Fuel Cell System Modeling and Analysis


DOE Hydrogen and Fuel Cells Program 2017 Annual Merit Review and Evaluation Meeting

Washington, D.C.

June 5-9, 2017

Project ID: FC017

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

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

**Budget**
- FY16 DOE Funding: $550 K
- Planned DOE FY17 Funding: $500 K
- Total DOE Project Value: $500 K

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

**Partners/Interactions**
- Eaton, Ford, UDEL/Sonijector
- SA, Aalto University (Finland)
- 3M, Ballard, Johnson-Matthey Fuel Cells (JMFC), UTRC, FC-PAD, GM
- IEA Annex 34
- Transport Modeling Working Group
- Durability Working Group
- U.S. DRIVE 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 and Relevance

Develop a validated system model and use it to assess design-point, part-load and dynamic performance of automotive (primary objective) and stationary (secondary objective) fuel cell systems (FCS)

- 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 FY2017 work

- Projected 44.9 $/kWₑ FCS cost at high volume manufacturing and 0.126 g/kWₑ Pt content with high performance (HP) d-PtNi/C cathode catalyst, reinforced 14-µm 850 EW membrane, and Q/ΔT = 1.45 kW/°C constraint
- Estimated 10% degradation in net FCS power with 40% decrease in d-PtNi/C cathode catalyst ECSA (0.05-0.15 mg/cm² Pt loading) due to cyclic potentials
- Showed the possibility of removing cathode humidifier if MEA membrane thickness is <14-µm thin, and stack inlet pressure is 2.5 atm or higher
- Demonstrated through a CFD model that H₂ recirculation blower can be eliminated by using a pulse ejector and maintaining <20% N₂ mole fraction to avoid fuel starvation
- Evaluated extreme conditions (cell voltage, manufacturing volume, Q/ΔT constraint) where high stack inlet pressures (4 atm) may offer advantages

Q: Stack heat load; ΔT: Stack coolant exit T – Ambient T
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

<table>
<thead>
<tr>
<th></th>
<th>Description</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Evaluate the performance of MEAs with de-alloyed PtNi/C cathode catalyst relative to the targets of 0.44 A/mg-PGM mass activity at 900 mV_{ir-free}, 1000 mW/cm² at rated power, and 300 mA/cm² at 800 mV.</td>
<td>12/16</td>
</tr>
<tr>
<td>2</td>
<td>Determine the comparative performance of four state-of-the-art MEAs with Pt, Pt-alloy and dealloyed Pt-alloy catalysts and electrode structures.</td>
<td>03/17</td>
</tr>
<tr>
<td>3</td>
<td>Model, update and project the durability of SOA catalysts and MEAs relative to the 2020 operating life target of 5000 h.</td>
<td>06/17</td>
</tr>
<tr>
<td>4</td>
<td>Update the performance and cost of an automotive fuel cell system with an advanced low-PGM catalyst relative to 2020 targets of 65% peak efficiency, Q/ΔT of 1.45 kW/K, and $40/kW cost.</td>
<td>09/17</td>
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</table>
Technical Accomplishments: Summary

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

- Dispersed Pt/C and de-alloyed PtNi/C catalyst systems
- De-alloyed PtNi/C catalyst system: durability on drive cycles
- De-alloyed Pt$_3$Ni$_7$/NSTF catalyst system
- Dispersed PtCo/C alloy catalyst systems

Air Management: Investigating integrated air management system with two-stage, high speed centrifugal compressor and air-foil bearings (Honeywell patent)

Water Management: Optimized cost of integrated PEFC stack and cross-flow humidifier

- Investigated FCS performance without cathode humidifier (3M collaboration)

Fuel Management: Evaluating the performance of anode system with a pulse injector in lieu of H$_2$ recirculation blower (collaboration with Ford & UDEL)

Thermal Management: Optimizing system performance and cost subject to Q/ΔT constraint

ΔT: Stack coolant exit T – Ambient T
1.1 Differential Cell Data

Variables: P, T, RH, X_{O2}, i

2. Overpotential Breakdown

\eta_s^c, \eta_s^a, iR_m^m, iR_\Omega^c, \eta_m

3. \eta_m Correlation

i_L(P, T, RH, X_{O2}), \eta_m(P, T, RH, X_{O2}, i/i_L)

4. Expanded Polarization Data

5. Mass Transfer Resistance

R_m(P, T, RH, X_{O2}, E, i)

6. Resistance Breakdown

R_d: Pressure Dependent
R_{cf}: Pressure Independent

7. Integral Cell Model

1+1D or 2+1D

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Variables: P, T, RH, X_{O2}, i

CCL Conductivity

\sigma_c(T, RH)

