and simulated hydrogen PEM fuel cell performance as a function of temperature and pressure (anode/cathode side).