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Fuel Cell Systems Analysis

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U.S. Department
of Energy

UChicago ►
Argonne_{LLC}

A U.S. Department of Energy laboratory
managed by UChicago Argonne, LLC

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

■ 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

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

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

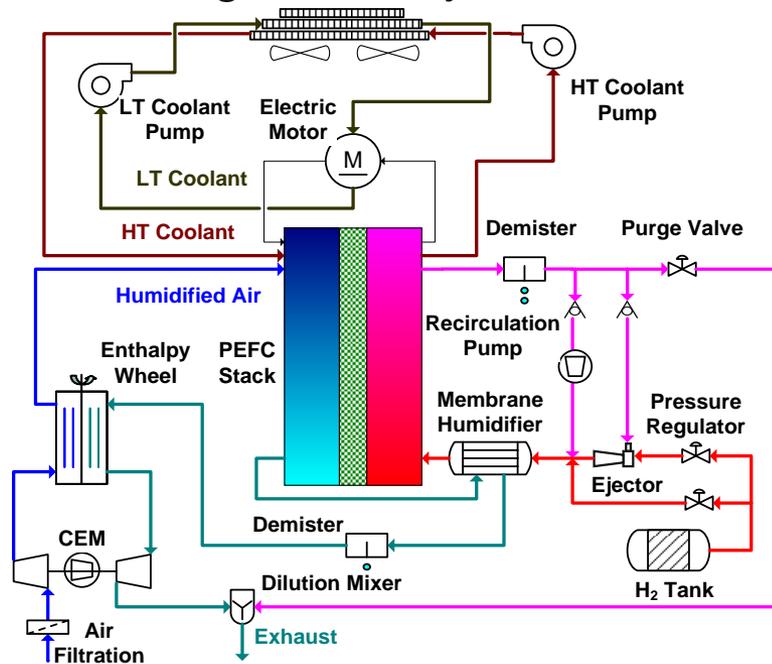
MEA: 3M's NSTFC, ternary Pt alloy, 0.3 mg-Pt/cm², organic whisker support, 3M PFSA membrane, 90°C

