

TOOLS AND TECHNIQUES FOR MODELING SOFC FUEL CELL PERFORMANCE

Alton J. Reich, Rupak Das, J. Vernon Cole, and Sandip Mazumder
CFD Research Corporation
215 Wynn Drive
5th Floor
Huntsville, AL 35805

ABSTRACT

Fuel cells have been utilized in certain specialized applications since the 1960's, however the technology has recently been the focus of a broad research and development effort. The next 10 years will likely produce practical, affordable fuel cells that are applied in fixed power generation, automotive, and even powered bicycle applications.

As the fuel cell becomes less of a research curiosity and more of an engineered commodity item, designers need tools to study and optimize the behavior of fuel cells. This paper discusses some of the questions that simulation can help fuel cell designers address.

Keywords: Fuel Cells, Multiphysics Simulation, CFD-ACE+

INTRODUCTION

To the average mechanical engineer, fuel cells appear to be the ultimate rechargeable battery. In automotive applications, they have many fewer moving parts than conventional internal combustion engines. They also provide higher efficiency, lower emissions, and appear to mesh well with other hybrid automobile technologies.

Fuel cells also scale relatively well. There are fuel cells that are being developed as an alternative to conventional rechargeable batteries for cellular phones, an application for which an internal combustion engine is completely unsuitable. On the higher power end of the spectrum, fuel cells are being developed for fixed, domestic power applications in which the fuel cell would provide both electrical power and hot water for remote homes and businesses.

Fuel cell designers are using the tools at their disposal to streamline the design process as much as possible in order to minimize design and production costs, and beat their competitors to the market. These tools include CAD for modeling the physical layout of the fuel cell stack and supporting equipment and FEA for structural analysis.

In fuel cell design one of the more important considerations is the interaction between the flow of reactant gases through the cell, electrophysics, and the temperature distribution within the cell. In the past, the performance of a fuel cell could only be assessed by constructing a prototype and testing it. Simulation tools did not exist that could accurately model all the necessary physics. Advances in multi-physics simulation make it possible to capture the physics involved in fuel cell operation. The CFD-ACE+ software package was used to perform a simulation of a simple cross-flow fuel cell, and describes the potential uses of the model.

Cross Flow Fuel Cell

A fairly simple cross flow fuel cell was considered for this paper because of the simplicity of the design. It allowed consideration of physics, rather than geometry, to dominate the discussion of fuel cell performance characteristics that can be assessed via simulation. The basic geometry is shown in Figures 1 and 2.

During operation, fuel flows from right to left in the upper layer of the cell and air flows from front to back in the lower layer of the cell. The reacting species (H₂ and O₂) diffuse toward the membrane at the center of the cell through the diffusion layers. In the Cathode Catalyst layer the oxygen undergoes a catalytic reaction in which it is split into two O⁻ ions. This liberates four electrons (for each O₂ molecule) that are sent through an external circuit.

The O^- ions migrate across the electrolyte layer to the anode catalyst layer where they release two electrons and react with an H_2 molecule to form water. The fuel cell is able to efficiently convert a chemical fuel into electric power with water as the primary by-product. (Although in certain types of fuel cells, some CO_2 is produced in the process that converts hydrocarbon fuel into H_2 .)

The basic input parameters used in setting up this simulation are provided in the tables that follow.

Table 1: Inlet Gas Properties

Gas	Mass Flow Rate, kg/sec	Temperature, K	Composition
Fuel	2.2E-5	1023	0.07 H ₂ , 0.03 H ₂ O, 0.9 N ₂ (mass fraction)
Air	6.4E-5	1023	0.23 O ₂ , 0.77 N ₂ (mass fraction)

Table 2: Porous Media Properties

Layer	Porosity	Permeability, m ²	Solid Thermal Conductivity, W/m K	Solid Electrical Conductivity, 1/Ω m
Anode Diffusion and Catalyst	0.5	1E-12	3.0	30000
Cathode Diffusion and Catalyst	0.5	1E-12	3.0	13000
Electrolyte	0.3	1E-18	3.0	1E-6 (non-conducting)

Table 3: Boundary Conditions

Location	Thermal BC	Electrical BC
Side Walls	T = 1023 K	J = 0 A/m ²
Anode Electrode	T = 1023 K	V = 0 V
Cathode Electrode	T = 1023 K	V = -0.01 -> -1.0 V

For this particular fuel cell model, the chemistry in the catalyst layers was set up to produce a fast reaction. This was done to make the overall operation of the cell diffusion limited. The reactions that were used were:

Table 4: Electrochemical Reactions

Location	Reaction	J ₀	α_A	α_C
Anode	$H_2 + O^- \rightarrow H_2O + 2e^-$	2E13	0.5	0.5
Cathode	$\frac{1}{2}O_2 + 2e^- \rightarrow O^-$	2E12	1.5	1.5

Note: α_A and α_C are the anodic and cathodic Tafel constants.

Simulations of solid oxide fuel cell performance can provide the design engineer with several solution parameters that are of interest. These include:

- The temperature distribution in the ceramic material that can be used to perform thermal stress analysis on the

ceramic. The ceramic is very brittle and the thermal stresses need to be minimized.

- The mass fraction of fuel in the cell. A lower mass fraction at the outlet indicates better utilization of the fuel.
- The current density in the fuel cell.
- The polarization curve which relates the current flowing through the cell to the potential difference across the cell.
- The overpotential between the catalyst layers.

