

# **Fuel Cells Systems Analysis**

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**Project ID: FC017**

This presentation does not contain any proprietary, confidential, or otherwise restricted information.

## Timeline

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

## Budget

- FY15 DOE Funding: \$555 K
- Planned DOE FY16 Funding: \$550 K
- Total DOE Project Value: \$550 K

## 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/Interactions

- Eaton, Ford, UDEL/Sonijector
- SA, Aalto University (Finland)
- 3M, Ballard, Johnson-Matthey Fuel Cells (JMFC), UTRC
- IEA Annex 34
- Transport Modeling Working Group
- Durability Working Group
- U.S. DRIVE fuel cell tech team

## Objectives and Relevance

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

- Support DOE in setting technical targets and directing component development
- Establish metrics for gauging progress of R&D projects
- Provide data and specifications to DOE projects on high-volume manufacturing cost estimation

Impact of FY2016 work

- Quantified the sources of 14-20% decrease in power density and 2.20 \$/kWe increase in cost due to the heat rejection ( $Q/\Delta T$ ) constraint.
- Identified the dominant NSTF catalyst degradation mechanism and determined that the cumulative fluoride release (CFR) must be limited to  $0.7 \mu\text{g}\cdot\text{cm}^{-2}$  for 10% performance degradation over 5000 h.
- Projected 25% increase in power density and 16.8% reduction in FCS cost by reducing anode Pt loading to  $0.02 \text{ mg}/\text{cm}^2$  and replacing  $\text{Pt}_{68}(\text{CoMn})_{32}/\text{NSTF}$  with  $\text{Pt}_3\text{Ni}_7/\text{NSTF}$  cathode catalyst and 20- $\mu\text{m}$  835 EW membrane with supported 14- $\mu\text{m}$  725 EW membrane.
- Demonstrated that, compared to a baseline unit, the V250 module (without expander) reduces parasitic power by 6.4% at full flow (92 g/s) and by 35% at quarter flow (25 g/s)



# Approach

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

- GCtool: Stand-alone code on PC platform
- GCtool-Autonomie: Drive-cycle analysis of hybrid fuel cell systems

Validate the models against data obtained in laboratories and test facilities inside and outside Argonne.

- Collaborate with external organizations

Apply models to issues of current interest.

- Work with U.S. DRIVE Technical Teams
- Work with DOE contractors as requested by DOE

|   |  |       |
|---|--|-------|
| 1 | In collaboration with 3M, formulate a test matrix for measuring the performance of de-alloyed Pt <sub>3</sub> Ni <sub>7</sub> /NSTF catalysts with cathode interlayer.   | 12/15 |
| 2 | Develop a model for the performance of MEAs using de-alloyed Pt <sub>3</sub> Ni <sub>7</sub> /NSTF catalysts with cathode interlayer relative to the targets of 0.44 A/mg-PGM mass activity and 720 mA/cm <sup>2</sup> -PGM specific activity at 900 mV <sub>iR-free</sub> , 1000 mW/cm <sup>2</sup> at rated power, and 300 mA/cm <sup>2</sup> at 800 mV. | 03/16 |
| 3 | In collaboration with 3M, develop and test strategies for mitigating the degradation of NSTF catalysts under long potentiostatic holds.  | 06/16 |
| 4 | Develop a model for the stability of NSTF catalyst and determine the MEA durability under automotive conditions relative to the target of 5000 h.  | 09/16 |

# Summary: Technical Accomplishments

**Stack:** Collaboration with 3M, JMFC/UTRC and Ballard in obtaining data to develop validated models for pressures up to 3 atm

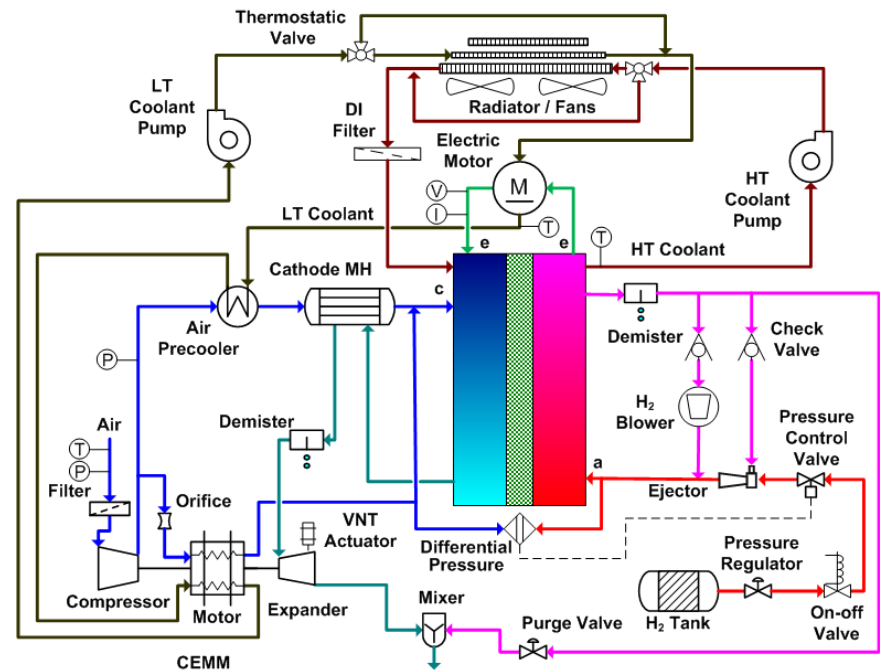
- Ternary PtCoMn/NSTF catalyst system: durability on drive cycles (**results #3 and #4**)
- De-alloyed Pt<sub>3</sub>Ni<sub>7</sub>/NSTF catalyst system (**results #1 and #2**)
- Dispersed Pt/C and de-alloyed PtNi/C catalyst systems (**ongoing**)

**Air Management:** Collaborating with Eaton and Ballard to develop and model Roots compressors and expanders and integrated air management system for automotive and bus applications (**ongoing**)

**Water Management:** Optimizing cost of integrated PEFC stack and cross-flow humidifier (**ongoing**)

**Fuel Management:** Collaboration with UDEL and Sonijector (**ongoing**)

**Thermal Management:** Optimize system performance and cost subject to  $Q/\Delta T$  constraint (**ongoing #1 and #2**)



Argonne 2015 & Interim 2016 FCS

# Effect of Q/ΔT Constraint on FCS Performance with NSTF Catalyst

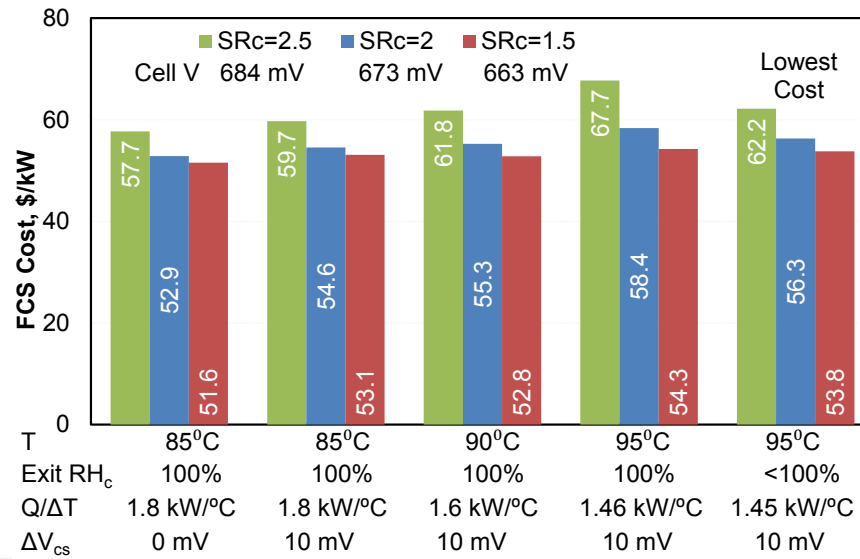
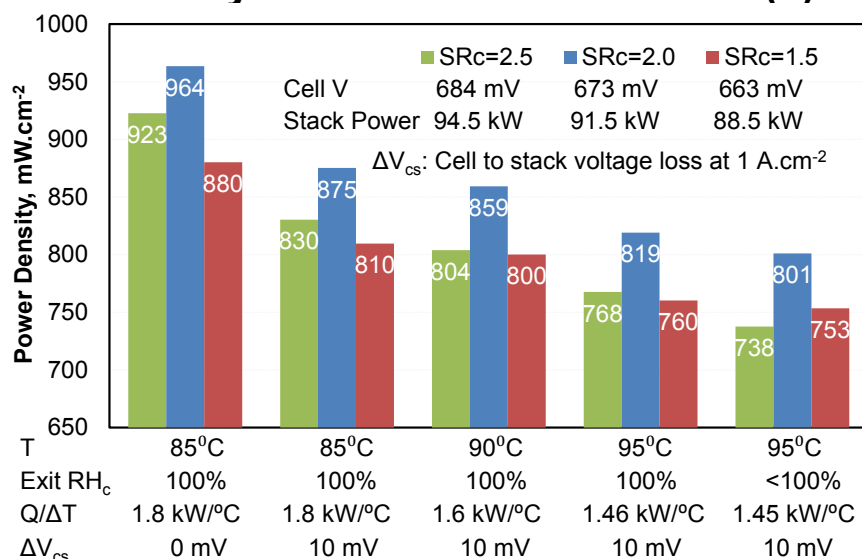
## Stack with PtCoMn/NSTF catalyst MEAs

- Cluster 1: Power density at 2.5 atm, 85°C, 100% exit RH and cell voltages needed to satisfy Q/ΔT constraint at 95°C and SRc = 1.5, 2.0 and 2.5
- Cluster 2: Effect of 10 mV cell-to-stack voltage degradation ( $\Delta V_{cs}$ ) at 1 A/cm<sup>2</sup>
- Clusters 3 and 4: Effect of raising temperature to 90-95°C to approach Q/ΔT target
- Cluster 5: Effect of drier operating conditions
- 14.4-20% decrease in power density from Cluster 1 to Cluster 4 conditions**

With respect to the baseline FCS cost for SR(c) = 1.5,  $\Delta V_{cs}$  = 0, 100% exit RH<sub>c</sub>, **2.20 \$/kWe projected increase\* in cost due to Q/ΔT constraint**

- 1.50 \$/kW<sub>e</sub> increase due to 10 mV  $\Delta V_{cs}$ ; 1.20 \$/kW<sub>e</sub> increase due to stack T raised from 85 to 95°C to meet Q/ΔT constraint; 0.50 \$/kW<sub>e</sub> decrease due to drier operating conditions, i.e., exit RH<sub>c</sub> < 100%

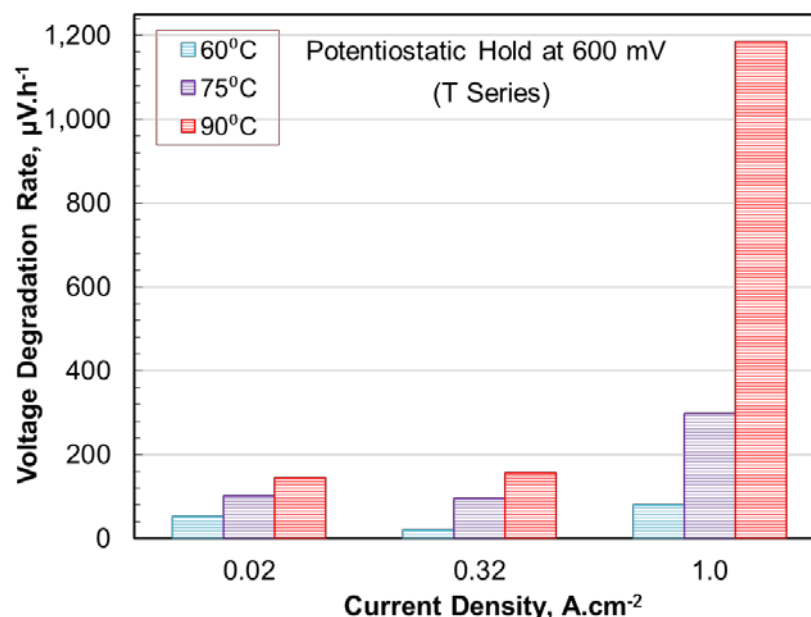
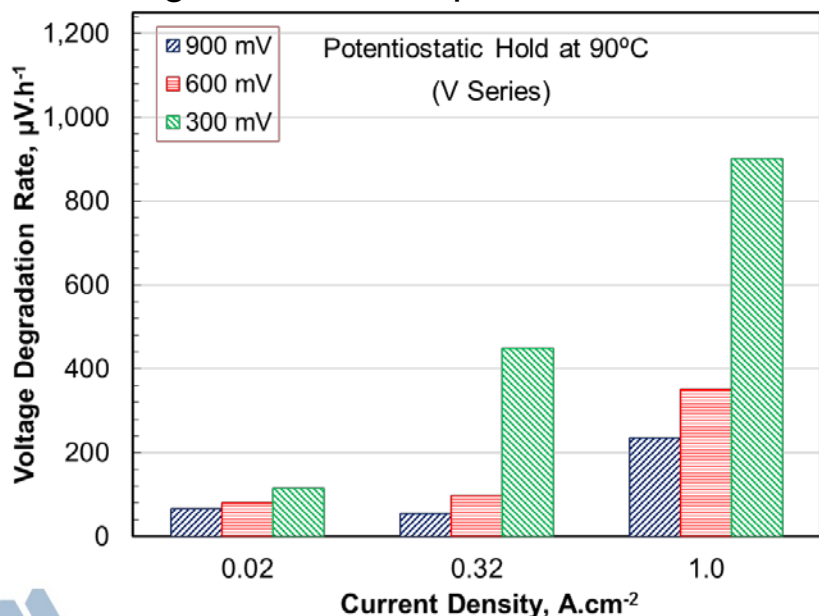
**Stack power density is highest and the stack cost is lowest at SRc = 2.0 but the overall system cost is lowest at SR(c) = 1.5**