Air Management: 2.5 bar peak, mixed-flow compressor, radial inflow turbine

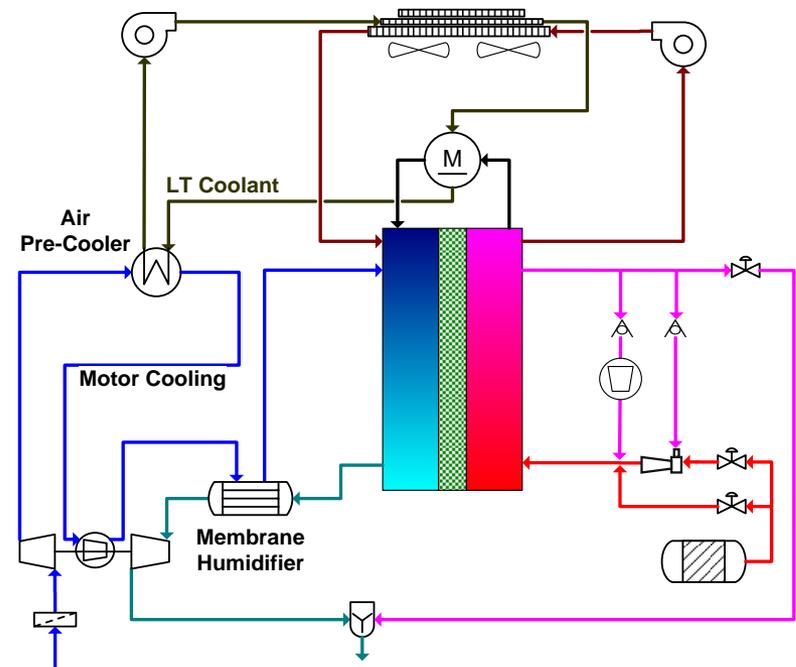
Water Management: EWH + MH

Thermal Management: HT + LT circuits, advanced automotive

Fuel Management: Ejector + blower, periodic purge



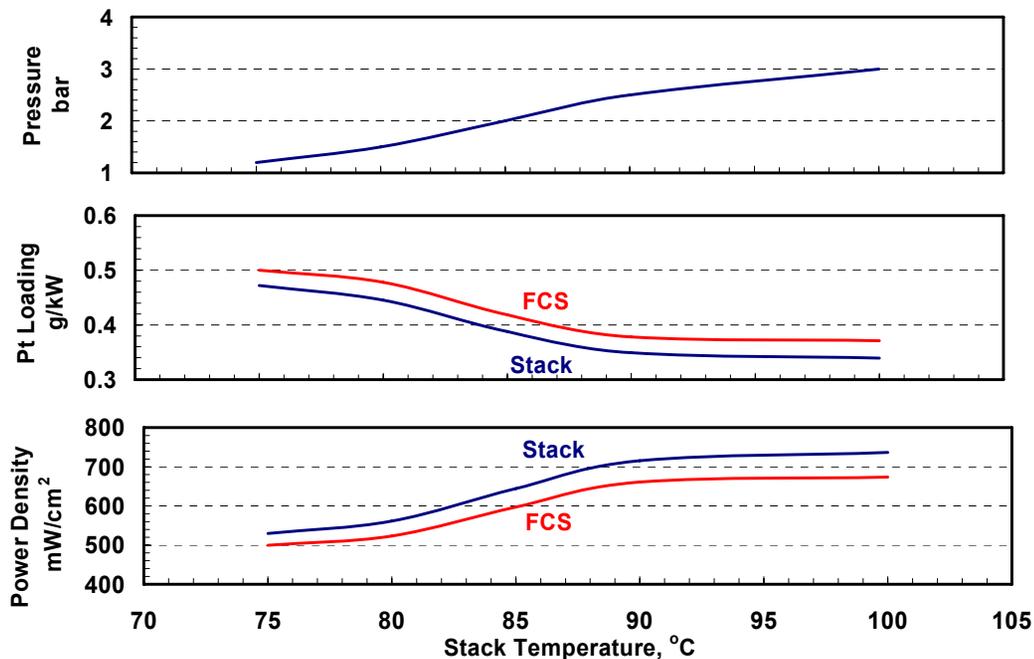
Reference System



An Alternate System

Stack Technology with NSTFC

- 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)

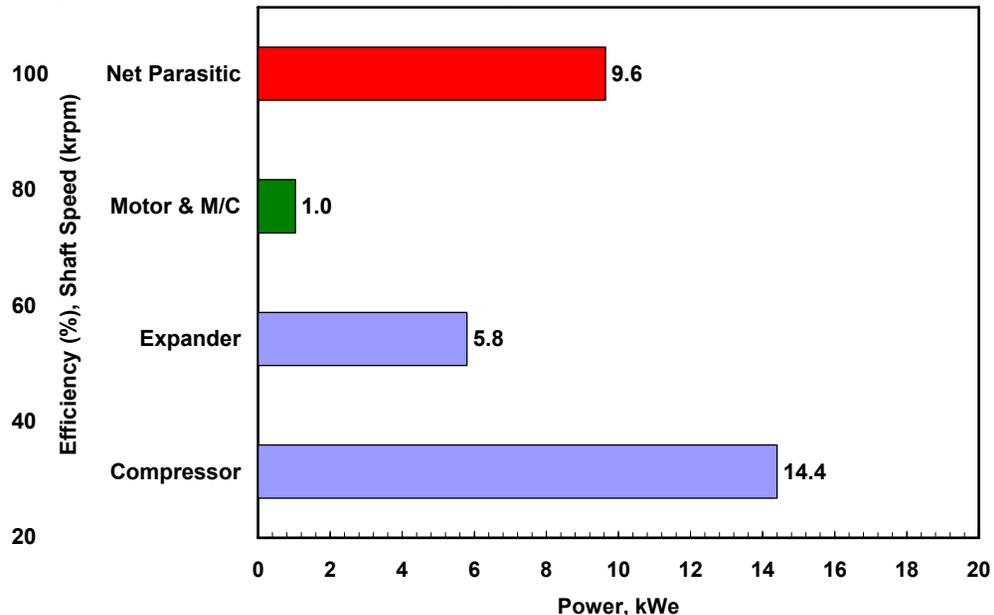
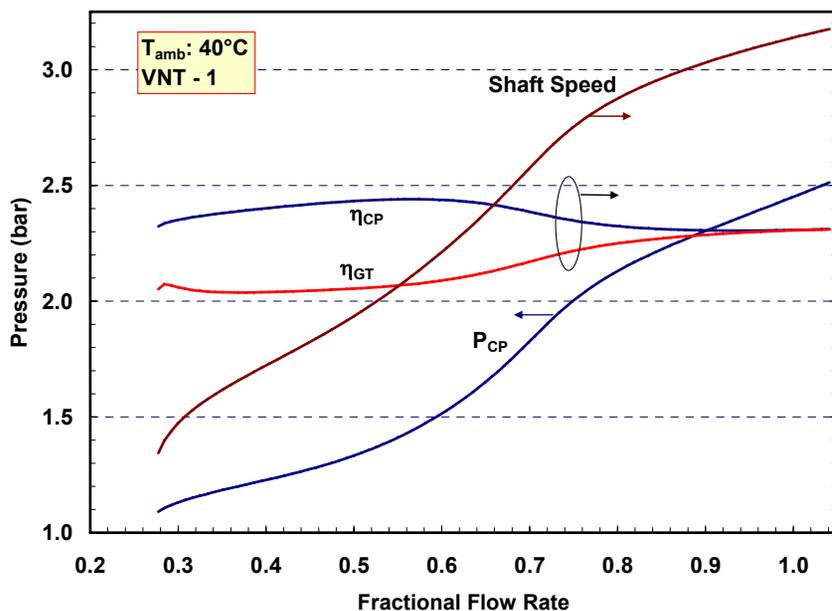