PtO_x Formation

\Theta(E)

Gas Resistance

R_g(P, T, RH, X_{O2})

GDL Resistance

\epsilon_T^d, \epsilon_T^w(E, i), \delta/\delta_d

Operating Conditions

Cell Design

FC-PAD

CCL Resistance

R_{cf}(T, RH, E, i)
Differential Cell Data

UTRC 12.25-cm² active area cell, triple serpentine flow channels, fixed flow rate 1(a) / 3(c) slpm, 5 minutes hold per point

- JMFC Catalyst: d-PtNi/C, 0.1 mg/cm² Pt loading, 60 m²/gPt ECSA (A_{Pt})
- BOL diagnostics: H₂-pump, H₂-xover, CV, EIS

<table>
<thead>
<tr>
<th>Test Series</th>
<th>Tests</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>X₀₂, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Effect of P</td>
<td>P, atm</td>
<td>1</td>
<td>1.5</td>
<td>2.5</td>
<td></td>
<td></td>
<td>100, 21, 10, 6, 2, 1</td>
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<tr>
<td>2. Effect of T</td>
<td>T, °C</td>
<td>90</td>
<td>80</td>
<td>70</td>
<td>60</td>
<td>45</td>
<td>100, 21</td>
</tr>
<tr>
<td>3. Effect of RH</td>
<td>Φ, %</td>
<td>100</td>
<td>85</td>
<td>70</td>
<td>55</td>
<td>30</td>
<td>100, 21, 10</td>
</tr>
</tbody>
</table>

Electrode conductivity (σₖ) from Galvanostatic impedance data for H₂/N₂ at 0.4 to 0.925 V with 5 mV perturbation

- σₖ has similar temperature and RH dependence as σₘ: σₖ = σₘf(εᵢ, τ)

σₘ: Membrane conductivity; εᵢ: Ionomer volume fraction; τ: Tortuosity for ion conduction
d-PtNi/C has 2X modeled mass activity of a-Pt/C that has nearly the same particle size

- d-PtNi/C and PtCo/C alloy have comparable mass activities
- Both d-PtNi/C and PtCo/C alloy systems meet the mass activity targets of 440 A/gPt
Mass Transfer Overpotentials

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

- Mass transfer overpotentials derived from pol curves do not correlate with mass activity
  \[
  \eta_m = E_N - E - i R^m_\Omega - \eta_c - \eta_a
  \]
- \( i_L \) defined as current density at which \( \eta_m = 450 \text{ mV} \)
- Limiting current densities are higher and mass transfer overpotentials are lower in NSTF MEAs than in dispersed catalyst MEAs with nearly same Pt loading
Model Calibration: Stack with d-PtNi/C Cathode Catalyst

High performance (HP) stack with d-PtNi/C cathode catalyst, 10°C rise in coolant T ($\Delta T_c$)
- 0.025(a)/0.1(c) mg/cm² Pt loading
- 850 EW, 14-µm (dry) chemically-stabilized, reinforced membrane, ~42 mΩ.cm² HFR(1)
- 20% higher $i_L$ reflecting better high surface-area carbon support (FC144)
- 47 mΩ.cm² electrode sheet resistance ($\delta_c/\sigma_c$) at 100% RH

Sources of Cell-to-Stack Derating in Power Density at Q/$\Delta T$ Relevant Conditions

2.5-atm Stack Inlet P, 95°C Stack T(2)
- Operating pressure, 2.5 atm inlet (i) vs. 2.5 atm outlet (o): 4.4%
- Air stoichiometry (SR(c)), 1.5 vs. 2.0: 7.3%
- Total derating: 11.3%

1.5 Stack Inlet P, 95°C Stack T(2)
- Operating pressure, 1.5 atm inlet vs. 1.5 atm outlet: 8.7%
- Air stoichiometry, 2.5 vs. 1.5: 6.9%
- RH$_{in}$, 51% vs. 70%: 2.3%

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(1) High-frequency resistance for 2.5-atm conditions; (2) Bipolar plate temperature at coolant exit
Projected Performance of Automotive FCS: HP d-PtNi/C Cathode Catalyst

Modeled optimal beginning of life (BOL) performance of automotive FCS subject to $Q/\Delta T=1.45$ kW/°C constraint: 0.125 mg/cm² total Pt loading; 850 EW, 14-μm chemically-stabilized, reinforced membrane

- Projected FCS cost and Pt content: 44.9 $/kW_e at 2.5 atm, and 0.126 g_{Pt}/kW_e at 2.5-atm stack inlet pressure, 95°C stack temperature
- Determined Optimum exit RH: ~100% at 2.5 atm and <60% at 1.5 atm

