

VII.H.7 Fuel Cell Systems Analysis

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Projected End Date: Project continuation and direction determined annually by DOE

Objectives

- Develop and validate a model for automotive fuel cell systems and periodically update it to assess the status of technology.
- Conduct studies to improve performance and packaging, to reduce cost, and to identify key R&D issues.
- Compare and assess alternative configurations and systems for transportation and stationary applications.
- Support DOE/FreedomCAR automotive fuel cell development efforts.

Technical Barriers

This project addresses the following technical barriers from the Fuel Cells section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- D. Thermal, Air and Water Management
- E. Compressors/Expanders
- F. Fuel Cell Power System Integration
- J. Startup Time/Transient Operation

Approach

- Develop, document and make available an efficient and versatile system design and analysis tool.
- Validate the models against data obtained in the laboratory and at Argonne's Fuel Cell Test Facility.
- Apply models to issues of current interest.

Accomplishments

- Developed a model for a membrane humidifier and validated it with available experimental data.
- Analyzed a proton exchange fuel cell (PEFC) system with a membrane humidifier in the cathode circuit.
- Validated the model for the enthalpy wheel humidifier with available experimental data and used it to address the issue of humidification in PEFC systems with high-temperature membranes.
- Developed a model for self-start of PEFC stacks from sub-freezing temperatures.
- Proposed and evaluated an alternative method of start-up from sub-freezing temperatures.

Future Directions

- Further develop the model on self-start of PEFC stacks from sub-freezing temperatures and analyze different start-up scenarios.
- Continue collaboration with Honeywell on thermal and water management.

- Participate in validation effort and explore combined heat and power applications of stationary PEFC systems.
- Continue to support DOE/FreedomCAR development efforts.

Introduction

While different developers are addressing improvements in individual components and subsystems in automotive fuel cell propulsion systems (i.e., cells, stacks, fuel processors, balance-of-plant components), we are using modeling and analysis to address issues of thermal and water management, design-point and part-load operation, and component-, system-, and vehicle-level efficiencies and fuel economies. Such analyses are essential for effective system integration.

Approach

Two sets of models are being developed. GCtool is a stand-alone code with capabilities for design, off-design, steady-state, transient and constrained optimization analyses of fuel cell systems. GCtool-ENG has an alternative set of models with a built-in procedure for translation to the MATLAB/SIMULINK platform commonly used in vehicle simulation codes such as PSAT.

Results

We have formulated a model for a counterflow, shell-and-tube membrane humidifier. The model considers heat and mass transfer between two streams separated by hollow tubes made of Nafion. It determines mass transfer from the gradient of the water content within the Nafion membrane and water diffusivity, which is a function of the local water content and temperature. The model was validated against experimental data obtained at Perma Pure LLC on a sub-scale unit (480 hollow tubes, 1.1 mm tube outer diameter, 64 μm membrane thickness, 17.8 cm active length) with wet air at 100% relative humidity (RH) and 80°C flowing on the shell side. The experiments were conducted with dry air at 25-70°C on the tube side. On a dry basis, the air flow rate varied between 1.7 and 8 g/s on the tube side and 1.5 to 7.2 g/s on the shell side. The pressure of the two air streams varied with flow rate between 1.3 and 2.5 atm. Figure 1 compares the model results with

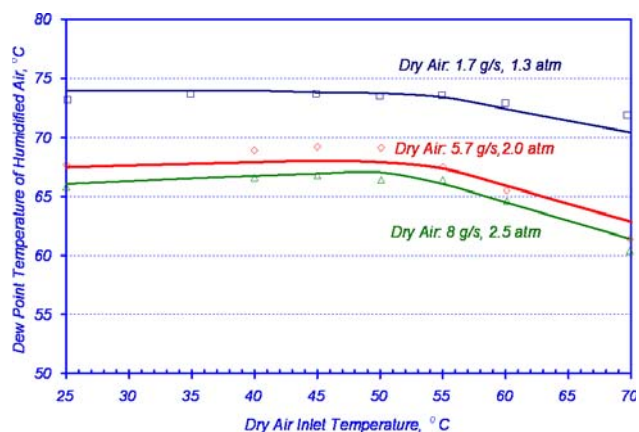


Figure 1. Variation of Dew Point Temperature of Humidified Air with Inlet Temperature

the measured dew point temperature of the humidified air. Both the model and the data indicate that the mass transfer peaks at about 50-55°C dry air temperature. Above this temperature range, the wet air stays hot and can become unsaturated, causing the water activity and hence the mass transfer to decrease. For dry air temperature below 50-55°C, the mass transfer is limited by the 100% saturation condition.