2008 Stack Reference Parameters

- 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

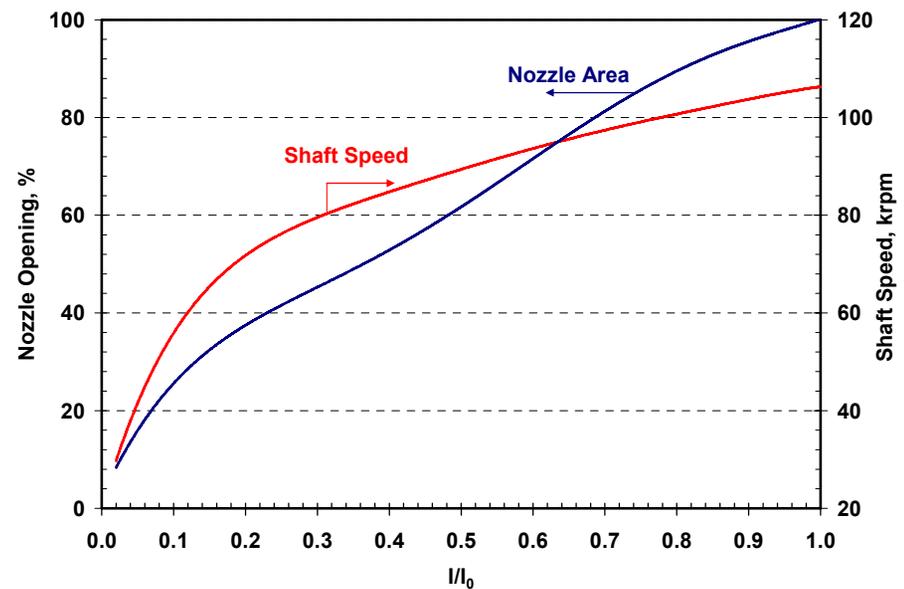
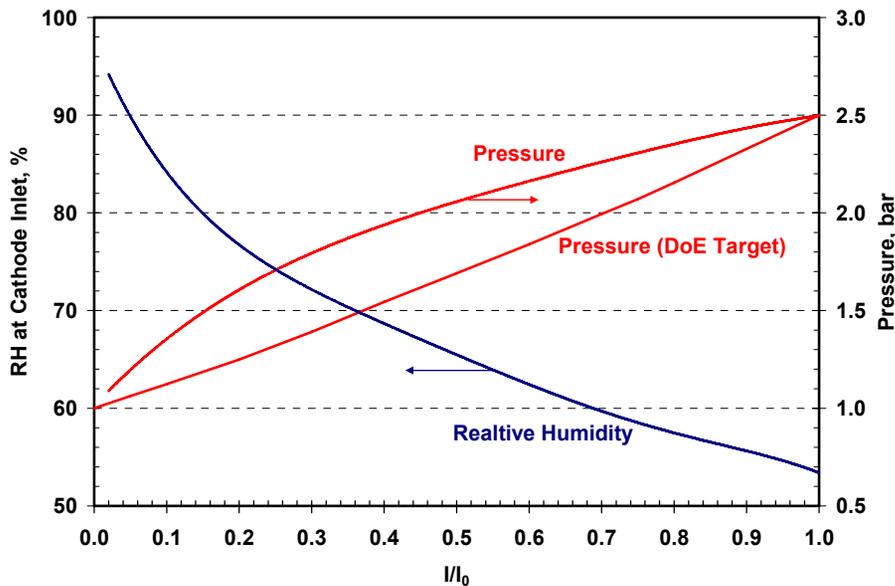
Performance of Integrated CEM Module

- Scalable compressor map from Honeywell data: pressure ratio (PR) and efficiency (η) 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



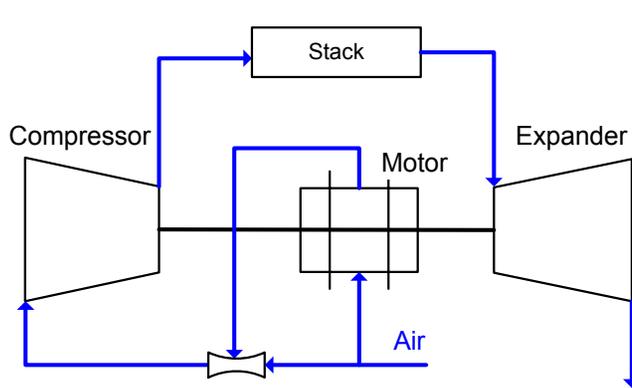
Integrated CEMM with Variable Area Nozzle