<table>
<thead>
<tr>
<th>P</th>
<th>CEM Power</th>
<th>Current Density</th>
<th>Cell Voltage</th>
<th>Power Density</th>
<th>Stack Pt Content</th>
<th>Pt Cost</th>
<th>Stack Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>atm</td>
<td>kW_e</td>
<td>A/cm²</td>
<td>mV</td>
<td>mW/cm²</td>
<td>g_{Pt}/kW_e</td>
<td>$/kW_e</td>
<td>$/kW_e</td>
</tr>
<tr>
<td>3.0</td>
<td>8.8</td>
<td>1.735</td>
<td>670</td>
<td>1162</td>
<td>0.108</td>
<td>5.8</td>
<td>18.6</td>
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<tr>
<td>2.5</td>
<td>7.0</td>
<td>1.651</td>
<td>663</td>
<td>1095</td>
<td>0.114</td>
<td>6.1</td>
<td>19.2</td>
</tr>
<tr>
<td>2.0</td>
<td>5.5</td>
<td>1.457</td>
<td>657</td>
<td>956</td>
<td>0.131</td>
<td>6.8</td>
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<tr>
<td>1.5</td>
<td>4.1</td>
<td>1.231</td>
<td>651</td>
<td>801</td>
<td>0.156</td>
<td>8.0</td>
<td>24.2</td>
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</table>

Cost correlations from Strategic Analysis (SA), 500,000 units/year, no H₂ blower
Optimum Pt Loading in HP d-PtNi/C Cathode Electrode*

Similar total overpotentials but current density is lower at lower Pt loadings in cathode ($L_{Pt(c)}$), 663-mV cell voltage

~33% lower power density at 0.05 mg/cm$^2$ Pt loading in cathode

Similar total overpotentials at 1.5 atm as at 2.5 atm but at much lower current densities, 651-mV cell voltage

Small differences in FCS cost may favor >0.10 mg/cm$^2$ Pt loading in cathode

*Conditions as in slide 10, $Q/\Delta T=1.45$ kW/°C, 95°C stack $T$, $\Delta T_c = 10$°C
Stability of d-PtNi/C Electrode under Cyclic Potentials

Collaboration with FC-106: Catalyst AST, 30,000 cycles

- Measured ECSA loss higher on trapezoid cycles (0.6-0.95 V, 700 mV/s) than on triangle cycles (0.6-925 V, 50 mV/s)
- Faster ECSA loss with extensive intra-cycle diagnostics
- WAXS indicates extensive leaching of Ni that depends on duty cycle

<10% decrease in specific activity even with >90% Ni loss from alloy catalyst

Linear correlation between mass activity and ECSA

Correlation between limiting current density and Pt surface roughness ($S_{Pt}$)

1) WAXS data from N. Kariuki and D. Myers (ANL)
To meet the target of 10% derating in net FCS power over lifetime, the acceptable ECSA loss ($\Delta A_{Pt}$) is limited to <40% for $L_{Pt(c)}=0.1$ mg/cm$^2$

- Small dependence of acceptable ECSA loss on Pt loading ($L_{Pt}$) although Pt loading may affect ECSA loss over cyclic potentials and startup/shutdown

- Regardless of Pt loading, increase in kinetic and mass transfer overpotentials contribute equally to voltage loss

- Additional degradation mechanisms involving other components (membrane, catalyst support) and fuel/air impurities to be included in future work

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### Data Table

<table>
<thead>
<tr>
<th>$\Delta A_{Pt}$, %</th>
<th>$L_{Pt(c)}$, mg/cm$^2$</th>
<th>FCS Net Power, kW$_e$</th>
<th>$\eta_{f}$, mV</th>
<th>$\eta_{c}$, mV</th>
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<tbody>
<tr>
<td>0</td>
<td>0.15</td>
<td>80.0</td>
<td>40.9</td>
<td>384</td>
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<td>25</td>
<td>0.10</td>
<td>75.7</td>
<td>67.4</td>
<td>400</td>
</tr>
<tr>
<td>50</td>
<td>0.10</td>
<td>71.5</td>
<td>76.3</td>
<td>413</td>
</tr>
<tr>
<td></td>
<td>0.05</td>
<td>80.0</td>
<td>97.7</td>
<td>423</td>
</tr>
<tr>
<td></td>
<td>0.05</td>
<td>75.4</td>
<td>79.7</td>
<td>436</td>
</tr>
<tr>
<td></td>
<td>0.05</td>
<td>75.5</td>
<td>102.5</td>
<td>432</td>
</tr>
<tr>
<td></td>
<td>0.05</td>
<td>75.5</td>
<td>72.8</td>
<td>447</td>
</tr>
<tr>
<td></td>
<td>0.05</td>
<td>66.7</td>
<td>39.3</td>
<td>459</td>
</tr>
</tbody>
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$P$: 2.5 atm
$T$: 95$^\circ$C
Collaborated with 3M (FC104) to design and conduct tests analyzing the effects of anode and cathode RH on performance of 5-cm² active-area differential cells