# Durability of NSTFC MEAs: Irreversible Degradation

Long holds at low potentials identified as the dominant degradation mechanism in NSTF catalysts

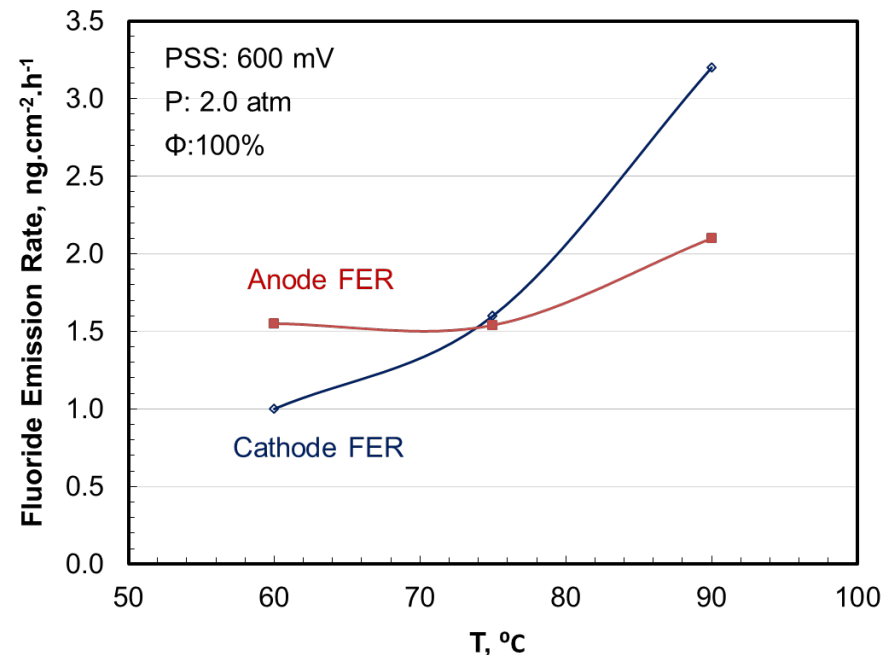
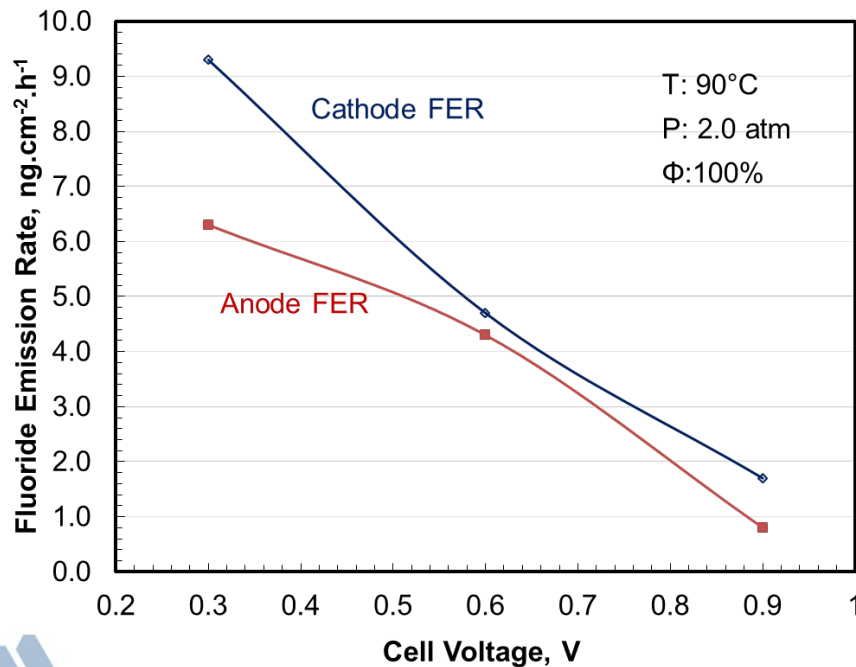
- Collaborated with 3M to run 700-h tests to expose 50-cm<sup>2</sup> cells: PtCoMn/NSTF catalysts, 0.15(c)/0.05(a) mg/cm<sup>2</sup> Pt loading; 3M 835EW 20- $\mu$ m unsupported, chemically stabilized membrane; 3M GDLs, 10% strain; quad-serpentine flow field; constant flow based on 2(c)/2(a) stoichiometry at current density at BOL hold potential
- Test protocol: periodic F<sup>-</sup> collection and partial reconditioning (1 TC) every 10 h, H<sub>2</sub>/air pol curves every 20 h, and more full reconditioning (3 TCs) every 40-80 h
- V Series: Potentiostatic hold at 0.3, 0.6 and 0.9 V at 90°C, 100% RH, SR(c) = 2
- T Series: Potentiostatic hold at 60, 75 and 90°C, 0.6 V
- Irreversible degradation defined as loss in cell voltage after normal recovery method: three thermal-conditioning (TC) cycles plus electrochemical characterization (EC) tests
- Voltage losses from polarization curves at 1.5 atm, 80°C, 100% RH



\* All exposure tests at 100/100% RH, 100/100 kPag H<sub>2</sub>/Air

# Fluoride Release Rates

- Fluoride release measured by ion chromatography of collected water samples
- F<sup>-</sup> concentrations are very low: 20 ppb or less
  - Measured fluoride emission rates (FER) on cathode and anode are similar
  - Fluoride release rates for NSTF catalysts are an order-of-magnitude smaller than for dispersed Pt/C catalysts with chemically stabilized and mechanically reinforced membranes
  - FER on cathode are higher at lower cell voltages, consistent with the observed dependence of H<sub>2</sub>O<sub>2</sub> production on potential in RRDE tests
  - 43.2 kJ/mol activation energy for temperature dependence of cathode FER





# Irreversible Increase in Kinetic Losses

Cathode ECSA ( $A_{Pt}$ ) loss is due to smoothing of whiskerettes and the resulting decrease in surface area.

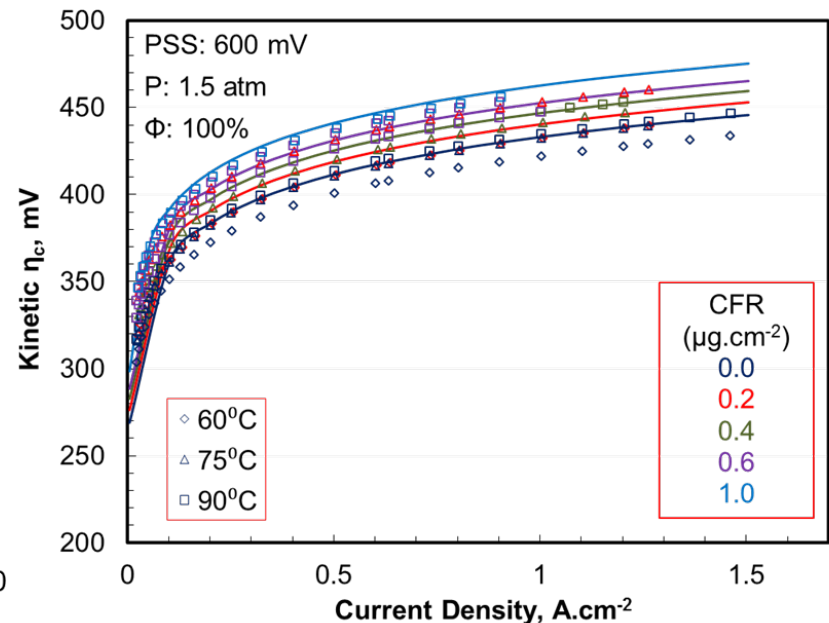
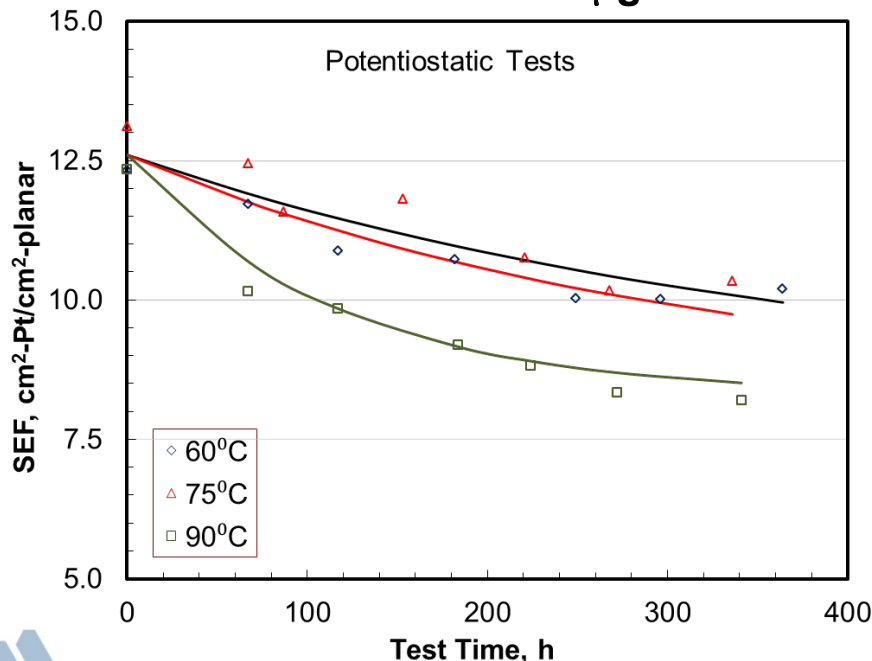
- Loss in cathode surface area enhance factor (SEF) is nearly independent of the hold potential
- Faster loss in SEF at higher exposure temperatures (48 kJ/mol activation energy ) but the maximum loss is limited to 30-40% as under cyclic potentials

Decrease in ORR specific activity ( $\text{mA}/\text{cm}^2\text{-Pt}$ ) suggests a kinetic loss mechanism separate from ECSA loss

- Exchange current density ( $i_0$ ,  $\mu\text{A}\cdot\text{cm}^2\text{-Pt}$ ) determined from polarization data at low current densities and correlated with CFR\*

Up to 65 mV increase in kinetic overpotential ( $\eta_c$ ) during the tests

- **Need to restrict CFR to  $<1 \mu\text{g}/\text{cm}^2$  to limit increase in  $\eta_c$  at EOL to  $<35 \text{ mV}^{**}$**



\*CFR: cumulative fluoride release ; \*\*half of allowed 10% voltage degradation at EOL