The validated model was used to analyze an 80-kW PEFC system with a membrane humidifier in which the dry air discharged from the compressor is pre-cooled to 60°C at rated power using low-temperature stack coolant at 55°C. Our analysis shows that it is preferable to pass the wet spent cathode air into the humidifier without separating any liquid water that forms in the PEFC stack. We estimate that 4500 Nafion tubes, 17.8 cm long and 2.85 m² membrane area, are needed to humidify the compressed air to 60% RH at 2.5 atm. Figure 2 shows that at the rated flow, the humidified air is cooled to 70°C from the compressor discharge temperature of 160°C, and it is heated to about 78°C from the 70°C compressor discharge temperature at one-tenth of the rated flow. At the 10% flow rate, RH of the humidified air can exceed 90%.

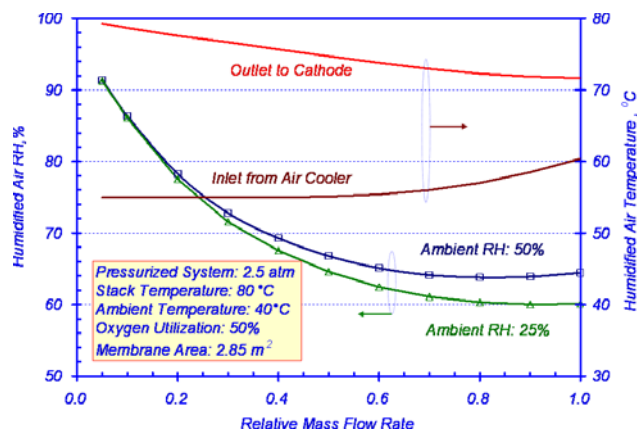


Figure 2. Performance of a Membrane Humidifier in a PEFC System

The enthalpy wheel (EW) model formulated in FY 2004 was validated against experimental data obtained on a sub-scale unit at Emprise Corporation. The validated EW model was used to estimate the extent to which air can be humidified by transferring moisture from the spent cathode air leaving a PEFC stack with a high-temperature membrane at 120°C. We estimated that compressed air at 2.5 atm can be humidified to 9-18% RH with a 14-cm-diameter, 15-cm-long EW in an 80-kW PEFC system. The RH can be increased to 20-30% if the EW is made twice as long. The corresponding levels of RH in an ambient-pressure system are 6-9% with 15-cm-long EW and 10-13% with a 30-cm-long EW (see Figure 3). Based on these analyses, we recommended to the High-Temperature Membrane Working Group that the membranes be capable of operating at relatively dry conditions.

In late FY 2004, we initiated the development of a two-dimensional simulation model to determine the conditions under which PEFC stacks can be self-started from sub-freezing temperatures. The model considers electrochemical reactions with species transport in a five-layer membrane electrode assembly [anode gas diffusion layer (GDL), anode catalyst layer, membrane, cathode catalyst layer, and cathode GDL], capillary transport of water across GDLs and porous catalysts, formation and melting of ice, effect of ice on electrochemical surface area (ECSA) and transport of species, and temperature distribution in bipolar plate flow channels and the membrane electrode assembly