- Anode: Ternary Pt₆₈(CoMn)₃₂, 0.019 mgPt/cm²
- Cathode: Binary Pt₃Ni₇/NSTF, 0.096 mgPt/cm², with 3M Type “B” cathode interlayer, 0.016 mgPt/cm²
- Membrane: 3M-S (reinforced) 725 EW PFSA with additive, 14 µm
- Diffusion Media: 3M “X3” cathode GDL (experimental backing, MPL), 3M 2979 cathode GDL

Developed models for effect of anode RH on HFR, ORR kinetics, limiting current and mass transfer overpotential

**Lower HFR under wet conditions**

**Lower limiting current density under wet conditions**

**Higher mass transfer losses under wet conditions**

All results for H₂/Air, P = 1.5 atm, T = 80°C
Water Transport in FCS w/o Cathode Humidifier

Self humidification of cathode by internal water transport from anode to cathode (and vice versa) across thin (14 μm) membrane

- Complete water balance at steady state: zero net transport
- Exit cathode RH is only a function of cell temperature and cathode SR
- Exit anode RH depends on cell temperature and anode SR

- Coolant flow concurrent with cathode flow
- Cathode inlet and outlet RHs do not depend on anode flow but cathode RH distribution depends on whether anode flow is co-flow or counter-flow

<table>
<thead>
<tr>
<th>P</th>
<th>1.5 atm</th>
</tr>
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<tbody>
<tr>
<td>ΔT_c</td>
<td>10°C</td>
</tr>
<tr>
<td>SR(c)</td>
<td>1.5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>T</th>
<th>RH(c)</th>
<th>RH(c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>75°C</td>
<td>22%</td>
<td>92%</td>
</tr>
<tr>
<td>80°C</td>
<td>18%</td>
<td>75%</td>
</tr>
<tr>
<td>85°C</td>
<td>14%</td>
<td>61%</td>
</tr>
<tr>
<td>90°C</td>
<td>12%</td>
<td>51%</td>
</tr>
</tbody>
</table>

- Parallel Flow
- Counter Flow

T: Coolant outlet temperature
Performance of FCS w/o Cathode Humidifier

All results for fixed 0.675 cell V, ΔT=10°C, SR(c)=1.5

Effect of cathode humidifier on stack power density
- Small improvement at low cell temperature
- Larger improvement at low operating pressure
- Larger improvement for parallel flow

Conclusions
- Cathode humidifier needed at 1.5 atm and >90°C, especially with parallel flow
- Small penalty in removing humidifier at 2.5 atm, especially with counter flow

Power density decreases if SR(a) < 2, but parasitic power too high if SR(a) > 2
Comparing fixed/variable area twin ejectors, hybrid ejector-recirculation pump, and pulse ejector

- CFD model of H₂ ejector with converging-diverging nozzle, undergoing testing and validation
- Process model of supersonic ejector with normal and oblique shocks, calibrated with laboratory data
- CFD model of pulse ejectors

Hybrid system with variable-area nozzle ejector (but not two-parallel ejectors) can meet flow and H₂ stoichiometry targets

Cost of recirculation blower: ~3.25 $/kWe

Modeled operating map of a fixed-area ejector with constant motive gas pressure (10.7 atm) and H₂ flow rate (1.38 g/s). Variable suction/delivery pressure

Entrainment: Ratio of suction to motive gas mass flow rate

Performance of Pulse Ejectors

Pulses of stack inlet/outlet pressure generated by opening (10 ms) and closing (90 ms) of H₂ injector

Depending on pulse width/frequency, there is threshold N₂ content for H₂ starvation at low current densities

Periodic variation of H₂ mole fraction, 0.1 A/cm² current density; H₂ on for 5 ms, off for 45 ms

Peak gas velocity depends on pulse width and controls the ability to remove liquid water and prevent its accumulation

Conclusion: May be feasible to replace hybrid ejector-recirculation pump with a pulse ejector, with limits on allowable N₂ build-up and pulse width
Air Management System

Study Objective: Evaluate possible advantage of air management system capable of delivering air at high pressures, up to 4 atm

2-Stage Centrifugal Compressor
- Mixed axial and flow compressors on a common shaft with air foil bearings (AFB); Honeywell US Patent 2015/0308456
- 3-phase brushless DC motor, liquid and air cooled; liquid-cooled motor controller
- Compressor power >20 kWₑ needed even if AFB/motor cooling air is recovered