- 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

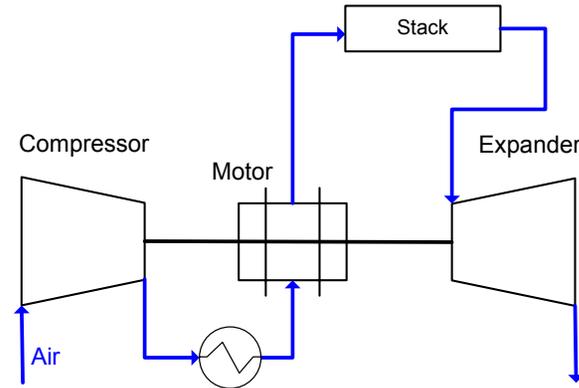


Alternate CEM Configurations

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



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

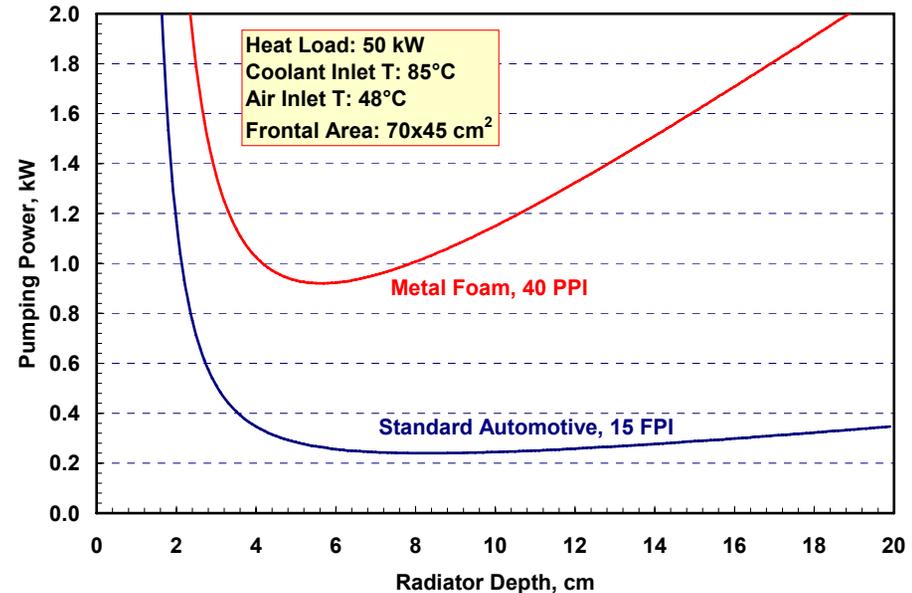
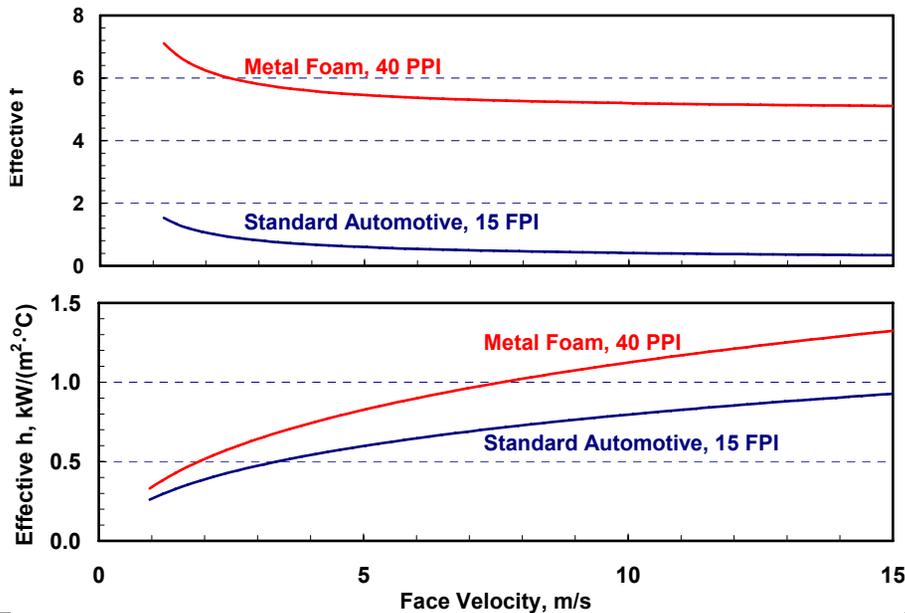


TC4: CEM with external heat exchanger

	Compressor		Efficiency		Power		
	Air Flow	P	CP	EXP	CP	EXP	Parasitic
	g/s	bar	%	%	kW	kW	kWe
TC5	91	2.57	69.4	75.3	14.0	6.3	9.1
TC1	110	2.50	72.6	75.5	14.5	6.1	9.9
TC2	110	2.50	72.6	75.5	14.5	7.4	8.3
TC3	91	2.56	73.1	75.5	12.3	6.3	7.0
TC4	91	2.62	73.2	75.4	12.5	6.3	7.3