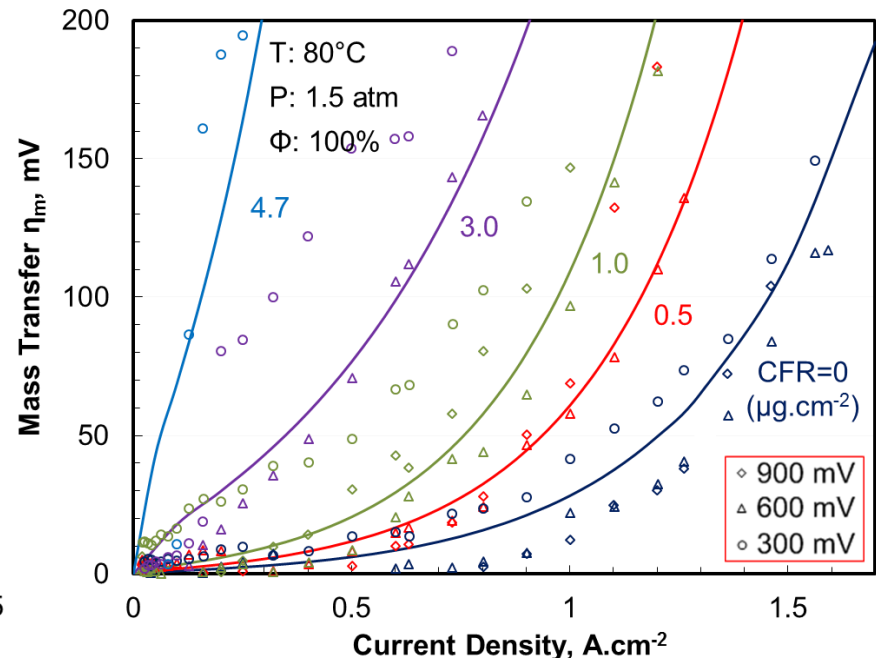
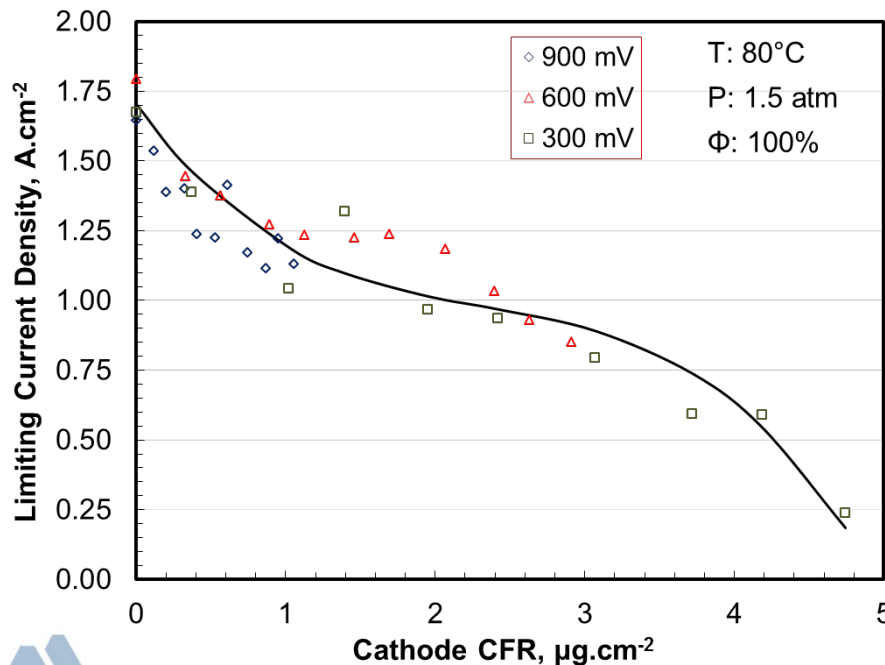
# Irreversible Increase in Mass Transfer Overpotentials

Limiting current density ( $i_L$ ) defined for convenience as the reference current density at which the mass transfer overpotential ( $\eta_m$ ) equals 300 mV

- $i_L$  can be correlated with CFR without any explicit dependence on hold potential or exposure temperature
- **2  $\mu\text{g}\cdot\text{cm}^{-2}$  suggested as the absolute upper limit of CFR for NSTF MEA:**  
Value at which  $i_L$  becomes  $<1 \text{ A/cm}^2$  at 3M standard conditions

Mass transfer overpotential ( $\eta_m$ ) correlated with  $i/i_L$  and the cumulative fluoride release at cathode (CFR)

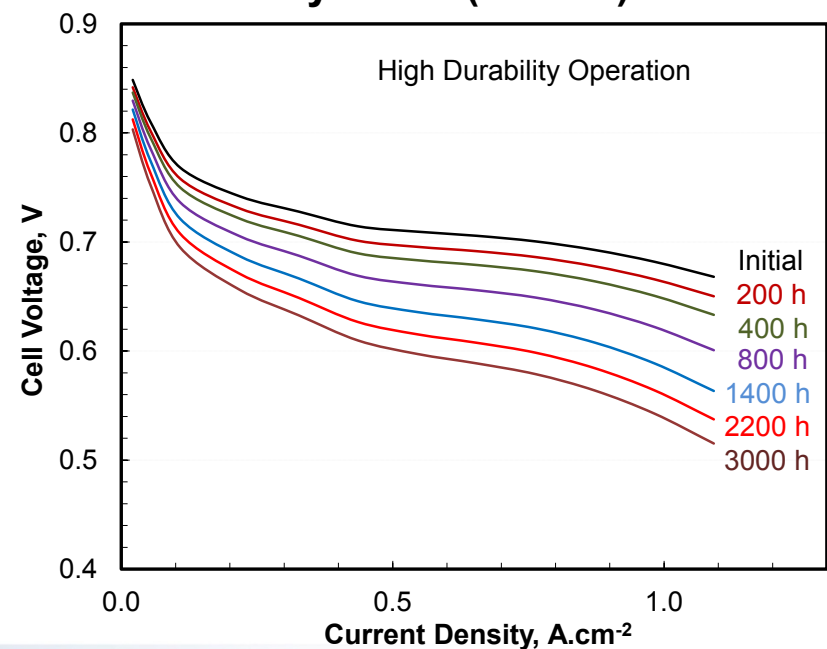
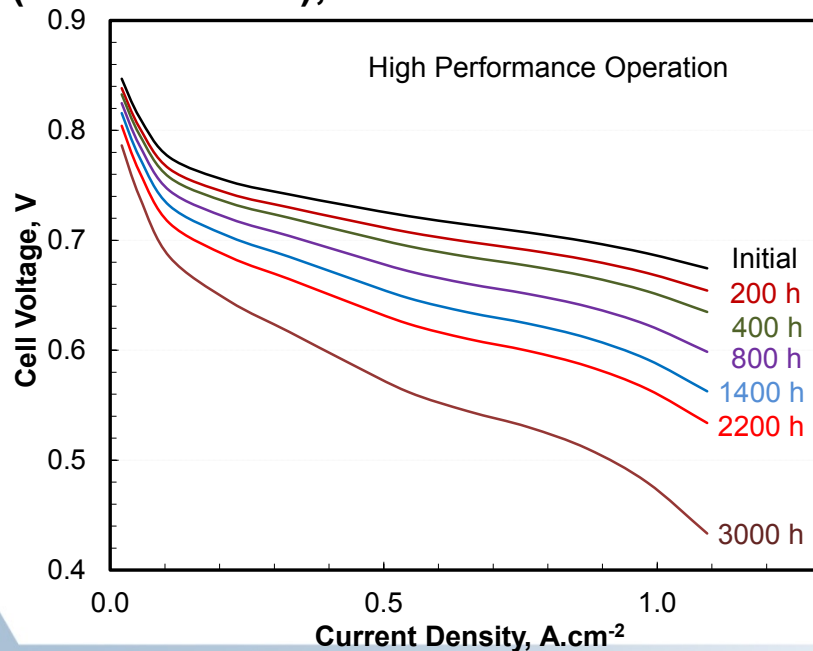
- **CFR has to be restricted to  $<0.5 \mu\text{g}\cdot\text{cm}^{-2}$  to limit increase in  $\eta_m$  at EOL to 35 mV at  $1 \text{ A/cm}^2$  (half of target 10% degradation at EOL)**



# Projected Durability of Stacks with NSTF MEA

Projected durability over lifetime represented as repeated FUDS and FHDS schedules

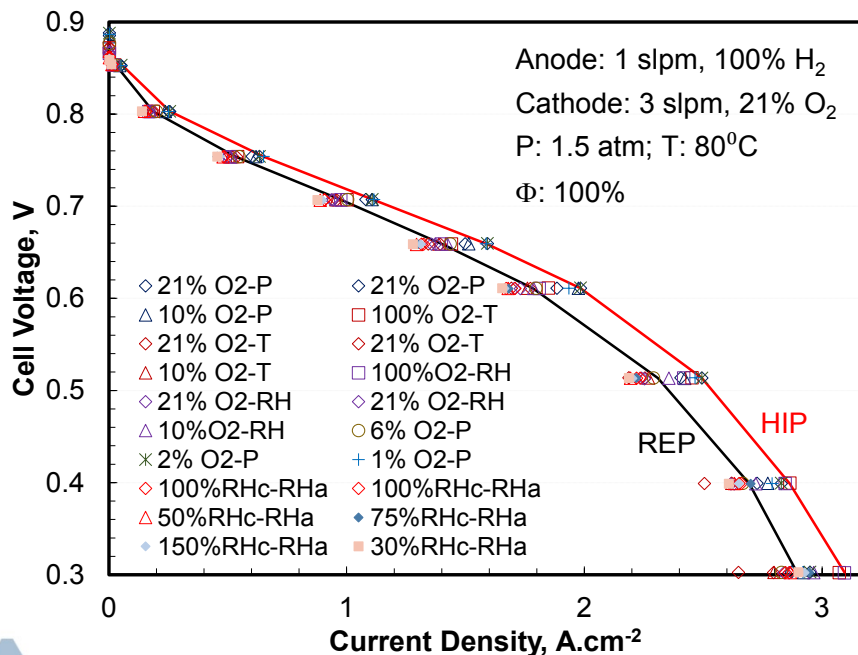
- Stack Design Point: 2.5 atm stack inlet pressure; 95°C coolant exit (stack) T;  $SR_c = 1.5$ ; 40°C ambient T; 1.45 kW/°C  $Q/\Delta T$  constraint
- High Performance: Coolant exit T (88°C at full power) and  $SR_c$  (1.7 at full power) determined for maximum performance; 25°C ambient T
- High Durability: Coolant exit T (80°C at full power) and  $SR_c$  for 1% lower than maximum efficiency; 25°C ambient temperature
- **Increased ORR kinetic losses contribute 30% and mass transfer losses contribute 70% of the projected 10% performance degradation at 800 h**
- **Need to limit CFR to 0.7  $\mu\text{g}\cdot\text{cm}^{-2}$  over 5,000 h**
- **Mitigation strategies: Improve catalyst and support to reduce ECSA loss by 50% (not as critical); More stable membrane to reduce FER by ~80% (critical)**



# Dealloyed Pt<sub>3</sub>Ni<sub>7</sub> /NSTF Catalyst with Cathode Interlayer (CI)

Collaborating with 3M (FC104) in designing tests on 5-cm<sup>2</sup> active-area differential cells and analyzing data to model performance of full-area (>250 cm<sup>2</sup>) cells

- Ternary Anode: Pt<sub>68</sub>(CoMn)<sub>32</sub>, 0.019 mg<sub>Pt</sub>/cm<sup>2</sup>
- Binary Cathode: Pt<sub>3</sub>Ni<sub>7</sub>/NSTF, dealloyed (JHU Chemistry), 0.096 mg<sub>Pt</sub>/cm<sup>2</sup>
- Membrane: 3M-S (supported) 725 EW PFSA with additive, 14 μm
- Anode GDL: 3M “X3” (Experimental backing, 3M hydrophobization, MPL)
- Cathode GDL: 3M 2979
- Cathode Interlayer: 3M Type “B”, 0.016 mg<sub>Pt</sub>/cm<sup>2</sup>



## Test Campaign

- 3 TCs (NFAL+RFAL) before each test series, 1 TC before polarization curves
- ~25% decrease in ECSA over ~735 h actual test time, 22.9 to 17.2 m<sup>2</sup>/g
- Test space: P: 1-3 bar; T: 45-90°C; X(O<sub>2</sub>): 1-21%, 100%; RH(a): 30-100%; RH(c): 30-150%; Q(H<sub>2</sub>): 1 slpm; Q(air): 3 slpm
- Performance metrics: HFR, H<sub>2</sub> x-over, mass activity, ECSA, short resistance