FCS Performance at 4-atm Stack Inlet P
- 5.3% increase in MEA power density if Q/ΔT constraint is imposed, SR(c)=1.5, 0.718 V required cell voltage
- 25% increase in MEA power density at the 2.5-atm operating cell voltage, 0.672 V
- At low manufacturing volume, 1000 units/year, the cost of 4-atm FCS is only 3.8% higher at same cell voltage, 0.672 V

Cost correlations from SA, 1,000 units/year, Ejector + H₂ blower
<table>
<thead>
<tr>
<th>Collaborations</th>
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</thead>
<tbody>
<tr>
<td><strong>Air Management</strong></td>
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</table>
| **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** | ANL-Autonomie (SA044), Aalto University (Fuel Cell Buses) |
| **H₂ Impurities** | 3M |
| **System Cost** | SA: Manufacturing Cost Analysis of Fuel Cell Systems and Transportation Fuel Cell System Cost Assessment (FC163) |
| **Dissemination** | IEA Annex 34, Transport Modeling Working Group, Durability Working Group, Catalyst 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
Proposed Future Work

1. Support DOE development effort at system, component, and phenomenological levels

2. Support SA in high-volume manufacturing cost projections, collaborate in life-cycle cost studies
   - 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
   - State-of-the-art low PGM Pt and Pt alloys (FC-PAD 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
   - Alternate electrode structures (FC-PAD FOA projects collaboration)

4. System architecture and balance-of-plant components
   - Air management system with centrifugal and Roots compressors and expanders (Honeywell/Eaton collaboration)
   - Fuel and water management systems: anode gas recirculation, internal/external humidification
   - Bipolar plates and flow fields for low pressure drops and uniform air/fuel distribution, cell to stack performance differentials

5. Incorporate durability considerations in system analysis
   - System optimization for cost, performance, and durability on drive cycles (Advanced alloy catalyst systems)
### Project Summary

<table>
<thead>
<tr>
<th><strong>Relevance:</strong></th>
<th>Independent analysis to assess design-point, part-load and dynamic performance of automotive and stationary FCS</th>
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</table>
| **Approach:**  | Develop and validate versatile system design and analysis tools  
                  Apply models to issues of current interest  
                  Collaborate with other organizations to obtain data and apply models |
| **Progress:**   | Projected 44.9 $/kW_e FCS cost and 0.126 g/kW_e Pt content with HP d-PtNi/C cathode catalyst, reinforced 14-μm 850 EW membrane, and Q/ΔT = 1.45 kW/°C constraint  
                  Estimated 11% degradation in net FCS power with 40% decrease in d-PtNi/C cathode catalyst ECSA (0.05-0.15 mg/cm² Pt loading) due to cyclic potentials  
                  Showed the possibility of removing cathode humidifier for MEA membrane thickness <14-μm thin, and stack inlet P >2.5 atm  
                  Demonstrated that H₂ recirculation blower can be eliminated with a pulse ejector and maintaining <20% N₂ mole fraction  
                  Evaluated favorable extreme conditions (cell voltage, volume of manufacturing, Q/ΔT constraint) for high stack inlet P (4 atm) |
| **Collaborations:** | 3M, Aalto University, Eaton, JMFC, SA, UTRC, UDEL/Sonjector |
| **Future Work:** | Fuel cell systems with emerging high activity catalysts  
                  Alternate balance-of-plant components  
                  System analysis with durability considerations on drive cycles |
Key recommendations and feedback

- Investigate dispersed systems, including PtCo catalysts
- Show parasitic losses for the air machine vs. inlet air pressure
- De-emphasize work on 3M nanostructured thin-film catalyst
- Closer cooperation with FC-PAD activities and projects
- Clarify interactions with SA, collaboration or source of cost correlations
- This is a good solid model and a good team

Work scope consistent with above recommendations

✓ Focused work on d-PtNi/C dispersed catalysts using differential cell data obtained in collaboration with JMFC and UTRC (FC-106)

✓ On-going work on differential cell data for PtCo/C dispersed catalysts in collaboration with FC-PAD and an industrial partner. Initial results on performance and durability are included in FC-PAD presentations. The PI is FC-PAD coordinator for modeling and validation thrust area.