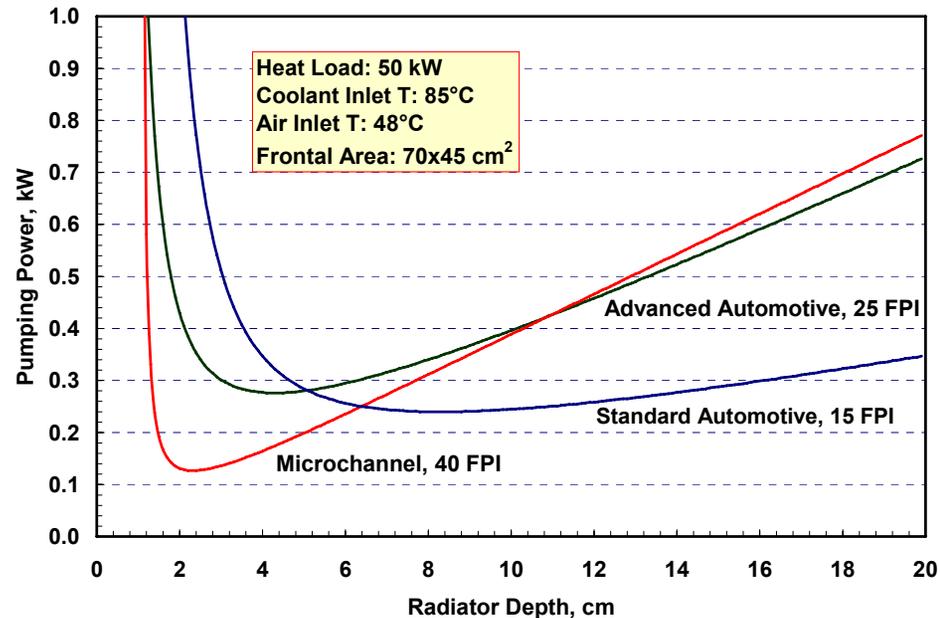
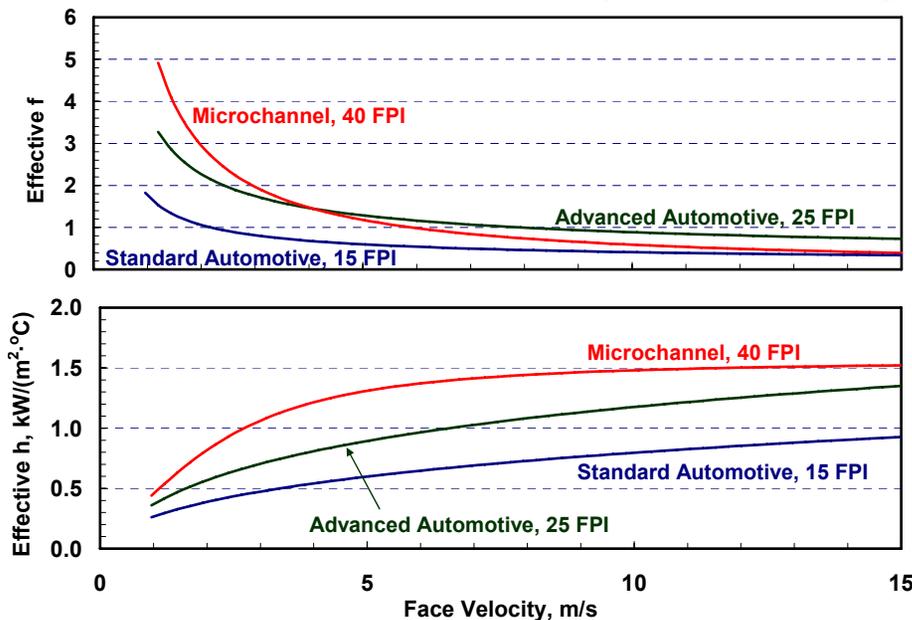
Thermal Management: Metal Foam Radiator

- 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.