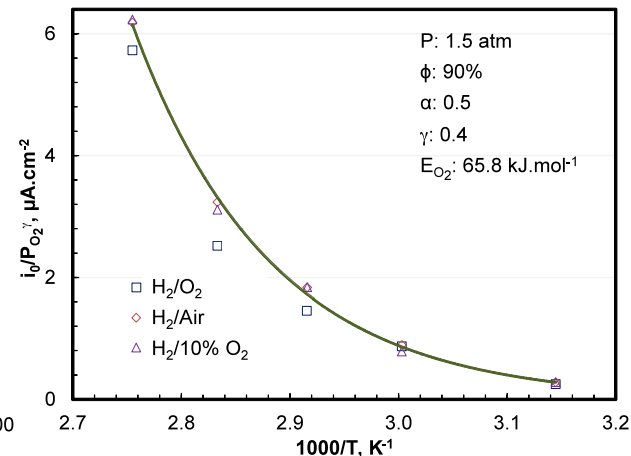
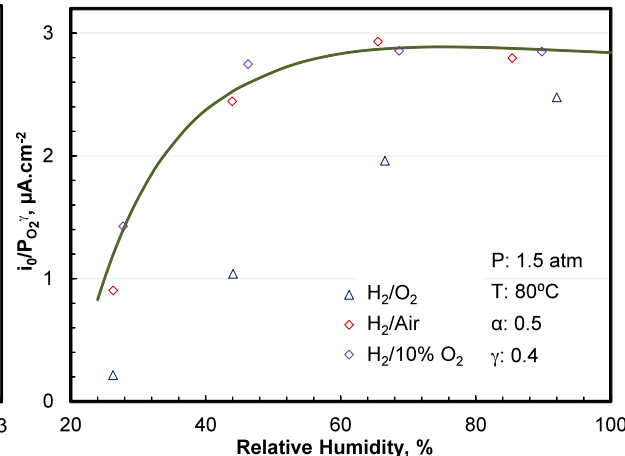
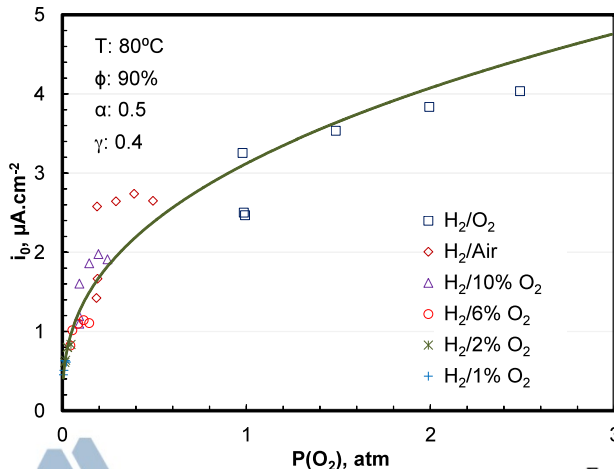
\*Differential cells have identical build as “Best of Class” (BOC) 50-cm<sup>2</sup> active area cells

# ORR Activity of d-Pt<sub>3</sub>Ni<sub>7</sub> /NSTF Catalyst with CI

Determined ORR kinetic parameters from IR and crossover corrected cell voltages at low current densities in H<sub>2</sub>/O<sub>2</sub> and H<sub>2</sub>/air.

- Modeled mass activities of the three catalyst systems are consistent with values measured using the 3M protocol
- Compared to the ternary Pt<sub>68</sub>(CoMn)<sub>32</sub>/NSTF catalyst, the mass activity of binary d-Pt<sub>3</sub>Ni<sub>7</sub>/NSTF catalyst with cathode interlayer is 78-144% higher.

| Cathode / Anode Catalyst                                       | Membrane          | Cathode / Anode Pt Loading            | Cathode ECSA               | Measured Mass Activity   | Modeled Mass Activity | Cell Designation |
|--|-------------------|---------------------------------------|----------------------------|--------------------------|-----------------------|------------------|
| C: Pt <sub>68</sub> (CoMn) <sub>32</sub>                       | 20 μm, 835 EW     | 0.1 mg/cm <sup>2</sup>                | 9.8 m <sup>2</sup> /g      | 180 A/g <sub>Pt</sub>    | 190 A/g <sub>Pt</sub> | 19478            |
| A: Pt <sub>68</sub> (CoMn) <sub>32</sub>                       |                   | 0.05 mg/cm <sup>2</sup>               |                            |                          |                       |                  |
| C: d-Pt <sub>3</sub> Ni <sub>7</sub>                           | 20 μm, 835 EW     | 0.125 mg/cm <sup>2</sup>              | 14.5±0.7 m <sup>2</sup> /g | 330±30 A/g <sub>Pt</sub> | 392 A/g <sub>Pt</sub> | 30086            |
| A: Pt <sub>68</sub> (CoMn) <sub>32</sub>                       |                   | 0.05 mg/cm <sup>2</sup>               |                            |                          |                       |                  |
| C: d-Pt <sub>3</sub> Ni <sub>7</sub> + Cathode Interlayer (CI) | 14 μm (S), 725 EW | 0.096 + 0.016 (CI) mg/cm <sup>2</sup> | 22±3 m <sup>2</sup> /g     | 380±60 A/g <sub>Pt</sub> | 334 A/g <sub>Pt</sub> | 36135            |
| A: Pt <sub>68</sub> (CoMn) <sub>32</sub>                       |                   | 0.019 mg/cm <sup>2</sup>              |                            |                          |                       |                  |

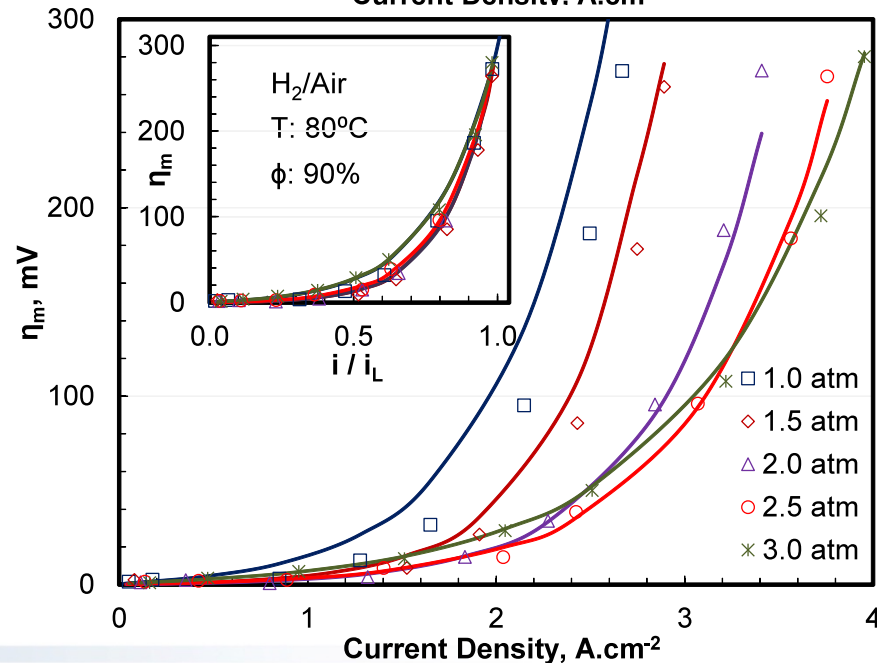
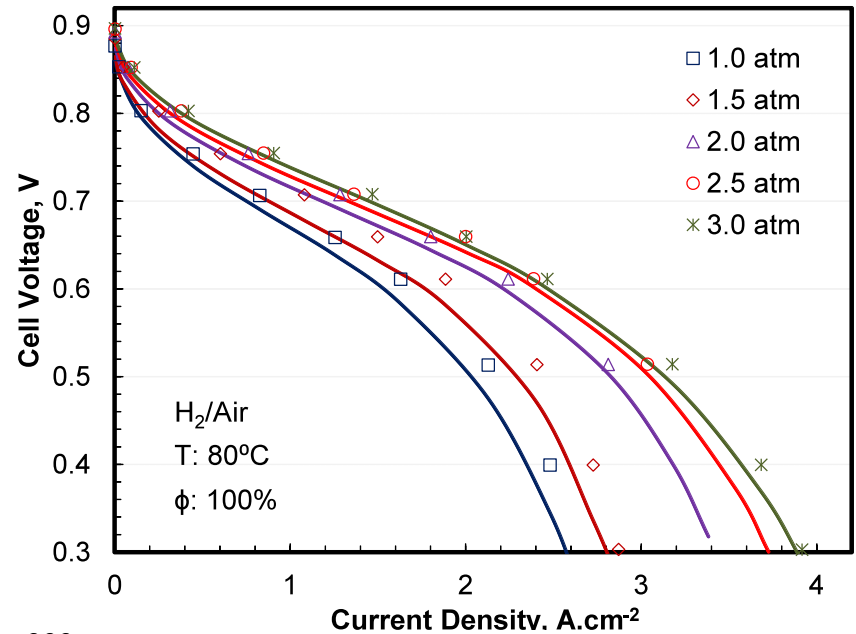
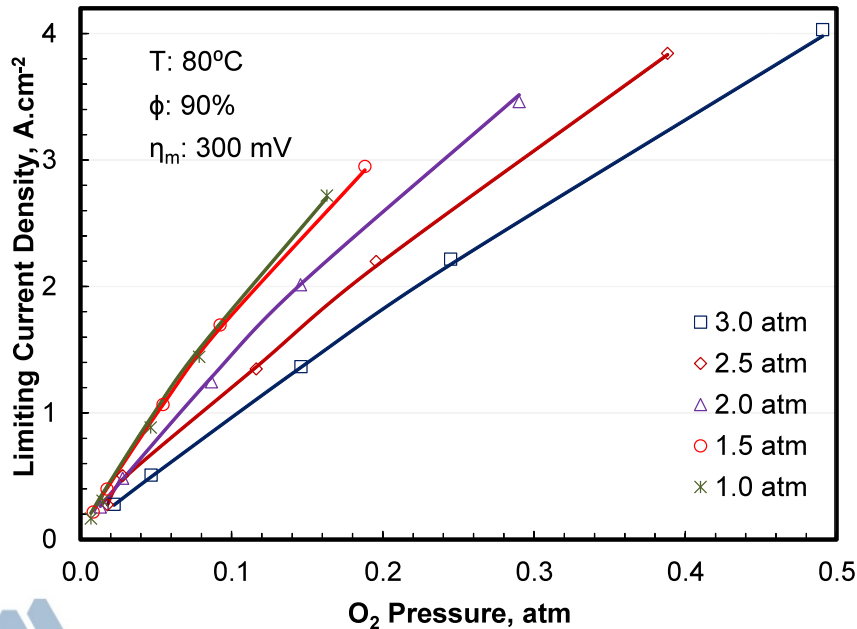


$$i + i_x = i_{0r} P_{O_2}^\gamma \phi^\beta e^{\frac{E_{O_2}}{R} \left( \frac{1}{T} - \frac{1}{T_r} \right)} e^{\frac{\alpha n F}{RT} \eta}$$

# Mass Transfer Overpotentials in d-Pt<sub>3</sub>Ni<sub>7</sub> /NSTF Catalyst with CI

Determined limiting current density ( $i_L$ ) and correlated mass transfer overpotential ( $\eta_m$ ) with reduced current density ( $i/i_L$ )

- $i_L$  defined as current density at which  $\eta_m = 300$  mV
- $\eta_m$  includes IR drop in the electrode
- Determined relationships between  $\eta_m$  (and  $i_L$ ) and all operating variables: P, T, X(O<sub>2</sub>), RH(a), RH(c),  $i/i_L$