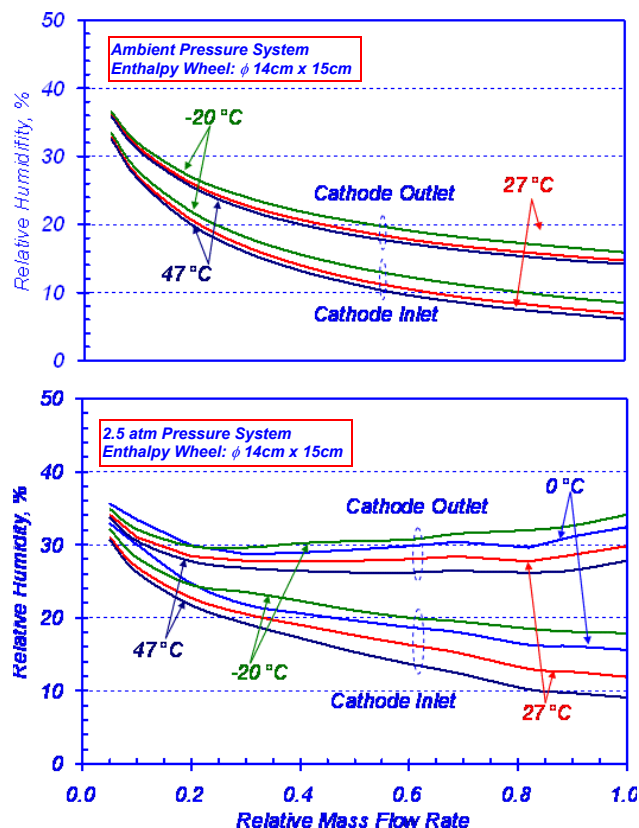


Figure 3. Performance of Enthalpy Wheel Humidifiers in Pressurized and Ambient-Pressure PEFC Systems

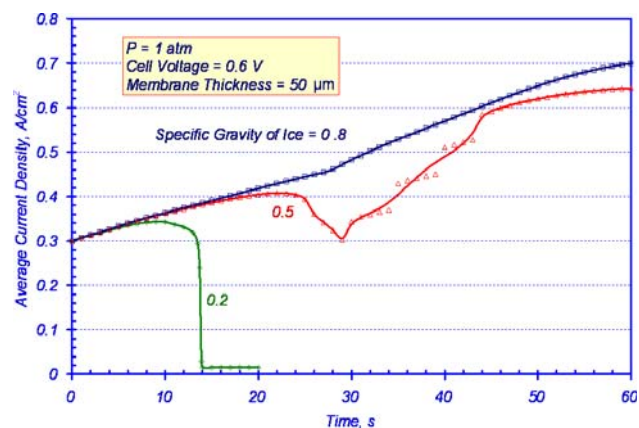


Figure 4. Sensitivity of Simulations to the Assumed Bulk Density of Ice

(MEA). Some preliminary results using the model are summarized below.

- Figure 4 shows the sensitivity of simulation results to the assumed bulk density of ice that

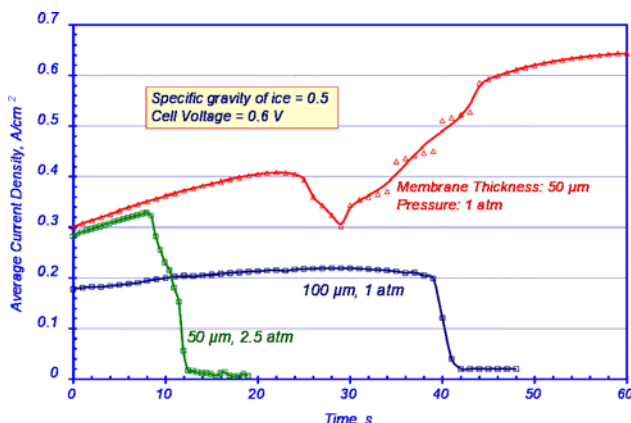


Figure 5. Simulated Effects of Membrane Thickness and Pressure on Self-Start from -20°C

forms within the cathode catalyst and cathode GDL. The simulation conditions are 1 atm operating pressure, 0.6 V cell voltage, 50 μm membrane thickness, 200- μm -thick GDL, 1.2 kW/kg stack specific power, Pt loading of 0.4 mg/cm^2 on cathode catalyst and 0.05 mg/cm^2 on anode catalyst, and -20°C initial temperature. With an assumed ice specific gravity of 0.2, the average current density initially increases with time as the MEA heats up, but the cathode catalyst is rapidly covered with ice so that the electrochemical reaction shuts down after about 15 s. Self-start is possible for an assumed ice specific gravity of 0.5, although there is an intermediate period of 25–30 s, during which the average current density decreases with time. The simulation indicates a smooth start-up from -20°C if the specific gravity of ice is assumed to be 0.8.