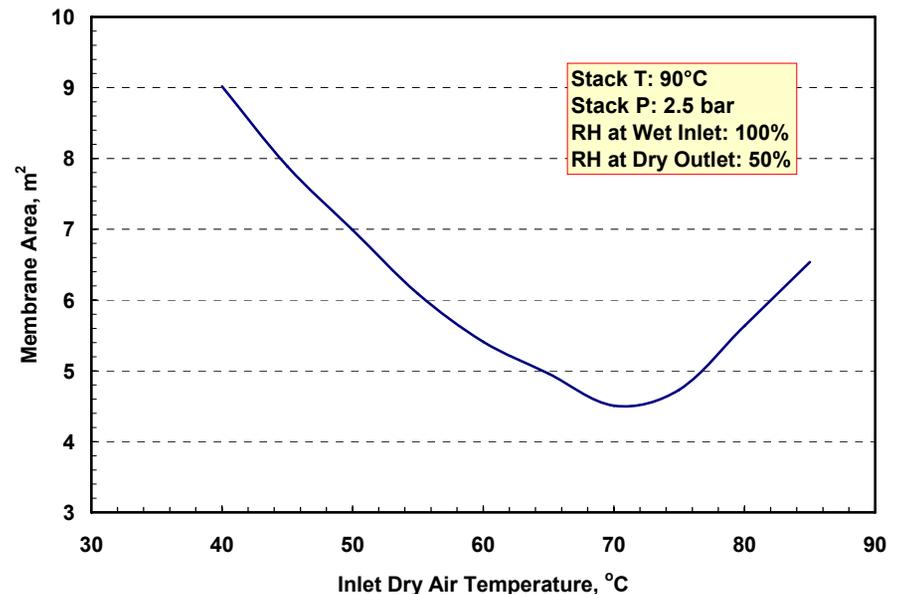
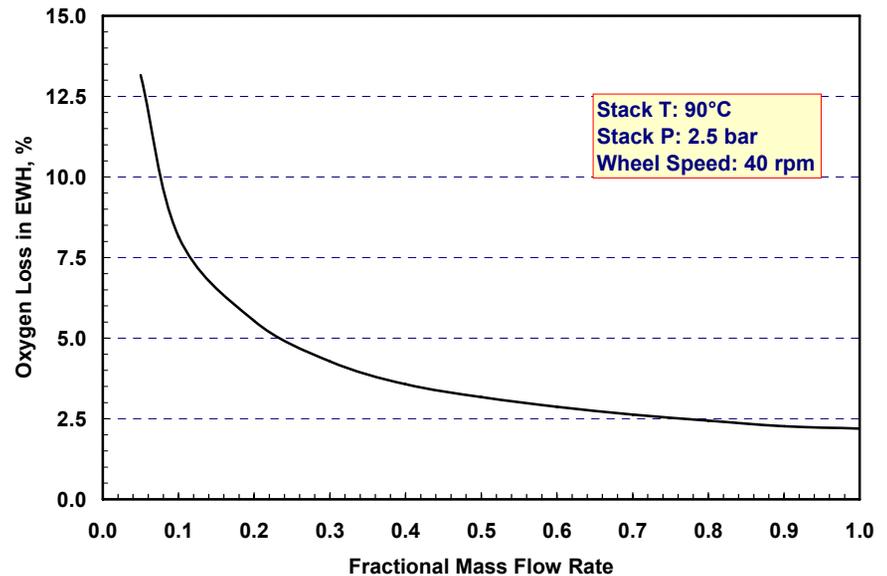
Thermal Management: Advanced Radiators

- 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 O₂ 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

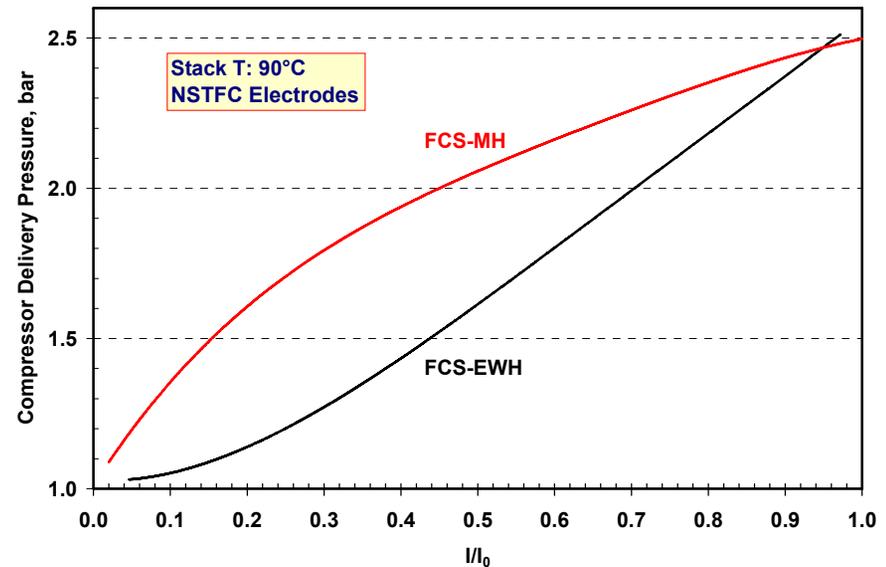


Impact of Humidifier on System Performance

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)

	EWH	MH
Pressure Drop, psi	0.2	0.3
Oxygen Loss, %	2.2	0
Compressor Power, kW	11.4	11.2
Expander Power, kW	7.1	6.5
CEM Motor Power, kWe	5.1	5.6
EW Motor Power, kWe	0.1	0
Air Precooling, kW	0	8.1
Volume, l	11	9
Weight, kg	10	4.5



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/desorption and oxidation reactions
 - Illustrated approach by running the model under different conditions and treating the simulation results as data.

