The Effects of Impurities on Fuel Cell Performance and Durability

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Project ID
#FC_24_Molter

FuelCell Energy

Hamilton Sundstrand
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Overview

Timeline

- Start March 2007
- End February 2011
- ~50% Complete

Barriers

- Establish Tolerance to Fuel and System Derived Impurities

Budget

- Total project funding $2,335,725
  - DOE share $1,868,580
  - Contractor share $467,145
- Funding Received in FY07 - $350K
- Funding Received in FY08 - $550K

Partners

- United Technologies Hamilton Sundstrand – Historical Contaminant Data
- FuelCell Energy, Inc., - Contaminant Test Support
- UConn CGFCC – Project Management, Testing

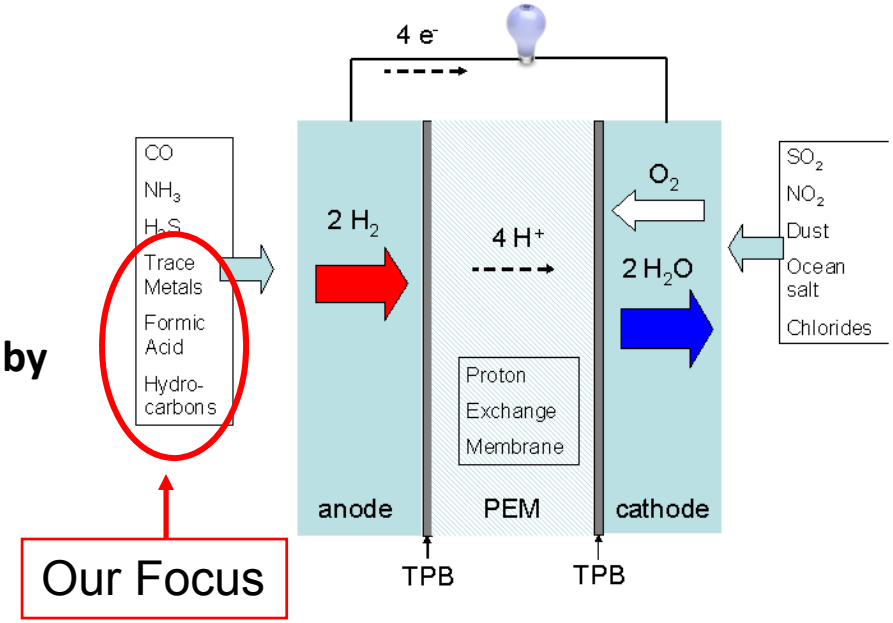
Relevance - Objectives

- **Overall Objective – Develop an Understanding of the Effects of Various Impurities on Fuel Cell Performance and Durability**
- **Specific Focus for Past Year**
  - **Screening of Hydrocarbon Impurities Per Standard Test Protocols to Identify Impurities of Concern**
  - **Quantification of Effects on Fuel Cell Performance**
  - **Effects of Cations on Membrane Properties**
  - **Develop Fundamental Models Based on Experimental Findings**

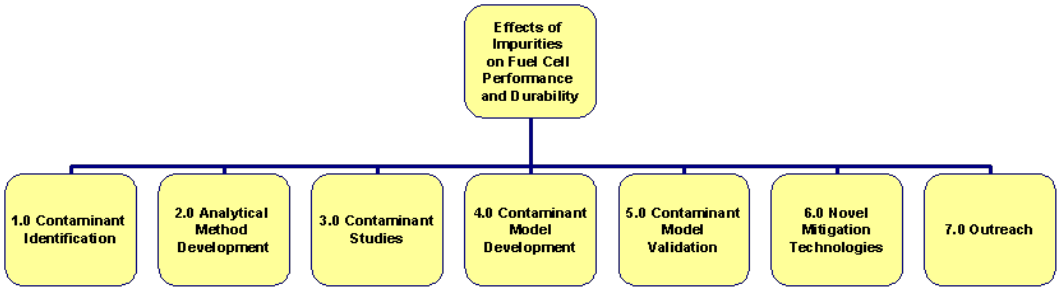
Task	Objectives
1.0 Contaminant Identification	• Identify specific contaminants and contaminant families present in both fuel and oxidant streams.
2.0 Analytical Method Development	• Development of analytical methods to study contaminants. • Experimental design of analytical studies. • Novel *in situ* detection methods.
3.0 Contaminant Studies	• Develop contaminant analytical models that explain these effects. • Establish an understanding of the major contamination-controlled mechanisms that cause material degradation in PEM cells and stacks under equilibrium and especially dynamic loading conditions
4.0 Contaminant Model Development	• Construct material state change models that quantify that material degradation as a foundation for multiphysics modeling • Establish the relationship between those mechanisms and models and the loss of PEM performance, especially voltage decay
5.0 Contaminant Model Validation	• Validate contaminant models through single cell experimentation using standardized test protocols.
6.0 Novel Mitigation Technologies	• Develop and validate novel technologies for mitigating the effects of contamination on fuel cell performance.
7.0 Outreach	• Conduct outreach activities to disseminate critical data, findings, models, and relationships etc. that describe the effects of certain contaminants on PEM fuel cell performance.