# Water Transport across Membrane

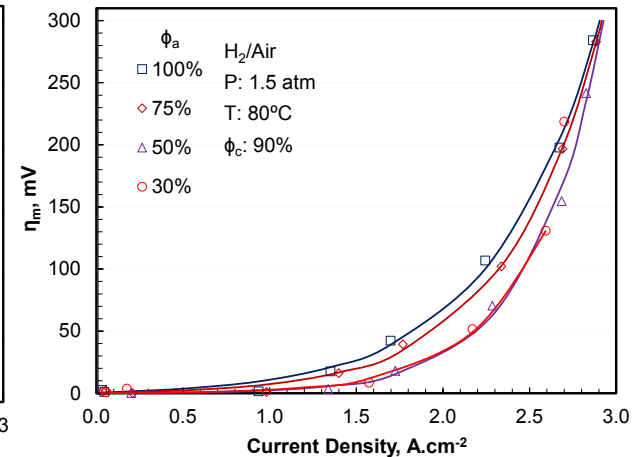
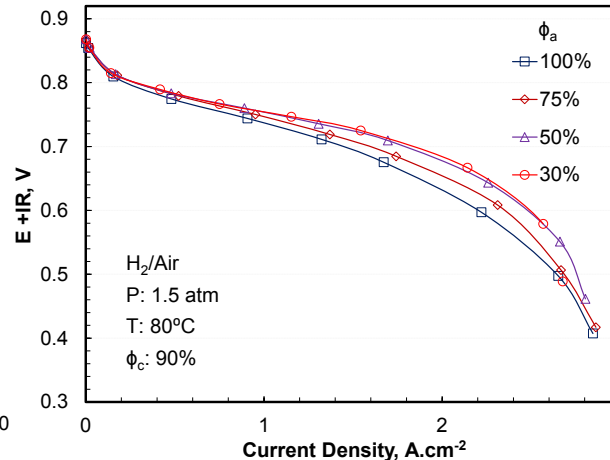
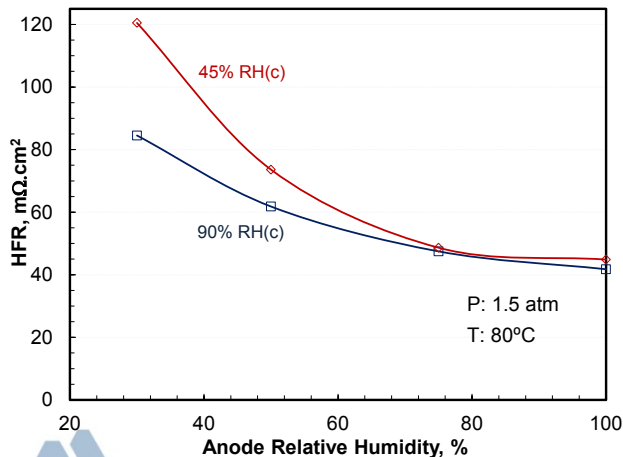
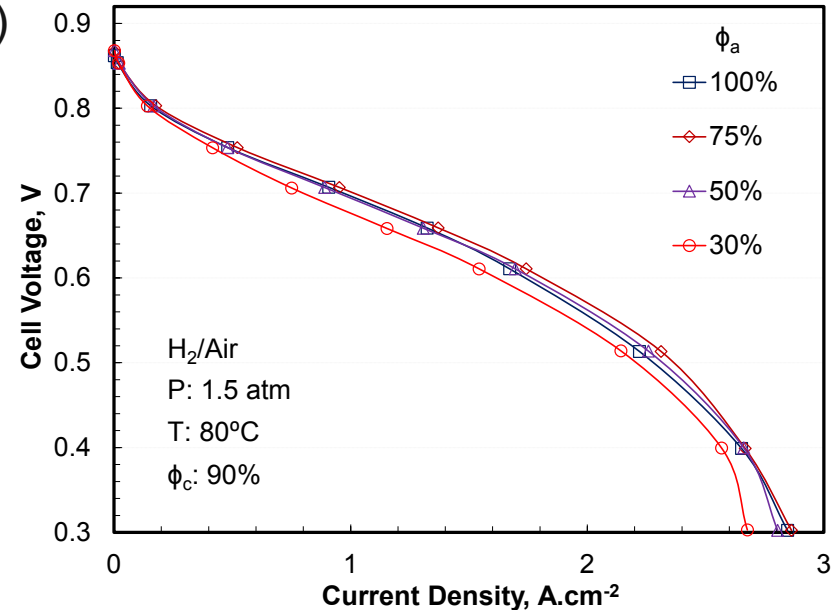
Special test series to investigate the effect of cathode-to-anode and anode-to-cathode water transport on differential cell performance

For given RH(c), there is an optimum RH(a) at which the cell voltage is highest.

- For 100% RH(c), the optimum RH(a) is ~75%.
- The lower the RH(c), the higher the optimum RH(a)

Trade-off between membrane Ohmic resistance and cathode flooding

- HFR (and  $E + IR$ ) always increases as RH(a) is lowered
- $\eta_m$  decreases as RH(a) is lowered





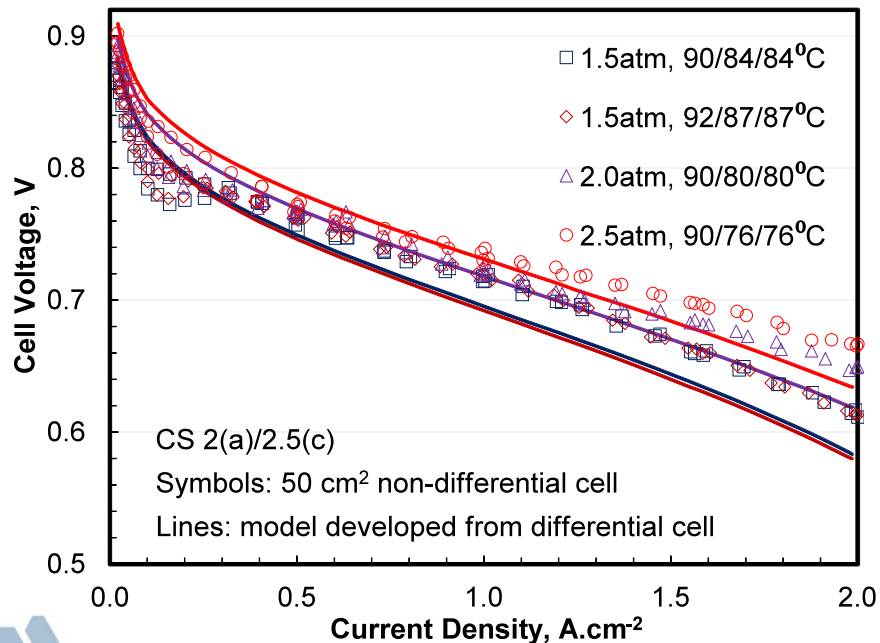
# Model Validation

Work underway to calibrate the performance model developed using differential cell data with 50-cm<sup>2</sup> cell data for finite cathode/anode stoichiometries and operating temperatures needed to satisfy the Q/ $\Delta$ T constraint.

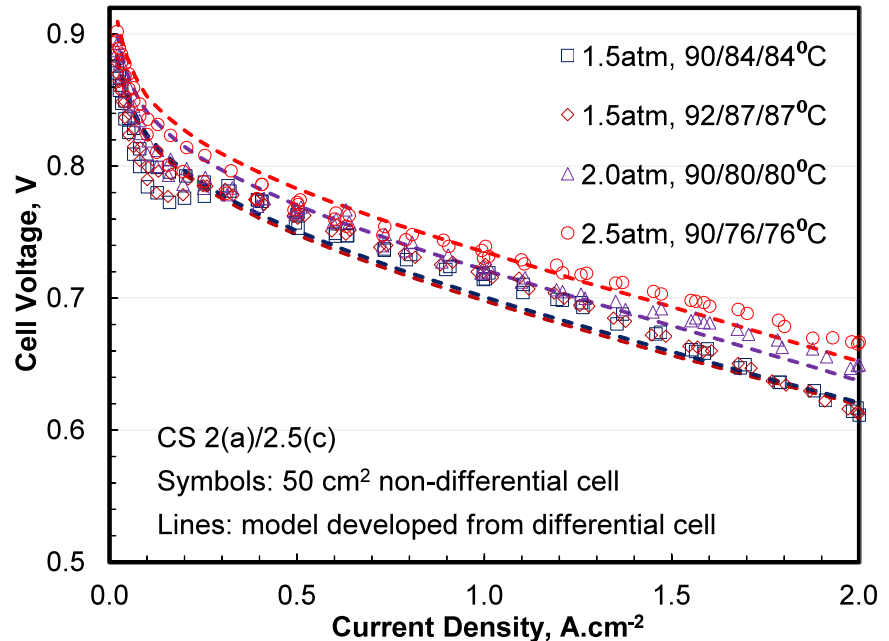
3M's BOC 50-cm<sup>2</sup> cell data are closer to the modeled results without mass transfer overpotentials.

- Parallel effort at GM to replicate 3M's BOC performance with identical cells and conditioning procedures
- Future validation of model with full-area short stack being built at GM

### Model results inclusive of $\eta_m$



### Model results exclusive of $\eta_m$



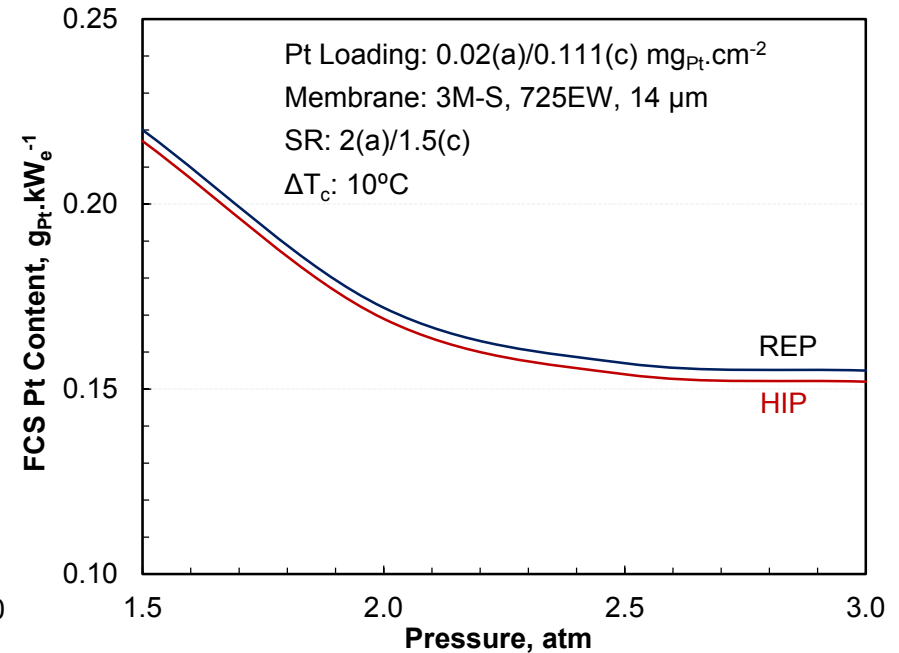
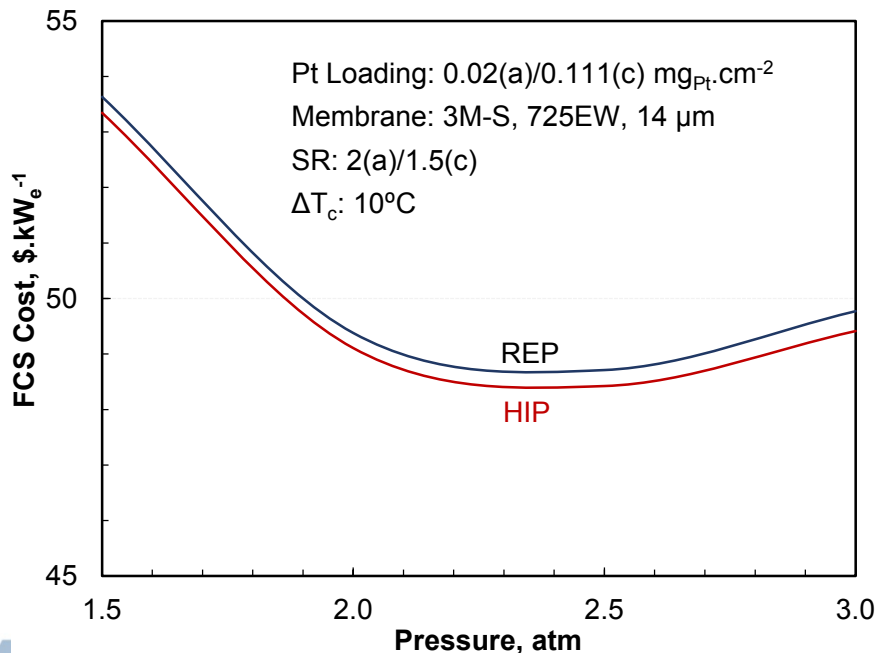


# Performance of Automotive FCS: d-Pt<sub>3</sub>Ni<sub>7</sub>/NSTF Catalyst with CI

Modeled optimal BOL\* performance of FCS with d-Pt<sub>3</sub>Ni<sub>7</sub>/NSTF catalyst and cathode interlayer subject to Q/ΔT constraint: 0.131 mg/cm<sup>2</sup> total Pt loading; 725 EW, 14 μm 3M-S membrane.