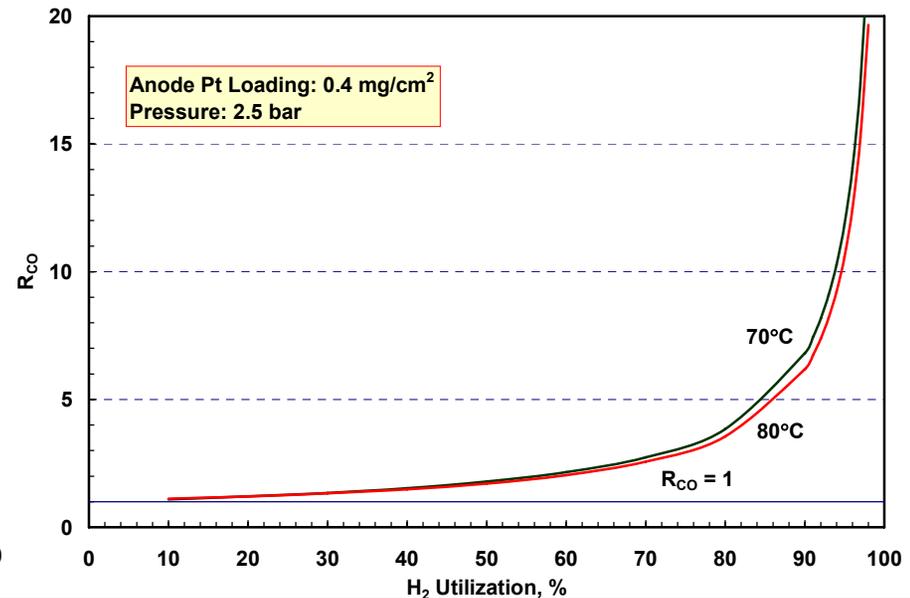
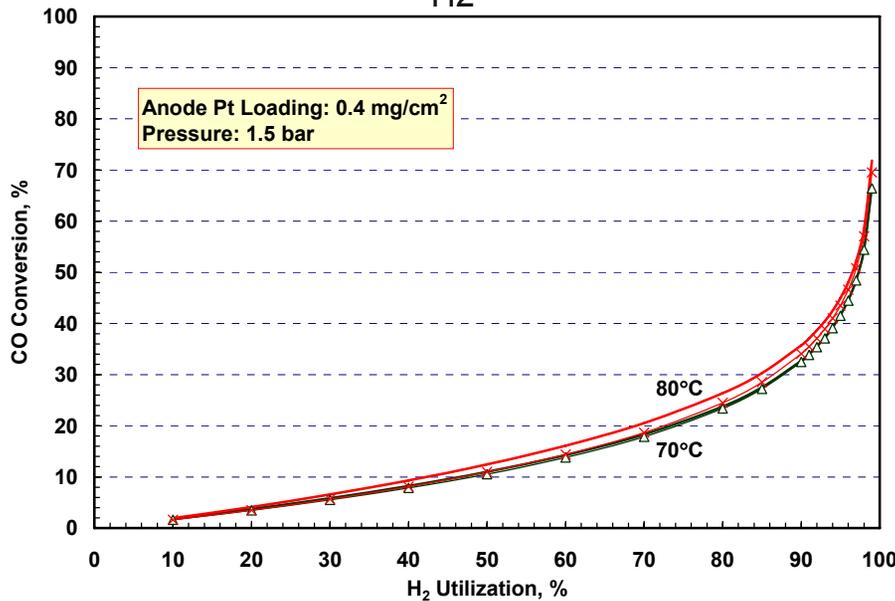
Effect of H₂ Utilization on CO Buildup

