Fuel Cell Systems Analysis

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Project ID: FC6
Overview

Timeline
- Start date: Oct 2003
- End date: Open
- Percent complete: NA

Budget
- FY08 funding: $500K
  DOE share: 100%
- FY07 funding: $500K

Barriers
- B. Cost
- C. Performance
- E. System Thermal and Water Management
- F. Air Management
- J. Startup and Shut-down Time, Energy/Transient Operation

Partners
- Honeywell CEM+TWM projects
- Emprise, PermaPure, PNNL
- 3M, LBL, TIAX
- H₂ Quality Working Group, HNEI, LANL
- IEA Annexes 17 and 20
- FreedomCAR fuel cell tech team

This project addresses system, stack and air management targets for efficiency, power density, specific power, transient response time, cold start-up time, start up and shut down energy.
Objectives

Develop a validated system model and use it to assess design-point, part-load and dynamic performance of automotive fuel cell systems.

- Support DOE in setting technical targets and directing component development
- Establish metrics for gauging progress of R&D projects
Approach

Develop, document & make available versatile system design and analysis tools.

- GCtool: Stand-alone code on PC platform
- GCtool_ENG: Coupled to PSAT (MATLAB/SIMULINK)

Validate the models against data obtained in laboratory and at Argonne’s Fuel Cell Test Facility.

Apply models to issues of current interest.

- Work with FreedomCAR Technical Teams
- Work with DOE contractors as requested by DOE
Technical Accomplishments

1. System analysis to update the status of technology
   - **Stack:** Analyzed performance of NSTFC stacks with reduced Pt loading at elevated T
   - **Air Management:** Working with Honeywell to build and validate compressor and expander maps and analyze performance of alternate configurations
   - **Thermal Management:** Working with Honeywell to evaluate performance of advanced automotive radiators
   - **Water Management:** Assisting Honeywell to determine performance of full-scale enthalpy wheel and membrane humidifiers
   - **FCS-HTM:** Began investigating performance of FCS with high temperature membranes
   - **Cost:** Assisted TIAX in projecting cost of Argonne FCS-2010 at high volume manufacturing

2. Impurity effects in support of H₂ Quality Working Group
   - Hosted a workshop and presented ANL models for impurity effects
   - Developed an approach for determining rate constants
   - Attended ISO-TC192 WG-12 meetings and provided modeling support
Argonne LT-PEFC System Configuration

**Reference System**

- **MEA:** 3M’s NSTFC, ternary Pt alloy, 0.3 mg-Pt/cm², organic whisker support, 3M PFSA membrane, 90°C
- **Air Management:** 2.5 bar peak, mixed-flow compressor, radial inflow turbine
- **Water Management:** EWH + MH
- **Thermal Management:** HT + LT circuits, advanced automotive
- **Fuel Management:** Ejector + blower, periodic purge

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**An Alternate System**

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Our analysis of 3M data for optimized electrode structure (0.15 mg-Pt(c)/cm²) shows 15% reduction in Pt loading (g/kW) at constant system efficiency.

We estimate >35% higher Pt loading for ambient pressure system (75°C cell temperature).

No further reduction in Pt loading by raising cell T above 100°C (3 bar).

**2008 Stack Reference Parameters**
- 2.5 bar, 90°C
- Pt loading: 0.15(c)/0.1(a) mg/cm²
- Total Pt loading: 0.35 g/kW
- Stack power density: 715 mW/cm²
Performance of Integrated CEM Module

- Scalable compressor map from Honeywell data: pressure ratio (PR) and efficiency ($\eta$) as functions of corrected rpm ($N_c$) & mass flow rate
- Scalable expander maps from Honeywell data for different nozzle areas: $PR(F_f, N_c)$ and $\eta(F_v, PR)$
- Model for matched compressor and expander on common shaft
  - Stack operating at 2.5 bar, 80°C, 91 g/s, $\Delta P=3$ psi, 100% RH exit
  - With a fixed nozzle, parasitic power > 5.4 kWe for 40°C ambient at rated power and pressure < specs for part load operation
**Integrated CEMM with Variable Area Nozzle**

- Developed a method to determine the nozzle area at part load for optimum performance.
- Determined compressor delivery pressure (nozzle area) by matching performance of a cathode membrane humidifier and a stack with 3M NSTFC (90°C cell temperature).
- With an actuator, the nozzle opening can be controlled to match any desired pressure vs. load profile.
Alternate CEM Configurations

- Proposed and analyzed alternate configurations to reduce the CEM parasitic power to 5.4 kWe