- Projected cost\*\* and Pt content: 48.4-48.7 \$/kW<sub>e</sub> at 2.2-2.5 atm, and 0.152-0.155 g<sub>Pt</sub>/kW<sub>e</sub> at 2.5-3.0 atm stack inlet pressure
- Optimal power density determined by HFR and ORR activity rather than mass transfer overpotentials

| P   | T  | Cell Voltage | Power Density      | Stack Pt Content                 | Pt Cost            | Stack Cost         |
|-----|----|--------------|--------------------|----------------------------------|--------------------|--------------------|
| atm | °C | mV           | mW/cm <sup>2</sup> | g <sub>Pt</sub> /kW <sub>e</sub> | \$/kW <sub>e</sub> | \$/kW <sub>e</sub> |
| 3.0 | 95 | 670          | 973                | 0.135                            | 7.3                | 21.1               |
| 2.5 | 95 | 663          | 941                | 0.139                            | 7.4                | 21.4               |
| 2.0 | 95 | 656          | 840                | 0.156                            | 8.2                | 22.9               |
| 1.5 | 95 | 651          | 645                | 0.203                            | 10.5               | 27.8               |



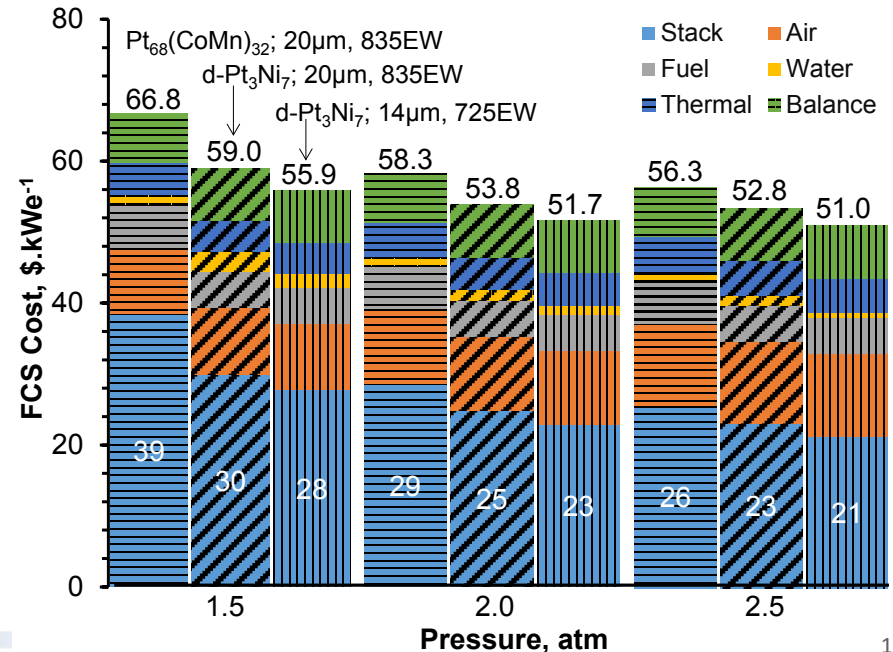
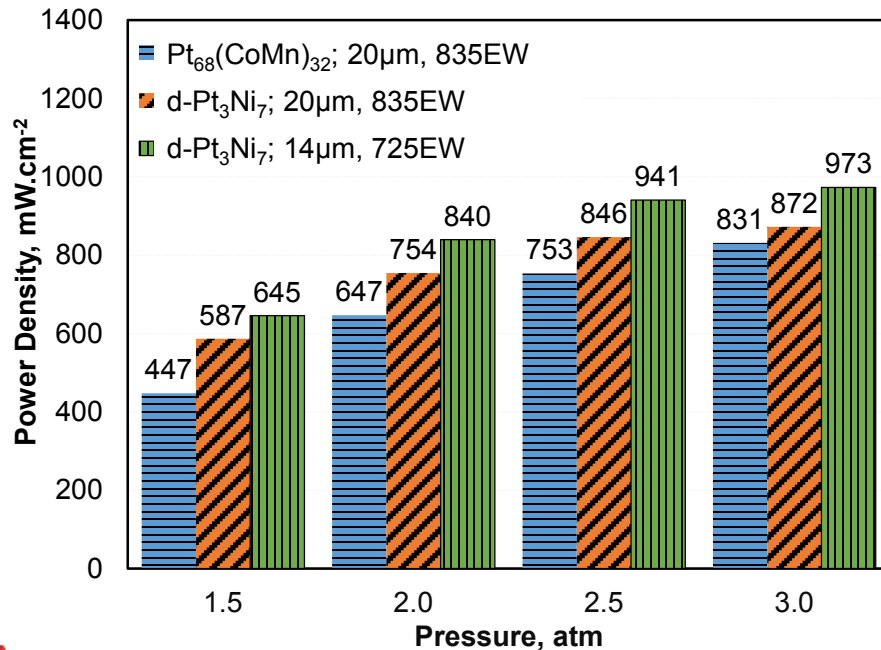
\*BOL: Beginning of life, \*\*Cost correlations from Strategic Analysis Inc. (SA)

# Comparative Cost and Performance of FCS with NSTF Catalysts

Improvement compared to the 2015 FCS with ternary catalyst

- 25% higher stack power density, including 12.3% due to higher ORR activity
- 16.8% lower stack cost, including 10% due to higher ORR activity

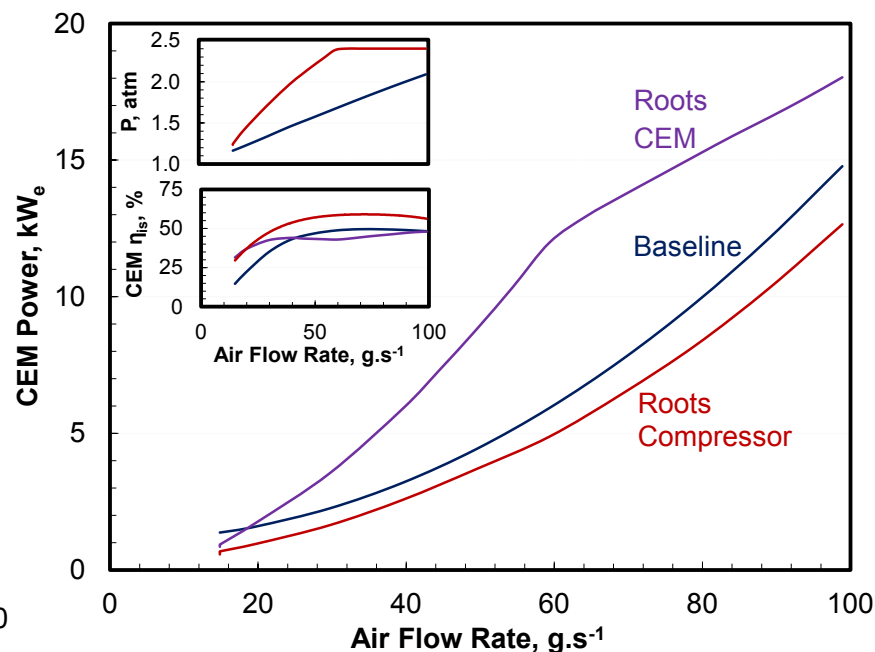
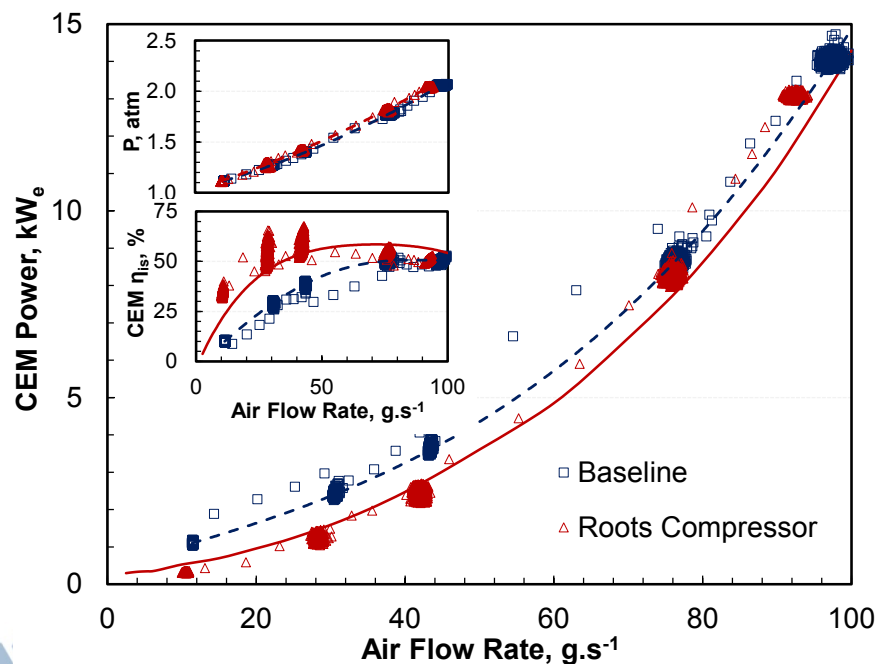
| Cathode / Anode Catalyst                                  | Membrane          | Cathode / Anode Pt Loading            | Power Density (2.5 atm) | Stack Cost (2.5 atm)     |
|---|-------------------|---------------------------------------|-------------------------|--------------------------|
| C: Pt <sub>68</sub> (CoMn) <sub>32</sub>                  | 20 μm, 835 EW     | 0.1 mg/cm <sup>2</sup>                | 753 mW/cm <sup>2</sup>  | 25.69 \$/kW <sub>e</sub> |
| A: Pt <sub>68</sub> (CoMn) <sub>32</sub>                  |                   | 0.05 mg/cm <sup>2</sup>               |                         |                          |
| C: d-Pt <sub>3</sub> Ni <sub>7</sub> + Cathode Interlayer | 20 μm, 835 EW     | 0.095 + 0.016 (Cl) mg/cm <sup>2</sup> | +12.3%                  | -10.0%                   |
| A: Pt <sub>68</sub> (CoMn) <sub>32</sub>                  |                   | 0.02 mg/cm <sup>2</sup>               |                         |                          |
| C: d-Pt <sub>3</sub> Ni <sub>7</sub> + Cathode Interlayer | 14 μm (S), 725 EW | 0.095 + 0.016 (Cl) mg/cm <sup>2</sup> | +25.0%                  | -16.8%                   |
| A: Pt <sub>68</sub> (CoMn) <sub>32</sub>                  |                   | 0.02 mg/cm <sup>2</sup>               |                         |                          |



# Roots Air Management System with Integrated Expander

Argonne is collaborating with Eaton-led team (FC103) to model and analyze Roots air management system and optimize it for use in Ballard fuel cell module

- Developed and validated performance maps for V250 Twin Vortices Series Roots compressor, Gen2 three-lobe V210 Roots expander, and 38-kW (peak power) motor and motor-controller
- Demonstrated that, compared to a baseline unit, the V250 module (without expander) reduces parasitic power by 6.4% at full flow (92 g/s) and by 35% at quarter flow (25 g/s)
- Demonstrated that the CEM efficiency\* decreases by 10 percentage-points at full flow if an expander is included because of higher operating pressures

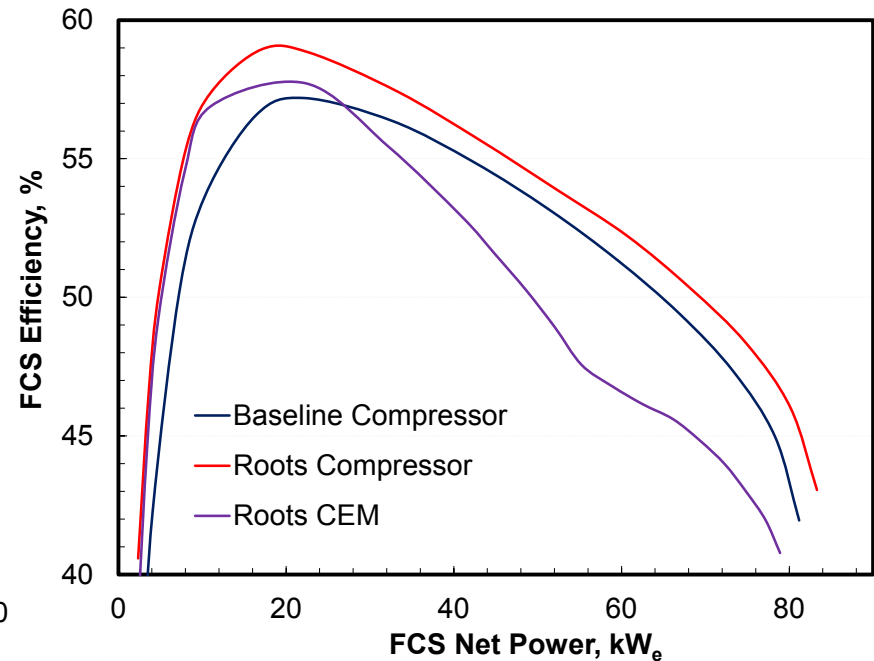
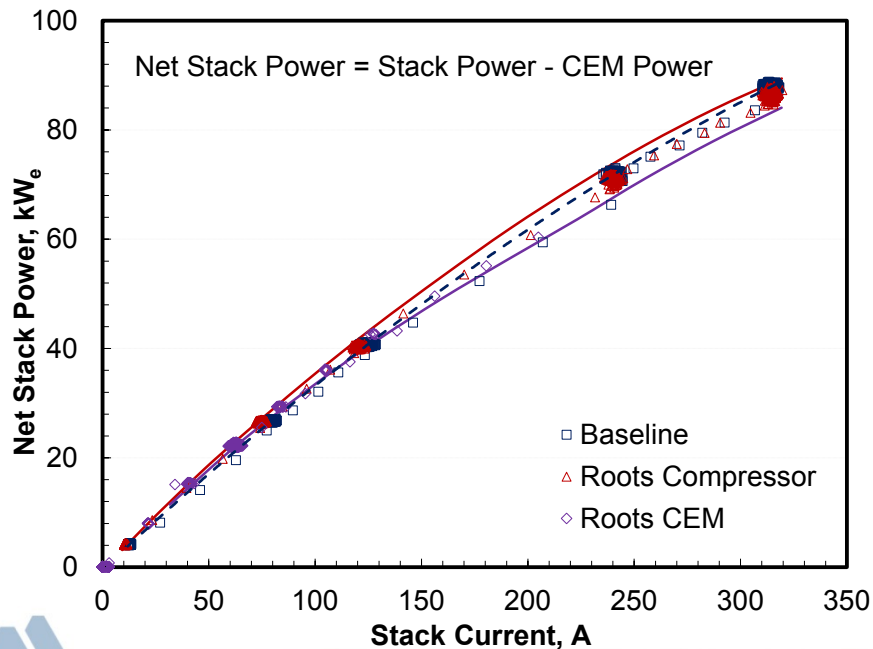


\*CEM efficiency: CEM Isentropic Power/CEM Input Power

# Projected FCS Performance with Roots Air Management System

Collaborated in formulating a test plan for a state-of-the-art, full-area automotive short stack and used the data to develop a stack model. Validated the model against data for a 100-kWe full stack.