✓ 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

✓ ANL is a subcontractor to SA on FC-018 project, responsible for supplying performance and design data. Plans and recent results are discussed in bi-weekly calls.
Technical Back-Up Slides
Publications and Presentations

Journal Publications

Conference Presentations

Meetings Organized
FCS with HP d-PtNi/C Cathode Catalyst: Critical Assumptions

PEFC Stack

- Membrane: 14-µm, 850 EW, PFSA Mechanically reinforced, with chemical additive
- Cathode Electrode: JMFC d-PtNi/C catalyst, 0.1 mgPt/cm², high surface-area carbon support, 850 EW ionomer, I/C=1.0
- Anode Electrode: Pt/C catalyst, 0.025 mgPt/cm², high surface-area carbon support
- Cathode/Anode GDL: Non-woven carbon paper with microporous layer (MPL), SGL 25BC, 235 µm nominal uncompressed thickness
- 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 mΩ.cm² 2X ICR*

Fuel Management System

- Hybrid ejector-recirculation pump
- 35% pump efficiency, 1% H₂ purge
- 3 psi pressure drop at rated power

*2X ICR: two-sided interfacial contact resistance

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 ΔP between compressor discharge and expander inlet at rated power

Heat Rejection System

- Two circuits: 75-95°C HT, 10°C ΔT
- 65°C LT coolant, 5°C ΔT
- 55% pump + 92% motor efficiency
- 45% blower + 92% motor efficiency
- 10 psi ΔP in stack and 5 psi in radiator

Water Management System

- Planar cross-flow humidifier with Gore’s M311.05 membrane
## Rated Power Performance of FCS with Alloy catalysts

<table>
<thead>
<tr>
<th>Stack Parameters</th>
<th>2017 FCS with d-PtNi/C Catalyst</th>
<th>2016 FCS with Binary NSTF Catalyst</th>
</tr>
</thead>
<tbody>
<tr>
<td>Membrane</td>
<td>Ionomer: 850 EW PFSA with chemical additive Substrate: Mechanical reinforcement Thickness: 14 μm</td>
<td>Ionomer: 3M 725 EW PFSA with chemical additive Substrate: 3M support Thickness: 14 μm</td>
</tr>
<tr>
<td>Cathode Catalyst</td>
<td>Electrode: d-PtNi₆ (0.1 mg/cm²), add washed Ink: organic, EW=850, V/C=1.0</td>
<td>d-Pt₃Ni₂ (0.095 mg/cm²) with Pt/C cathode interlayer (0.016 mg/cm²)</td>
</tr>
<tr>
<td>Anode Catalyst</td>
<td>Pt/C (0.025 mg/cm²)</td>
<td>Pt₈S(CoMn)₃₂/NSTF (0.019 mg/cm²)</td>
</tr>
<tr>
<td>Stack Gross Power</td>
<td>88.1 kW</td>
<td>88.2 kW</td>
</tr>
<tr>
<td>Stack Voltage (Rated)</td>
<td>250 V</td>
<td>300 V</td>
</tr>
<tr>
<td>Number of Active Cells</td>
<td>377 cells (also 376 cooling cells)</td>
<td>453 cells (also 452 cooling cells)</td>
</tr>
<tr>
<td>Stack Gross Power Density</td>
<td>2.84 kW/L</td>
<td>2.49 kW/L</td>
</tr>
<tr>
<td>Stack Gross Specific Power</td>
<td>3.45 kW/kg</td>
<td>2.99 kW/kg</td>
</tr>
<tr>
<td>Stack Inlet Pressure</td>
<td>2.5 bar</td>
<td>2.5 bar</td>
</tr>
<tr>
<td>Stack Coolant Temperature</td>
<td>84°C (inlet), 94°C (outlet)</td>
<td>83.9°C (inlet), 93.9°C (outlet)</td>
</tr>
<tr>
<td>Stack Air Inlet/Outlet RH</td>
<td>Inlet: 75% RH at 84°C; Outlet: 100% RH at 94°C</td>
<td>Inlet: 50% RH at 85°C; Outlet: 88% RH at 95°C</td>
</tr>
<tr>
<td>Stack Fuel Inlet/Outlet RH</td>
<td>Inlet: 42% RH at 94°C; Outlet: 100% RH at 84°C</td>
<td>Inlet: 43% RH at 95°C; Outlet: 105.7% RH at 85°C</td>
</tr>
<tr>
<td>Cathode/Anode Stoichiometry</td>
<td>1.5 (cathode) / 2.0 (anode)</td>
<td>1.5 (cathode) / 2.0 (anode)</td>
</tr>
<tr>
<td>Cell Area</td>
<td>213 cm² (active), 346 cm² (total)</td>
<td>208 cm² (active), 333 cm² (total)</td>
</tr>
<tr>
<td>Cell Voltage</td>
<td>663 mV</td>
<td>663 mV</td>
</tr>
<tr>
<td>Current Density</td>
<td>1.651 A/cm²</td>
<td>1.418 A/cm²</td>
</tr>
<tr>
<td>Crossover Current Density</td>
<td>4.2 mA/cm² @ 80°C, 100% RH, 1 atm P₆2</td>
<td>5.0 mA/cm²</td>
</tr>
<tr>
<td>Power Density</td>
<td>1095 mW/cm²</td>
<td>941 mW/cm²</td>
</tr>
<tr>
<td>Balance of Plant</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Humidifier Membrane Area</td>
<td>0.8 m²</td>
<td>0.53 m²</td>
</tr>
<tr>
<td>Air Pre-cooler Heat Duty</td>
<td>6.3 kW</td>
<td>5.7 kW</td>
</tr>
<tr>
<td>CEM Motor and Motor Controller Heat Duty</td>
<td>3.0 kW</td>
<td>3.0 kW</td>
</tr>
<tr>
<td>Main Radiator Heat Duty</td>
<td>78.9 kW</td>
<td>79.8 kW</td>
</tr>
<tr>
<td>CEM Power</td>
<td>Compressor shaft power: 10.3 kW</td>
<td>Compressor shaft power: 10.4 kW</td>
</tr>
<tr>
<td></td>
<td>Expander shaft power out: 4.7 kW</td>
<td>Expander shaft power out: 4.7 kW</td>
</tr>
<tr>
<td></td>
<td>Net motor and motor controller: 7.0 kW &amp;</td>
<td>Net motor and motor controller: 7.1 kW &amp;</td>
</tr>
<tr>
<td>Fan and Pump Parasitic Power</td>
<td>0.5 kWₑ (coolant pump), 0.3 kWₑ (H₂ recirculation pump), 0.345 kWₑ (radiator fan)</td>
<td>0.5 kWₑ (coolant pump), 0.3 kWₑ (H₂ recirculation pump), 0.345 kWₑ (radiator fan)</td>
</tr>
</tbody>
</table>
Distributed ORR kinetic model