For this particular fuel cell, these model results are shown in Figures 3 through 6 for a bias voltage of $-0.8V$. The cell polarization curve shown in Figure 7 was generated by performing a parametric study using the same model input file used to generate Figures 3 through 6. The parametric study was run automatically using the SimManager software package. The input to SimManager is a table of applied voltages that should be applied to a particular boundary of the model. SimManager then takes care of the sequential set up and execution of the set of simulations. Figures 8 and are screen shots that show the steps required to run the parametric to generate the cell polarization curve. The user then extracts the output data, in this case the current corresponding to each input voltage, and plots it. The polarization curve defines the relationship between current and voltage for each element in the fuel cell stack. The designer uses this information to decide how each element should be connected in the overall circuit.

Summary and Conclusions

The simulations performed for this paper show that simulation tools have matured and advanced to a point where they can be applied to the design of fuel cell stacks. Simulation tools, such as CFD-ACE+, can be used to predict the performance of fuel cells with respect to several output quantities of interest including temperature, species mass fraction, current density, and overpotential.

Simulation tools can also help to optimize other portions of the overall fuel cell system including reformers, distribution manifolds, heat exchangers and pumps.

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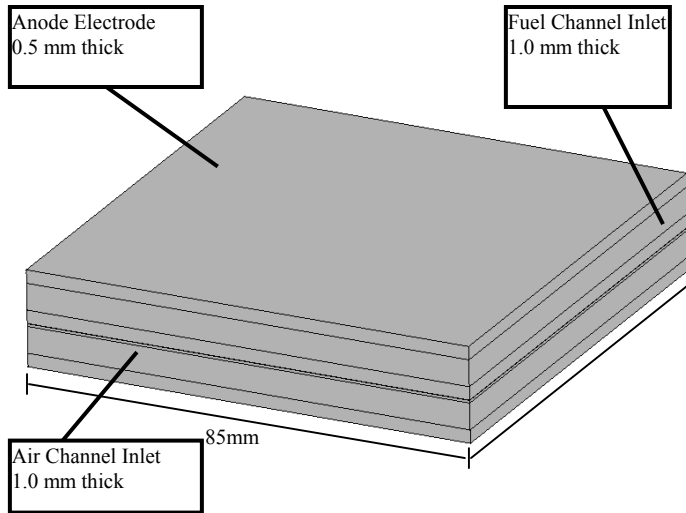


Figure 1: Fuel Cell Geometry

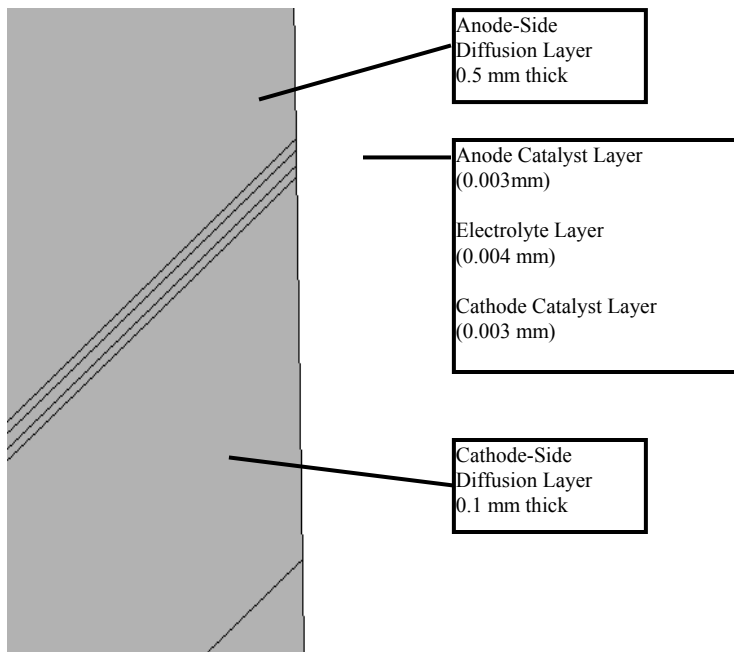


Figure 2: Membrane Geometry Details

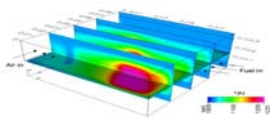


Figure 3: Cell Temperature Distribution – Isometric View

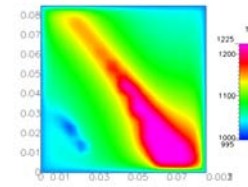


Figure 4: Cell Temperature Distribution – Top View Through Electrolyte Layer

Figure 5: Hydrogen Mass Fraction – Isometric View

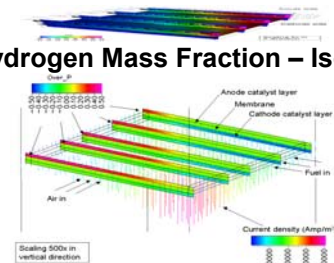


Figure 6: Current Density and Overpotential – Isometric

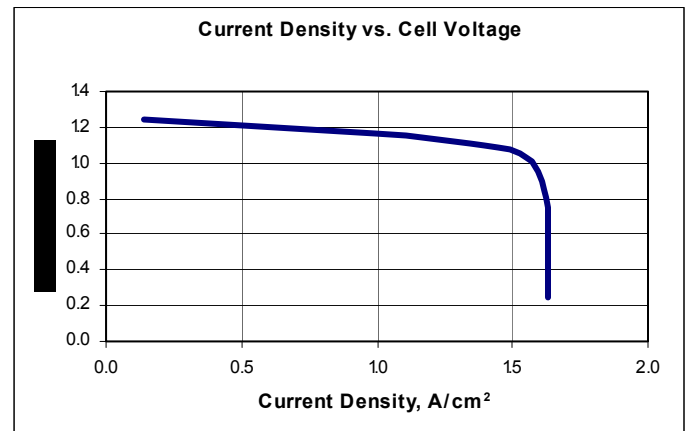


Figure 7: Cell Polarization Curve

Figure 8: Parametric Study – Model Specification

Figure 9: Parametric Study – Case List