- Demonstrated that the Roots compressor module can increase the net stack power (stack power–CEM power) by 1.5-10% at 100-25% power. Stack redesign (higher P and T, lower  $\Delta P$ ) required to fully realize the benefits with the expander.
- Developed FCS model for electric buses and projected 2.7 %-point improvement in system efficiency at rated power with Roots compressor (w/o expander)
- With Aalto University, showed 2-6% increase in bus fuel economy on US drive cycles with Roots compressor. Conducting life cycle analyses with SA and Aalto.



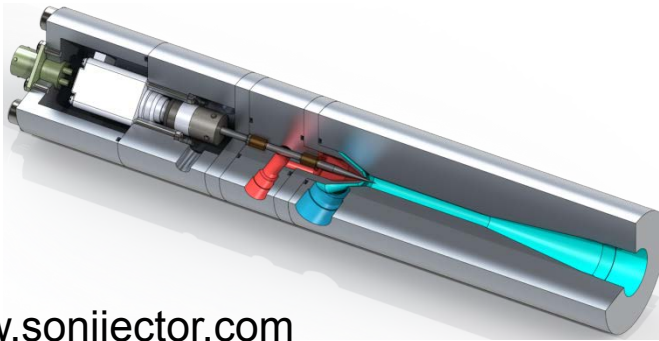
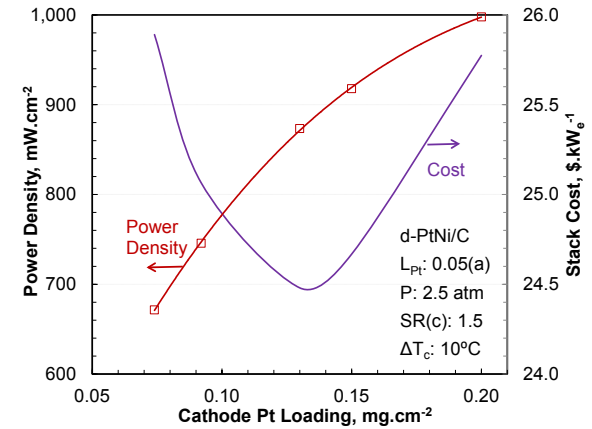
# Summary of Work in Progress

## De-alloyed PtNi/C cathodes (FC106: UTRC, JMFC)

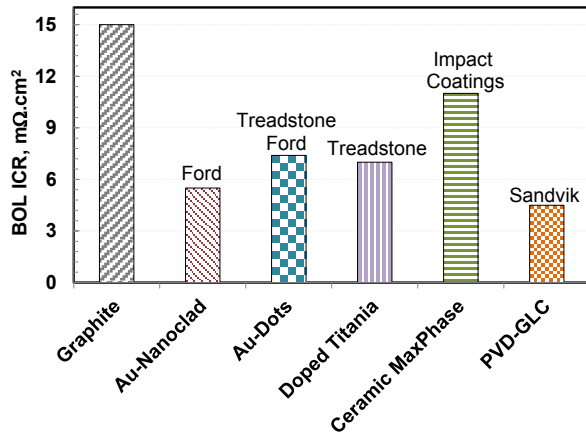
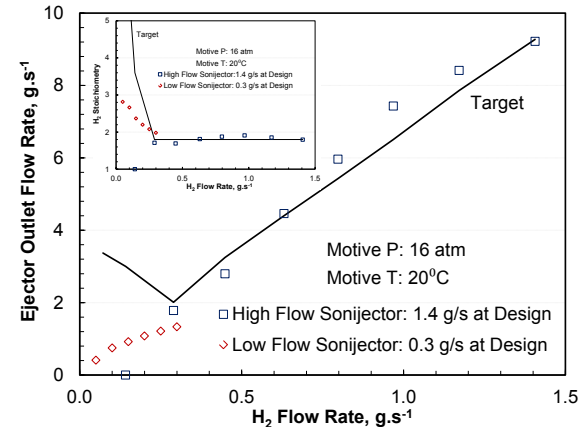
- Finalizing the preferred electrode parameters for cost and performance: ink (aqueous vs. organic), pre-treatment (acid washed vs. non-washed), ionomer EW, anode Pt loading.

## Fuel Management System (UDEL/Sonijector)

- Comparing variable area twin ejectors, hybrid ejector-recirculation pump, and pulse ejectors.

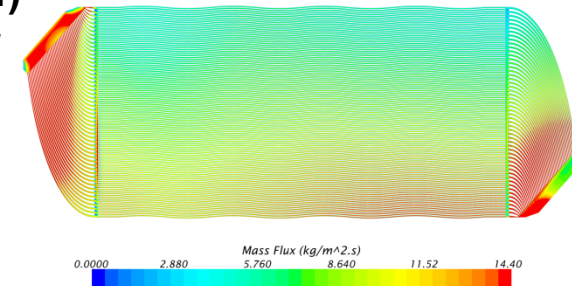


[www.sonijector.com](http://www.sonijector.com)



## Metal Bipolar Plates (IEA Annex 34)

- CFD simulations of two-phase flow in non serpentine flow-fields:  $\Delta P$ , flow uniformity, achievable active areas
- Stability of coatings and contact resistances



## Collaborations

|                           |  |
|---------------------------|--|
| Air Management            | Eaton: Roots Air Management System with Integrated Expander (FC103)  |
| Stack                     | 3M: High Performance, Durable, Low Cost Membrane Electrode Assemblies for Transportation (FC104)                 |
|                           | Ballard/Eaton: Roots Air Management System with Integrated Expander (FC103)                                      |
|                           | JMFC and UTRC: Rationally Designed Catalyst Layers for PEMFC Performance Optimization (FC106)                    |
| Water Management          | Gore, Ford, dPoint: Materials and Modules for Low-Cost, High-Performance Fuel Cell Humidifiers (FC067)           |
| Thermal Management        | 3M, Honeywell Thermal Systems  |
| Fuel Management           | 3M, University of Delaware (Sonijector)  |
| Fuel Economy              | Aalto University (Fuel Cell Buses)   |
| H <sub>2</sub> Impurities | 3M, ISO-TC-192 WG  |
| System Cost               | SA: Manufacturing Cost Analysis of Fuel Cell Systems and Transportation Fuel Cell System Cost Assessment (FC018) |
| Dissemination             | IEA Annex 34, Transport Modeling Working Group, Durability Working Group   |

- Argonne develops the fuel cell system configuration, determines performance, identifies and sizes components, and provides this information to SA for high-volume manufacturing cost estimation
- Conducting joint life-cycle cost studies with SA and Aalto University

## Future Work

1. Support DOE development effort at system, component, and phenomenological levels (ongoing)
2. Support SA in high-volume manufacturing cost projections, collaborate in life-cycle cost studies (ongoing)
  - Optimize system parameters considering costs at low-volume manufacturing
  - Life cycle cost study for fuel cell electric buses (work with Ballard, Eaton, SA)
3. Alternate MEAs with advanced alloy catalysts
  - De-alloyed Pt<sub>3</sub>Ni<sub>7</sub>/NSTF (3M collaboration)
  - De-alloyed PtNi on high surface-area carbon support (ANL catalyst project with JMFC and UTRC as partners), calibrate/validate model on larger area cells
  - State-of-the-art low PGM Pt and Pt alloys (FC-PAD collaboration)
4. System architecture and balance-of-plant components
  - Air management system with Roots compressors and expanders (Eaton collaboration)
  - Fuel and water management systems: anode gas recirculation (ongoing)
  - Bipolar plates and flow fields for low pressure drops and uniform air/fuel distribution, cell to stack performance differentials (ongoing)
5. Incorporate durability considerations in system analysis
  - System optimization for cost, performance, and durability on drive cycles (NSTF and d-PtNi/C catalyst systems)



# Project Summary

|                 |   |
|-----------------|---|
| Relevance:      | Independent analysis to assess design-point, part-load and dynamic performance of automotive and stationary FCS   |
| Approach:       | Develop and validate versatile system design and analysis tools<br>Apply models to issues of current interest<br>Collaborate with other organizations to obtain data and apply models   |
| Progress:       | Quantified the sources of 14-20% decrease in power density and 2.20 \$/kWe increase in cost due to $Q/\Delta T$ constraint.<br>Identified the dominant NSTF catalyst degradation mechanism and determined that the cumulative fluoride release must be limited to 0.7 mg.cm <sup>-2</sup> for 10% performance degradation over 5000 h.<br>Projected 25% increase in power density and 16.8% reduction in FCS cost by reducing anode Pt loading to 0.02 mg/cm <sup>2</sup> and switching to d-Pt <sub>3</sub> Ni <sub>7</sub> /NSTF cathode catalyst with supported 14- $\mu$ m 725 EW membrane.<br>Demonstrated that, compared to a baseline unit, the V250 module (without expander) reduces parasitic power by 6.4% at full flow (92 g/s) and by 35% at quarter flow (25 g/s) |
| Collaborations: | 3M, Aalto University, Eaton, JMFC, SA, UTRC, UDEL/Sonijector  |
| Future Work:    | Fuel cell systems with emerging de-alloyed catalysts<br>Alternate balance-of-plant components<br>System analysis with durability considerations on drive cycles   |



## Reviewers' Comments

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Generally favorable reviews with recommendations to

- More work on NSTF degradation including effect of temperature
- Continue the good progress toward end-of-life (EOL) analysis and system-level tradeoffs
- Maintain high degree of collaboration with material and component developers
- Scale back NSTF and Eaton collaborations until these are closer to maturation
- Incorporate down-the-channel stack model in GCtool
- More work on bipolar plates, flow fields and other BOP components

Work scope consistent with above recommendations

- ✓ Collaborated with 3M to identify the dominant degradation mechanism, and conducting long-duration tests at different temperatures
- ✓ Projected performance degradation on drive cycles and quantified desired reductions in fluoride emission rates
- ✓ Maintained and expanded collaborations with material and component developers and other projects
- ✓ Investigating non-NSTF advanced catalysts, with emphasis on low-PGM alloys
- ✓ All system analysis work is based on 1D+1D or 2D+1D down-the-channel stack model, co- or counter-flowing anode and cathode streams, anode recycle, etc.
- ✓ On-going parallel work on bipolar plates, flow fields, fuel system, alternate system architecture



# Technical Back-Up Slides



# Publications and Presentations

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## Journal Publications

R. K. Ahluwalia, X. Wang, W. B. Johnson, F. Berg, and D. Kadylak, “Performance of a Cross-Flow Humidifier with a High Flux Water Vapor Transport Membrane,” *Journal of Power Sources*, Vol. 291, pp. 225-238, 2015.

R. K. Ahluwalia, X. Wang, and A. J. Steinbach, “Performance of Advanced Automotive Fuel Cell Systems with Heat Rejection Constraint,” *Journal of Power Sources*, Vol. 309, pp. 178-191, 2016.

## Conference Presentations

R. K. Ahluwalia, X. Wang, and J-K Peng “Fuel Cells Systems Analysis,” US DRIVE Fuel Cell Tech Team Meeting, Southfield, MI, July 15, 2015.

R. L. Borup, R. Mukundan, Dusan Spornjak, D. Langlois, R. Ahluwalia, D. D. Papadias, Karren More, and Steve Grot, “Carbon Corrosion in PEM Fuel Cells During Drive Cycle Operation,” 228<sup>th</sup> ECS Meeting, Phoenix, AZ, Oct. 11-15, 2015.