<table>
<thead>
<tr>
<th>Compressor</th>
<th>Efficiency</th>
<th>Power</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air Flow</td>
<td>CP</td>
<td>EXP</td>
</tr>
<tr>
<td>P</td>
<td>%</td>
<td>%</td>
</tr>
<tr>
<td>g/s</td>
<td>bar</td>
<td></td>
</tr>
<tr>
<td>TC5</td>
<td>91</td>
<td>2.57</td>
</tr>
<tr>
<td>TC1</td>
<td>110</td>
<td>2.50</td>
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<tr>
<td>TC2</td>
<td>110</td>
<td>2.50</td>
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<tr>
<td>TC3</td>
<td>91</td>
<td>2.56</td>
</tr>
<tr>
<td>TC4</td>
<td>91</td>
<td>2.62</td>
</tr>
</tbody>
</table>

TC5: Based on Honeywell Patent US 7,056,132 B2

TC4: CEM with external heat exchanger
Thermal Management: Metal Foam Radiator

- Honeywell data confirms literature values for permeability of commercial metal foams and inertial drag coefficient.

- Our analysis shows that foams (40 PPI, 92% porosity) can have 30-40% higher effective heat transfer coefficients ($h$) than standard automotive louver fins (15 FPI) but also 6-15 times higher skin friction coefficients ($f$).

- For given frontal area and grill/underhood design, ANL radiator model shows much larger pumping power for commercial foams.
Thermal Management: Advanced Radiators

- Compared performance of advanced automotive (AAR, louver fins, 25 FPI), microchannel (plain rectangular fins, 40 FPI) and standard automotive radiators (SAR, louver fins, 15 FPI).
- AAR 50% more compact than SAR but slightly higher pumping power
- Microchannel radiator significantly more compact than SAR and also requires lower pumping power.
  - Honeywell to validate this result and address the issues of manufacturability and fouling
Water Management: Humidification Systems

- Working with Honeywell to validate models for enthalpy wheel (EWH) and membrane humidifiers (MH) developed from data with subscale modules
  - End-seal leakage in EWH
  - Maldistribution in MH
- Expanded EWH model to include $O_2$ leakage by volume exchange
  - Advantage of reduced leakage at lower rpm offset by larger unit size
  - 10-15% leakage at low loads
- MH module can be made compact by pre-cooling compressed air to 70°C
Impact of Humidifier on System Performance

Comparison between EWH & MH

- Smaller CEM parasitic power with EWH
- MH requires a precooler; low-grade Q difficult to reject
- EWH: At constant rpm, $T_{dp}$ increases as flow rate is reduced (effect of lower dry air inlet $T$, residence time)
- MH: With a precooler, $T_{dp}$ decreases at part load (effect of lower $P$ with fixed nozzle area)
- System with MH needs to operate at higher pressures at part load (lower system efficiency)

<table>
<thead>
<tr>
<th></th>
<th>EWH</th>
<th>MH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure Drop, psi</td>
<td>0.2</td>
<td>0.3</td>
</tr>
<tr>
<td>Oxygen Loss, %</td>
<td>2.2</td>
<td>0</td>
</tr>
<tr>
<td>Compressor Power, kW</td>
<td>11.4</td>
<td>11.2</td>
</tr>
<tr>
<td>Expander Power, kW</td>
<td>7.1</td>
<td>6.5</td>
</tr>
<tr>
<td>CEM Motor Power, kWe</td>
<td>5.1</td>
<td>5.6</td>
</tr>
<tr>
<td>EW Motor Power, kWe</td>
<td>0.1</td>
<td>0</td>
</tr>
<tr>
<td>Air Precooling, kW</td>
<td>0</td>
<td>8.1</td>
</tr>
<tr>
<td>Volume, l</td>
<td>11</td>
<td>9</td>
</tr>
<tr>
<td>Weight, kg</td>
<td>10</td>
<td>4.5</td>
</tr>
</tbody>
</table>
Summary of On-going System Studies

1. Stack
   - ORR kinetics at high temperature and low relative humidity
   - Advanced dispersed Pt/C electrodes
2. Air Management System
   - Better definition of motor and bearing cooling requirements
   - Detailed motor map: efficiency as a function of torque and rpm
3. Thermal Management System
   - Value function for trade-off study
   - Validation of microchannel radiator performance
4. Water Management System
   - Fuel cell system with PNNL microchannel humidifier
   - Validation of full-scale enthalpy wheel and membrane humidifier models
5. Fuel Management System
   - Dynamic pressure control
   - Passive recirculation
   - Elimination of anode humidifier
Modeling Impurity Effects for Fuel H₂ Quality