- Figure 5 shows the influence of operating pressure (1 atm vs. 2.5 atm) and membrane thickness (50 μm vs. 100 μm) on start-up from -20°C . Our simulations indicate that start-up from cold is more difficult under pressurized conditions because of more rapid build-up of ice on the cathode catalyst. The start-up is more difficult with a thicker membrane because the delicate balance between Joule heating (proportional to the square of current density) and loss of ECSA due to ice formation (proportional to the current density) shifts toward the latter.

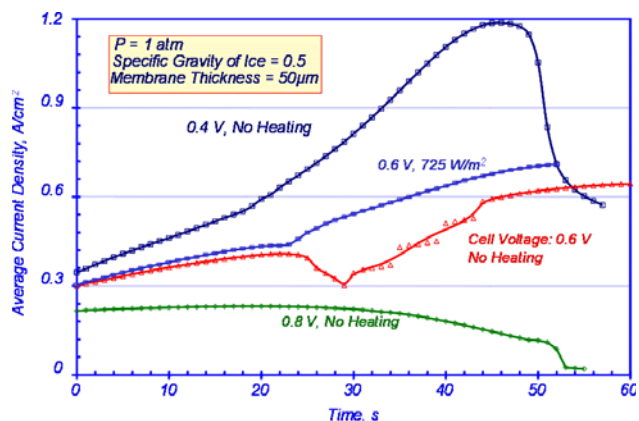


Figure 6. Simulated Effects of Cell Voltage and Electrical Heating on Self-Start from -20°C

- Finally, Figure 6 shows the effects of cell voltage and resistive heating of the stack on start-up from -20°C . Our simulations indicate that self-start is more feasible at a cell voltage of 0.4 V rather than 0.8 V. Also, the start-up is faster and more robust if the bipolar plate can be electrically heated.

Conclusions

- A membrane humidifier for a PEFC stack operating at 80°C can be made more compact if the inlet temperature of the dry air is maintained within a narrow temperature range and liquid water formed in the cathode channels is fed to the humidifier.
- From system considerations, the high-temperature membranes under development should be capable of operating at relatively dry conditions, i.e., $<13\%$ RH at ambient pressure and $<30\%$ RH at 2.5 atm.
- Preliminary results from our simulations indicate that self-start of PEFC stacks from sub-freezing temperatures is favored under the following conditions: ambient pressure, low cell voltage, thin membranes, and electrical heating of the bipolar plate.

FY 2005 Publications/Presentations

1. R. K. Ahluwalia, X. Wang, and A. Rousseau, "Fuel Economy of Hybrid Fuel Cell Vehicles," *Journal of Power Sources*, (in print), 2005.
2. R. K. Ahluwalia and X. Wang, "Direct Hydrogen Fuel Cell Systems for Hybrid Vehicles," *Journal of Power Sources*, 139, 152-164, 2005.
3. R. K. Ahluwalia, X. Wang A. Rousseau and R. Kumar, "Fuel Economy of Hydrogen Fuel Cell Vehicles," *Journal of Power Sources*, 130, 192-201, 2004.
4. R. K. Ahluwalia, X. Wang, and A. Rousseau, "Fuel Economy of Fuel Cell Hybrid Vehicles," *2004 Fuel Cell Seminar*; San Antonio, TX, November 1-5, 2004.
5. R. K. Ahluwalia, X. Wang, R. Kumar, "Fuel Cell Systems for Hybrid Vehicles," *2004 International PEM Fuel Cell Conference*, Hsinchu, Taiwan, October 14-15, 2004.
6. R. K. Ahluwalia and X. Wang, "Performance of Hybrid Fuel Cell Vehicles," *Annex XX Meeting*, Stuttgart, Germany, September 28, 2004.
7. R. K. Ahluwalia and X. Wang, "Systems Level Perspective on Humidification in Direct Hydrogen Fuel Cell Systems with a High-Temperature Membrane," *USDOE High Temperature Membrane Working Group Meeting*, Philadelphia, PA, May 27, 2004.
8. R. K. Ahluwalia and X. Wang, "Startup of PEFC Stacks from Sub-Freezing Temperatures," *DOE Workshop on Fuel Cell Operations at Sub-Freezing Temperatures*, Phoenix, AZ, February 1-2, 2005.
9. R. K. Ahluwalia and X. Wang, "Fuel Cell Systems for Hybrid Vehicles," *DaimlerChrysler Research and Technology*, Ulm, Germany, September 27, 2004.