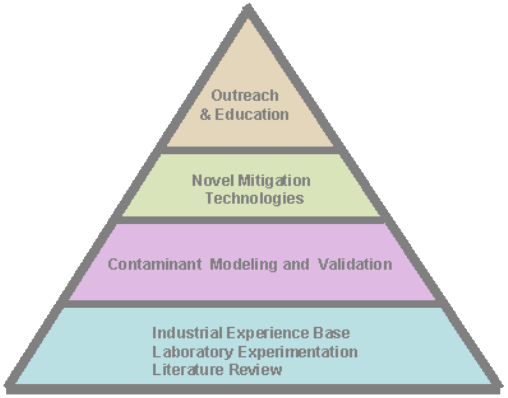
Approach

- **Initiate Studies by Leveraging Existing Database From Prior Work**
  - **DOE Sponsored Activity**
  - **USFCC Data**
  - **Prior Electrolysis Product Experience**
  - **Ongoing Literature Review**
- **Focus on Specific Contaminants/Concentrations Identified by DOE/Others**
- **Use Standardized Test Protocols Where Appropriate to Investigate Contaminant Effects**
- **Develop Empirical Models Based on Our Findings**



Project Work Plan/Deliverables





Deliverables

- Validated Contaminant Models Based on Performance and Durability Data Collected
- New Mitigation Technologies

Outreach

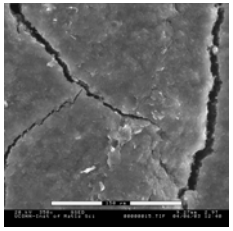
- Papers, Workshops, Technical Interchange, Etc.

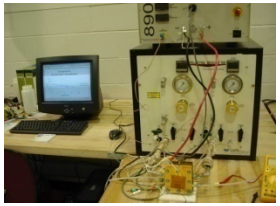
Task	Milestone	Date Year/Quarter
1.0 Contaminant Identification	• Contaminant Identification Review With DOE Sponsor & Industry Focus Group	Y1/Q2
2.0 Analytical Method Development	• Validate Analytical Methods For Studying Contaminants With Ersatz Gases	Y1/Q4
3.0 Contaminant Studies	• Establish an Understanding of the Major Contamination-Controlled Mechanisms that Cause Material Degradation	Y2/Q4
4.0 Contaminant Model Development	• Determine the Relationship Between Contaminant Mechanisms and the Loss of PEM Performance, Especially Voltage Decay.	Y3/Q4
5.0 Contaminant Model Validation	• Validate Contamination Models Through Single Cell Experimentation Using Standardized Test Protocols and a DOE Approved Test Matrix	Y4/Q1
6.0 Novel Mitigation Technologies	• Demonstrate Novel Technologies for Mitigating the Effects of Contamination on Fuel Cell Performance	Y4/Q4
7.0 Outreach	• Dissemination of Results Through Reports (DOE Approved), Papers and Workshops	Continuous
8.0 Project Management and Reporting	• Program Written Reports and Program Reviews	Continuous

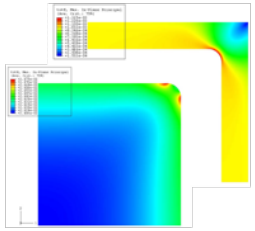
Roles of Participants

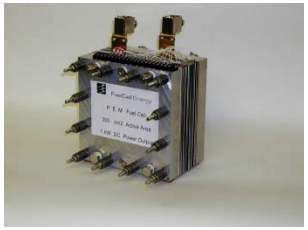
The Universtiy of Connecticut
Connecticut Global Fuel Cell Center
Program Lead

United Technologies Hamilton Sundstrand	The University of Connecticut Institute for Materials Science	The University of Connecticut School of Engineering	FuelCell Energy Inc.
Advise on Fate of Contaminants	Gas Analyses/Surface Studies	Contaminant Testing Modeling & Mitigation Strategies	Contaminant Identification Fuel Cell Testing
•Electrolysis Contaminant Experience •Prior Contaminant Studies	•Surface Studies/Equipment •Gas Purity Analyses	•Fuel Cell Testing •Modeling/Transport Expertise •Industry Relationships	•Gas Contaminant Experience •Fuel Cell Test Experience