- Hosted a workshop at ANL and detailed our model for effects of CO, CO₂, H₂S, NH₃ and N₂ in fuel H₂ on performance of cells.
- Attended ISO-TC194-WG12 meeting and obtained agreement on use of ANL model in setting H₂ quality standards.
- Published a paper on buildup of CO and CO₂ in closed anode gas circuit and optimum recycle ratio (purge rate).
- Attended NA Fuel H₂ Quality Team meeting and explained apparent discrepancy in ANL models results and JARI data on impurity buildup.
- Proposed new approach for determining rate constants using data for CO conversion and anode overpotential:
  - Sequential determination of parameters for electrochemical oxidation, adsorptions/desorptions and oxidation reactions.
  - Illustrated approach by running the model under different conditions and treating the simulation results as data.
Effect of H₂ Utilization on CO Buildup

- Apparent discrepancy between ANL model results and JARI data
  \[ \Phi_{CO} = 1 - \frac{\dot{N}_{CO}^{out}}{\dot{N}_{CO}^{in}} \]

  \[ R_{CO} = \frac{C_{CO}^{out}}{C_{CO}^{in}} = \frac{1 - \Phi_{CO}}{1 - \Phi_{H2}} \]

- \( R_{CO} = 1 \) (no buildup of CO ) if \( \Phi_{H2} = \Phi_{CO} \)
- \( R_{CO} > 1 \) if \( \Phi_{H2} > \Phi_{CO} \): ANL model for 70% H₂ utilization
- \( R_{CO} < 1 \) if \( \Phi_{H2} < \Phi_{CO} \): JARI data for 17-25% H₂ utilization
- ANL simulations: At constant current density (1 A/cm²), \( \Phi_{CO} \) is a function of \( \Phi_{H2} \) and membrane thickness
Effect of Pt Loading and Stack Temperature

- Examples of how the model, after validation, can be used to help in setting fuel quality standards
- Decrease in stack efficiency/cell voltage at reduced Pt loading in part due to the bridge-site mechanism for CO poisoning
- At lower temperature, reduced CO tolerance due to slower desorption ($\Delta H_{CO}$) and electrochemical oxidation ($E_{CO}$) rates
Approach for Determining Rate Constants in CO Poisoning Model

- Operate in H₂ Pump Mode under conditions of high $\eta_a$ and determine CO conversion for different CO concentrations at constant $J_H$.
- Repeat Step 1 at different $J_H$ and cell T.
- Operate in FC mode to determine $O_2$ selectivity for CO oxidation.

<table>
<thead>
<tr>
<th>Step</th>
<th>Reaction</th>
<th>Fitting Input</th>
<th>Fitting</th>
<th>Input</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$M_2 - CO + H_2O \Rightarrow 2M + CO_2 + 2H^+ + 2e^-$</td>
<td>$a_{CO}$</td>
<td>0.15</td>
<td>0.15</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_{CO}^e$, mol/m²Pt</td>
<td>$7 \times 10^{-10}$</td>
<td>$6 \times 10^{-10}$</td>
</tr>
<tr>
<td>2</td>
<td>$CO + 2M \Leftrightarrow M_2 - CO$</td>
<td>$\beta$</td>
<td>0.13</td>
<td>0.10</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$E_{CO}^o$, kJ/mol</td>
<td>41.1</td>
<td>39.7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_{CO}^o$, mol/(m²Pt/bar)</td>
<td>$5 \times 10^{-3}$</td>
<td>$6 \times 10^{-3}$</td>
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<tr>
<td></td>
<td></td>
<td>$E_{CO}^f$, kJ/mol</td>
<td>67.2</td>
<td>65</td>
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<tr>
<td></td>
<td></td>
<td>$\Delta H_{CO}^f$, kJ/mol</td>
<td>148</td>
<td>150</td>
</tr>
<tr>
<td>3</td>
<td>$M_2 - CO + \frac{1}{2} O_2 \Rightarrow 2M + CO_2$</td>
<td>$\Delta E_s$, kJ/mol</td>
<td>95.7</td>
<td>94.0</td>
</tr>
<tr>
<td></td>
<td>$M - H + \frac{1}{2} O_2 \Rightarrow M + H_2O$</td>
<td>$k_s$</td>
<td>$2 \times 10^{-5}$</td>
<td></td>
</tr>
</tbody>
</table>

- Working with HNEI to validate the approach
  - Meaningful only if changes in CO concentration can be measured accurately
  - Approach valid even if model assumptions have to be modified
  - Additional information from analyzing the transient data
Future Work

1. System Analysis
   - Support DOE/FreedomCAR development effort at system, component and phenomenological levels
   - Collaborate with 3M on durability, reduced Pt loading, elevated T operation of stacks
   - Continue cooperation with Honeywell to validate air, thermal and water management models
   - Support PNNL on development of microchannel humidifier
   - Provide feedback to LBNL and others on systems issues related to development of high-temperature membranes

2. Hydrogen Quality
   - Work with HNEI on validating CO impurity model
   - Collaborate with LANL on H₂S and mixed impurity effects
   - Support the Hydrogen Quality Working Group and the Codes and Standards Technical Team