R. K. Ahluwalia, D. D. Papadias, R. L. Borup, R. Mukundan, and D. Sporniak, “Mechanism and Kinetics of Carbon Corrosion in Polymer Electrolyte Fuel Cells during Drive Cycles,” 228<sup>th</sup> ECS Meeting, Phoenix, AZ, Oct. 11-15, 2015.

R. K. Ahluwalia, and N. L. Garland, “Report from the Annexes: Annex 34,” IEA AFC ExCo 51<sup>st</sup> Meeting, Phoenix, AZ, Oct. 15-16, 2015.

Rajesh Ahluwalia and Sunita Satyapal, “ U.S. Department of Energy Hydrogen and Fuel Cells Program,” Eco-Mobility 2025<sup>Plus</sup>, Vienna, Austria, November 9-10, 2015.

R. K. Ahluwalia, D. D. Papadias, J. K. Thompson, H. M. Meyer III, M. P. Brady H. Wang, J. A. Turner, R. Mukundan, and R. Borup, “Performance Requirements of Bipolar Plates for Automotive Fuel Cells,” IEA Annex 34 Meeting, Vienna, Austria, Nov. 11, 2015.

## Meetings Organized

R. K. Ahluwalia, “IEA Advanced Fuel Cells Annex 34: Fuel Cells for Transportation,” Vienna, Austria, Nov. 11, 2015.



# FCS with NSTF Catalysts: Critical Assumptions and Issues

## PEFC Stack

- Membrane: 14- $\mu\text{m}$ , 725 EW, PFSA (supported). Or 20- $\mu\text{m}$ , 835 EW, PFSA (unsupported). Both with chemical additive.
- Cathode Catalyst: Binary d-Pt<sub>3</sub>Ni<sub>7</sub>/NSTF (0.096 mg<sub>Pt</sub>/cm<sup>2</sup>) with Pt/C cathode interlayer (0.016 mg<sub>Pt</sub>/cm<sup>2</sup>). Or ternary Pt<sub>68</sub>(CoMn)<sub>32</sub>/NSTF (0.1 mg<sub>Pt</sub>/cm<sup>2</sup>).
- Anode Catalyst: Ternary Pt<sub>68</sub>(CoMn)<sub>32</sub>/NSTF (0.05 or 0.019 mg<sub>Pt</sub>/cm<sup>2</sup>)
- Cathode GDL: 3M 2979
- Anode GDL: 3M "X3" (Experimental backing, 3M hydrophobization, MPL)
- Seals/Frames: PET subgasket (3M patent)
- Bipolar Plates: 3-mil (0.075 mm) 316 SS substrate with Treadstone coating, 0.5 mm land, 0.7 mm channel, 0.4 mm depth. 62.5% active area, 15 m $\Omega$ .cm<sup>2</sup> 2X ICR\*.

## Fuel Management System

- Hybrid ejector-recirculation pump
- 35% pump efficiency, 1% H<sub>2</sub> purge
- 3 psi pressure drop at rated power

## Air Management System

- Integrated centrifugal compressor-expander-motor module (Honeywell), air foil bearings (AFB)
- Mixed axial flow compressor
- Inflow radial expander, variable area nozzle
- 3-phase brushless DC motor, liquid and air cooled; liquid-cooled motor controller
- Efficiencies at rated power: 71% compressor, 73% expander, 89.5% motor, 89.5% controller
- Turn-down: 20
- 5 psi  $\Delta\text{P}$  between compressor discharge and expander inlet at rated power

## Heat Rejection System

- Two circuits: 75-95°C HT, 10°C  $\Delta\text{T}$  65°C LT coolant, 5°C  $\Delta\text{T}$
- 55% pump + 92% motor efficiency
- 45% blower + 92% motor efficiency
- 10 psi  $\Delta\text{P}$  in stack and 5 psi in radiator

## Water Management System

- Planar cross-flow humidifier with Gore's M311.05 membrane

\*2X ICR: two-sided interfacial contact resistance

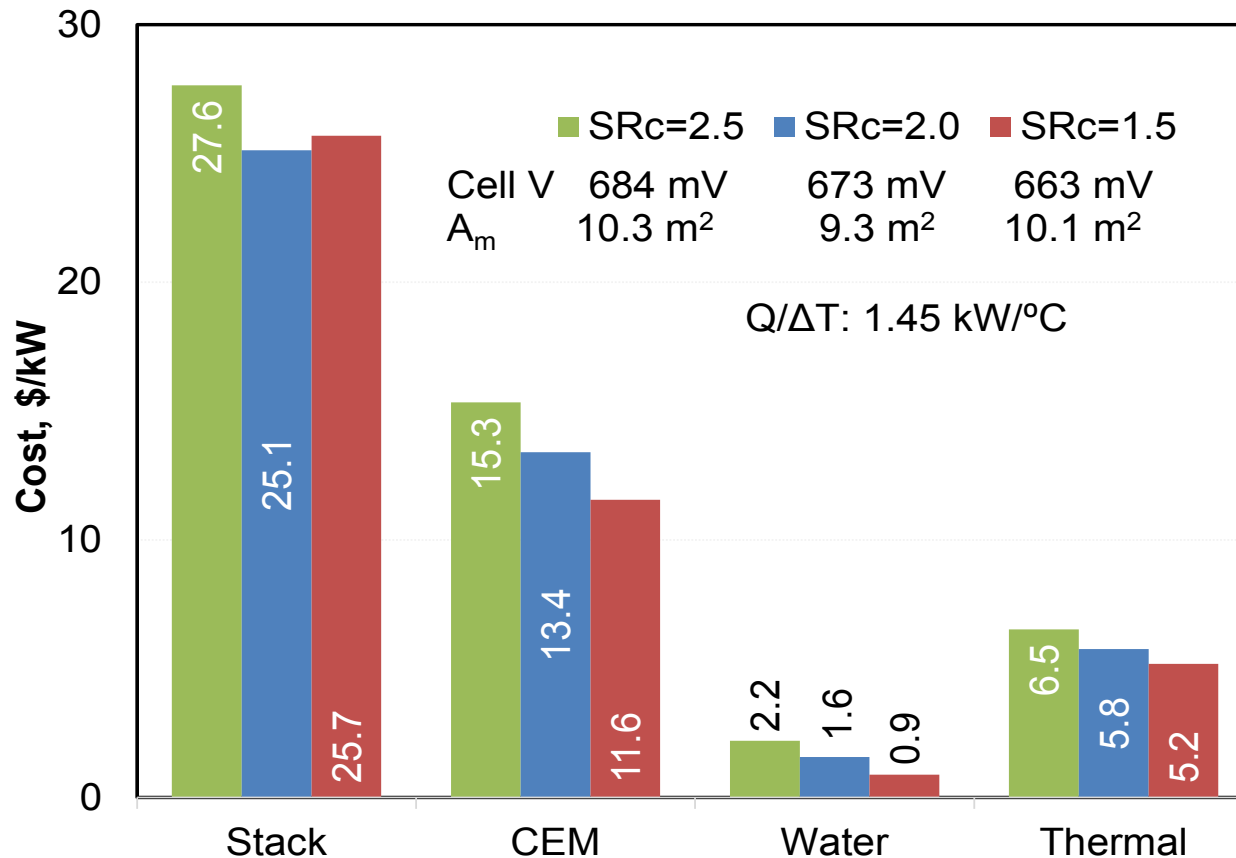
# Rated Power Performance of FCS with NSTF catalysts

| Stack Parameters                         | 2015 FCS with Ternary NSTF Catalyst  | 2016 FCS with Binary NSTF Catalyst   |
|--|--|--|
| Membrane                                 | Ionomer: 3M 835 EW PFSA with chemical additive<br>Substrate: None<br>Thickness: 20 $\mu\text{m}$                           | Ionomer: 3M 725 EW PFSA with chemical additive<br>Substrate: 3M support<br>Thickness: 14 $\mu\text{m}$   |
| Cathode Catalyst                         | $\text{Pt}_{68}(\text{CoMn})_{32}/\text{NSTF}$ (0.1 $\text{mg}_{\text{Pt}}/\text{cm}^2$ )                                  | d- $\text{Pt}_3\text{Ni}_7$ (0.095 $\text{mg}_{\text{Pt}}/\text{cm}^2$ ) with Pt/C cathode interlayer (0.016 $\text{mg}_{\text{Pt}}/\text{cm}^2$ ) |
| Anode Catalyst                           | $\text{Pt}_{68}(\text{CoMn})_{32}/\text{NSTF}$ (0.05 $\text{mg}_{\text{Pt}}/\text{cm}^2$ )                                 | $\text{Pt}_{68}(\text{CoMn})_{32}/\text{NSTF}$ (0.019 $\text{mg}_{\text{Pt}}/\text{cm}^2$ )  |
| Stack Gross Power                        | 88.2 kW  | 88.2 kW  |
| Stack Voltage (Rated)                    | 300 V  | 300 V  |
| Number of Active Cells                   | 453 cells (also 452 cooling cells)   | 453 cells (also 452 cooling cells)   |
| Stack Gross Power Density                | 2.7 kW/L (without insulation but with end plates)  | TBD  |
| Stack Gross Specific Power               | 2.67 kW/kg (without insulation but with end plates)  | TBD  |
| Stack Inlet Pressure                     | 2.5 bar  | 2.5 bar  |
| Stack Coolant Temperature                | 84.1°C (inlet), 94.1°C (outlet)  | 83.9°C (inlet), 93.9°C (outlet)  |
| Stack Air Inlet/Outlet RH                | Inlet: 56% RH at 85°C; Outlet: 91% RH at 95°C  | Inlet: 50% RH at 85°C; Outlet: 88% RH at 95°C  |
| Stack Fuel Inlet/Outlet RH               | Inlet: 43% RH at 95°C; Outlet: 102% RH at 85°C   | Inlet: 43% RH at 95°C; Outlet: 105.7% RH at 85°C   |
| Cathode/Anode Stoichiometry              | 1.5 (cathode) / 2.0 (anode)  | 1.5 (cathode) / 2.0 (anode)  |
| Cell Area                                | 259 $\text{cm}^2$ (active), 414 $\text{cm}^2$ (total)  | 208 $\text{cm}^2$ (active), 333 $\text{cm}^2$ (total)  |
| Cell Voltage                             | 662 mV   | 663 mV   |
| Current Density                          | 1.138 $\text{A}/\text{cm}^2$   | 1.418 $\text{A}/\text{cm}^2$   |
| Crossover Current Density                | 3.4 $\text{mA}/\text{cm}^2$  | 5.0 $\text{mA}/\text{cm}^2$  |
| Power Density                            | 754 $\text{mW}/\text{cm}^2$  | 941 $\text{mW}/\text{cm}^2$  |
| <b>Balance of Plant</b>                  |  |  |
| Humidifier Membrane Area                 | 0.479 $\text{m}^2$   | 0.53 $\text{m}^2$  |
| Air Pre-cooler Heat Duty                 | 6.7 kW   | 5.7 kW   |
| CEM Motor and Motor Controller Heat Duty | 3.0 kW   | 3.0 kW   |
| Main Radiator Heat Duty                  | 79.5 kW  | 79.8 kW  |
| CEM Power                                | Compressor shaft power: 10.4 kW<br>Expander shaft power out: 4.7 kW<br>Net motor and motor controller: 7.1 $\text{kW}_e$   | Compressor shaft power: 10.4 kW<br>Expander shaft power out: 4.7 kW<br>Net motor and motor controller: 7.1 $\text{kW}_e$                           |
| Fan and Pump Parasitic Power             | 0.5 $\text{kW}_e$ (coolant pump), 0.3 $\text{kW}_e$ ( $\text{H}_2$ recirculation pump), 0.345 $\text{kW}_e$ (radiator fan) | 0.5 $\text{kW}_e$ (coolant pump), 0.3 $\text{kW}_e$ ( $\text{H}_2$ recirculation pump), 0.345 $\text{kW}_e$ (radiator fan)                         |

## Breakdown of System Cost

All three systems satisfy  $Q/\Delta T$  target at 2.5 atm stack inlet pressure and 95°C coolant exit temperature

- Stack power density is highest and the stack cost is lowest at  $SRc = 2.0$  but the overall system cost is lowest at  $SRc = 1.5$
- CEM is the second largest contributor to the overall system cost
- >1 \$/kW<sub>e</sub> variation in costs of water and thermal systems over  $SRc = 1.5 - 2.5$



# Performance Degradation during Differential Cell Tests

Polarization data for FC104 (d- Pt<sub>3</sub>Ni<sub>7</sub>/NSTF with Pt/C cathode Interlayer) at start and end of tests, ~735 h of actual test time

- Open Symbols: Pressure series data at beginning of tests (BOT)
- Solid Symbols: Repeat pressure series data at end of tests (EOT)
- Solid Lines: Model results