- For Tafel kinetics, the ORR and CCL Ohmic overpotentials are separable

\[ \eta_c = \eta_s^c + iR_\Omega \left( \frac{i\delta_c}{b\sigma_c} \right) \]

\[ i = i_0 (1 - \theta) e^{-\frac{\omega \theta}{RT}} e^{\frac{\alpha nF}{RT} \eta_s^c} \]

- An optimization algorithm required to determine \( i_0 \) and \( \omega \)

\[ i_0 = i_{0r} e^{-\frac{\Delta H_S^c}{RT} \left( \frac{1}{T} - \frac{1}{T_r} \right) P_{O_2}^{-\gamma} \left( \frac{\lambda}{\lambda_0} \right)^\beta} \]

- Solid solution model for PtO\(_x\) formation using cyclic voltammetry at \( 80^\circ C \), 100% RH, 1.5 atm, 0.5 l/s 4%\( H_2 \) & 0.5 l/s \( N_2 \), 30-min constant potential hold

\( Pt + H_2O = PtOH + H^+ + e^- \)

\( PtOH = PtO + H^+ + e^- \)

\( \theta = \theta_{PtOH} + \theta_{PtO} \)

Mass Transfer Overpotential Correlation

- Mass transfer overpotentials derived from pol curves do not correlate with mass activity
  \[ \eta_m = E_N - E - iR^m - \eta_c - \eta_a \]

- Product representation of \( i_L \) - current density at which \( \eta_m = 450 \text{ mV} \)
  \[ i_L = i_L(P,P_{O2})f_1(T)f_2(\Phi) \]

- Mass transfer overpotential correlation
  \[ \ln(\frac{\eta_m}{\eta_{mL}}) = F(P,T,X_{O2},\Phi,i/i_L) \]