- Apparent discrepancy between ANL model results and JARI data

$$\Phi_{CO} = 1 - \dot{N}_{CO}^{out} / \dot{N}_{CO}^{in}$$

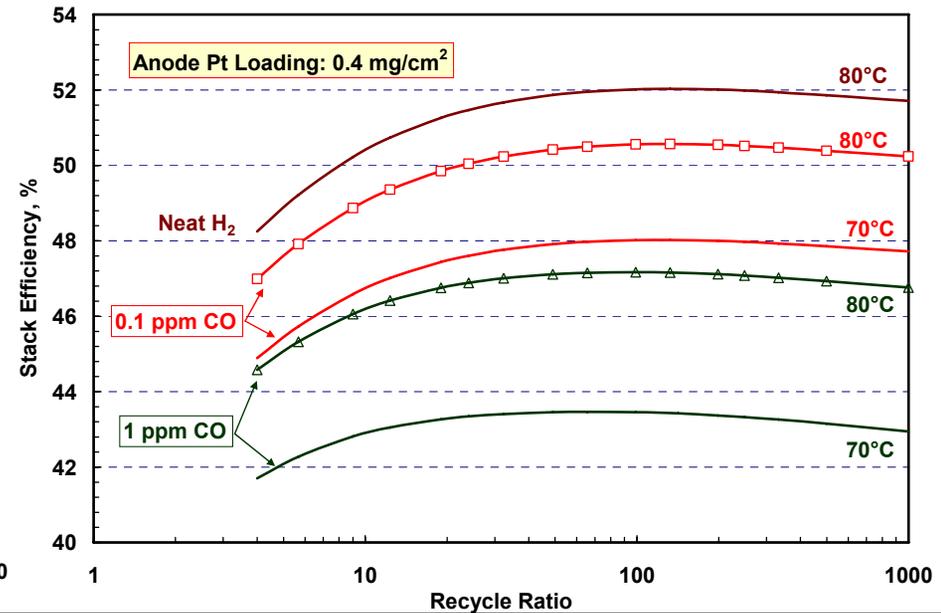
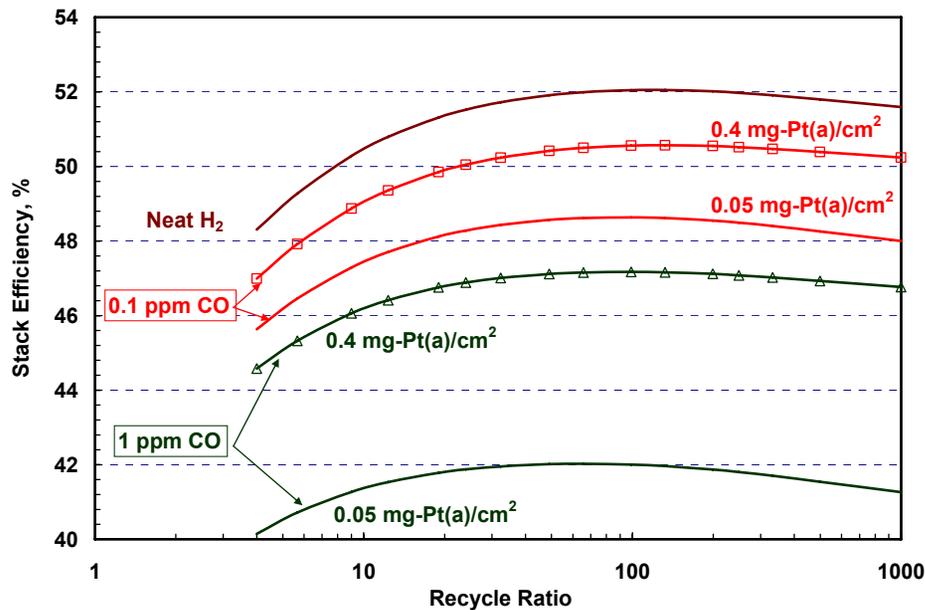
$$R_{CO} = \frac{C_{CO}^{out}}{C_{CO}^{in}} = \frac{1 - \Phi_{CO}}{1 - \Phi_{H_2}}$$

- $R_{CO} = 1$ (no buildup of CO) if $\Phi_{H_2} = \Phi_{CO}$
- $R_{CO} > 1$ if $\Phi_{H_2} > \Phi_{CO}$: ANL model for 70% H₂ utilization
- $R_{CO} < 1$ if $\Phi_{H_2} < \Phi_{CO}$: JARI data for 17-25% H₂ utilization
- ANL simulations: At constant current density (1 A/cm²), Φ_{CO} is a function of Φ_{H_2} 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 (ΔH_{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 η_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 O₂ selectivity for CO oxidation.

Step			Fitting	Input		Fitting	Input
1	$M_2 - CO + H_2O \Rightarrow 2M + CO_2 + 2H^+ + 2e^-$	α_{CO}	0.15	0.15	$k_{CO}^e, \text{mol/m}^2_{Pt}$	7×10^{-10}	6×10^{-10}
2	$CO + 2M \Leftrightarrow M_2 - CO$	β	0.13	0.10	$E_{CO}^a, \text{kJ/mol}$	41.1	39.7
		$k_{CO}^a, \text{mol}/(\text{m}^2_{Pt} \text{ bar})$	5×10^{-3}	6×10^{-3}	$k_{CO}^d, \text{mol/m}^2_{Pt}$	4.7×10^{-15}	4.4×10^{-15}
		$E_{CO}^e, \text{kJ/mol}$	67.2	65	$\Delta H_{CO}^d, \text{kJ/mol}$	148	150
3	$M_2 - CO + \frac{1}{2} O_2 \Rightarrow 2M + CO_2$ $M - H + \frac{1}{2} O_2 \Rightarrow M + H_2O$	$\Delta E_s, \text{kJ/mol}$	95.7	94.0	k_s	2×10^{-5}	

- 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