- \( \eta_m \) correlation used to obtain expanded polarization data
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>annealed</td>
</tr>
<tr>
<td>A&lt;sub&gt;Pt&lt;/sub&gt;</td>
<td>Pt electrochemical specific area</td>
</tr>
<tr>
<td>b</td>
<td>Tafel slope</td>
</tr>
<tr>
<td>Cl</td>
<td>cathode interlayer</td>
</tr>
<tr>
<td>d</td>
<td>de-alloyed</td>
</tr>
<tr>
<td>E</td>
<td>cell voltage</td>
</tr>
<tr>
<td>E&lt;sub&gt;N&lt;/sub&gt;</td>
<td>Nernst potential</td>
</tr>
<tr>
<td>i</td>
<td>current density</td>
</tr>
<tr>
<td>i&lt;sub&gt;0&lt;/sub&gt;</td>
<td>exchange current density</td>
</tr>
<tr>
<td>i&lt;sub&gt;0r&lt;/sub&gt;</td>
<td>reference exchange current density</td>
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<tr>
<td>i&lt;sub&gt;L&lt;/sub&gt;</td>
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<tr>
<td>L&lt;sub&gt;Pt&lt;/sub&gt;</td>
<td>Pt loading</td>
</tr>
<tr>
<td>n</td>
<td>no of electrons</td>
</tr>
<tr>
<td>P</td>
<td>pressure</td>
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<td>R</td>
<td>gas constant</td>
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<tr>
<td>R&lt;sub&gt;cf&lt;/sub&gt;</td>
<td>CCL O&lt;sub&gt;2&lt;/sub&gt; transport resistance</td>
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<td>R&lt;sub&gt;cs&lt;/sub&gt;</td>
<td>cell to stack additional resistance</td>
</tr>
<tr>
<td>R&lt;sub&gt;d&lt;/sub&gt;</td>
<td>GDL O&lt;sub&gt;2&lt;/sub&gt; transport resistance</td>
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<tr>
<td>R&lt;sub&gt;g&lt;/sub&gt;</td>
<td>gas channel O&lt;sub&gt;2&lt;/sub&gt; transport resistance</td>
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<tr>
<td>R&lt;sub&gt;m&lt;/sub&gt;</td>
<td>mass transfer resistance</td>
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<tr>
<td>R&lt;sub&gt;c&lt;/sub&gt;</td>
<td>cathode ionic resistance</td>
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<tr>
<td>R&lt;sub&gt;Ω&lt;/sub&gt;</td>
<td>high-frequency resistance (HFR)</td>
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<tr>
<td>RH</td>
<td>relative humidity</td>
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<tr>
<td>SR</td>
<td>stoichiometry</td>
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<tr>
<td>S&lt;sub&gt;Pt&lt;/sub&gt;</td>
<td>Pt surface roughness</td>
</tr>
<tr>
<td>T</td>
<td>temperature</td>
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<tr>
<td>T&lt;sub&gt;r&lt;/sub&gt;</td>
<td>reference temperature, 353 K</td>
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<tr>
<td>X</td>
<td>mole fraction</td>
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<tr>
<td>Δ&lt;sub&gt;H&lt;/sub&gt;&lt;sup&gt;c&lt;/sup&gt;</td>
<td>ORR activation energy</td>
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<tr>
<td>α</td>
<td>symmetry factor</td>
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<tr>
<td>β</td>
<td>relative humidity dependence</td>
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<tr>
<td>γ</td>
<td>O&lt;sub&gt;2&lt;/sub&gt; partial pressure dependence</td>
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<tr>
<td>δ&lt;sub&gt;c&lt;/sub&gt;</td>
<td>cathode electrode thickness</td>
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<tr>
<td>δ&lt;sub&gt;d&lt;/sub&gt;</td>
<td>GDL thickness</td>
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<tr>
<td>δ&lt;sub&gt;l&lt;/sub&gt;</td>
<td>liquid layer thickness</td>
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<td>ε&lt;sub&gt;i&lt;/sub&gt;</td>
<td>ionomer volume fraction</td>
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<td>ε/τ in dry portion of GDL</td>
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<tr>
<td>ε&lt;sub&gt;t&lt;/sub&gt;</td>
<td>ε/τ in wet portion of GDL</td>
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<tr>
<td>η&lt;sub&gt;a&lt;/sub&gt;</td>
<td>anode overpotential</td>
</tr>
<tr>
<td>η&lt;sub&gt;c&lt;/sub&gt;</td>
<td>cathode overpotential</td>
</tr>
<tr>
<td>η&lt;sub&gt;m&lt;/sub&gt;</td>
<td>mass transfer overpotential</td>
</tr>
<tr>
<td>η&lt;sup&gt;a&lt;/sup&gt;&lt;sub&gt;s&lt;/sub&gt;</td>
<td>HOR kinetic overpotential</td>
</tr>
<tr>
<td>η&lt;sup&gt;c&lt;/sub&gt;&lt;sub&gt;s&lt;/sub&gt;</td>
<td>ORR kinetic overpotential</td>
</tr>
<tr>
<td>θ</td>
<td>oxide coverage</td>
</tr>
<tr>
<td>λ</td>
<td>water uptake</td>
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<tr>
<td>σ&lt;sub&gt;c&lt;/sub&gt;</td>
<td>cathode ionic conductivity</td>
</tr>
<tr>
<td>σ&lt;sub&gt;m&lt;/sub&gt;</td>
<td>membrane conductivity</td>
</tr>
<tr>
<td>τ</td>
<td>tortuosity</td>
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