Test Matrix
Hydrocarbons and Halogenated Compounds

- Initiate Testing With Methane – Practice Molecule
- Establish Analytical Techniques, Test Protocols, Basic Performance Models
- Export Data in Common Format to Working Groups for Further Modeling
- Contaminant Strategy
  - Near Term Focus – Hydrocarbons and Halogenated Compounds
  - Choice Based on Industry Input
  - Start With High Level – Dilute if Effects are Noted
  - Empirical Models – Near Term
  - Multi-Physics Models – Long Term

Test Matrix
Hydrocarbons and Halogenated Compounds

- Focus on Molecules that May be Present in Hydrogen Fuel Stream
- Impurity Choices Based on Industry Input & Literature Review
- Determine Effects of:
  - Molecule Functionality
  - Molecule Size (ie. # Carbons)

Already Tested

In Process

Test Strategy

Alkanes

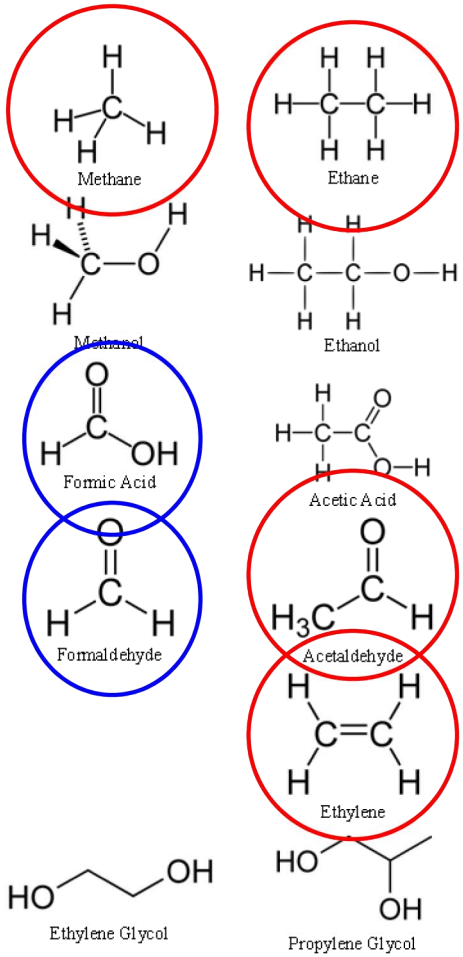
Alcohols

Organic Acids

Aldehydes

Alkenes

Glycols



Specifications for Draft CD

Component	ISO/SAE Specs
Hydrogen	99.97+
Sulfur (as H_2S)/total S	4 ppb
CO	.2 ppm
CO_2	2 ppm
NH_3	.1 ppm
NMHC/Total HCs	2 ppm
Particulates	1 ug/L (10 um size)
Total non H_2 gases	<.03% (300ppm)
Water	5 ppm
Oxygen	5 ppm
He	300 ppm
N_2 + Ar	100 ppm
Formaldehyde	10 ppb
Formic acid	.2 ppm
Total halogenates	50 ppb

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Test Protocol

Hydrocarbons and Halogenated Compounds

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MEA Definition

Parameter	Value (Early)	Value (Recent)
Membrane	Nafion® 212	Nafion® 212
Anode Loading	0.4 mg/cm^2	0.4 mg/cm^2
Anode Type	50% Pt on C	50% Pt on C
Cathode Loading	0.2 mg/cm^2	0.4 mg/cm^2
Cathode Type	50% Pt on C	50% Pt on C
MEA OEM	Ion Power	Ion Power
Cell Area	25 cm^2	25 cm^2
OEM	Fuel Cell Technologies	Fuel Cell Technologies

Operating Conditions

Parameter	Value (Early)	Value (Recent)
Anode Temperature	80°C	80°C
Cathode Temperature	80°C	73°C
Cell Temperature	80°C	80°C
Anode Humidity	100%	100%
Cathode Humidity	100%	75%
Anode Stoich	1.3	2.0
Cathode Stoich	2.0	2.0
Anode Flow	Commensurate with Current Density	
Cathode Flow	Commensurate with Current Density	
Anode Pressure	25 psig	25 psig
Cathode Pressure	25 psig	25 psig

Strategy

- Use Commercially Available MEA's
- Start Test at High Concentration (Screening Test)
- Reduce Concentration to Projected Spec. Levels if Effects are Noted, Otherwise Move On
- Move Toward Lower Catalyst Loadings (Projected Commercial)

Cell Conditioning and Tests Performed in Accordance With Standardized Protocols

- H_2 Crossover Per Appendix 1
- ECA Measurement Per Appendix 2
- Cell Conditioning and Verification per section 3.1
- Polarization Under Standard Hardware Conditions 0 – 1.2 A/cm^2. Repeat 3 times.
- Durability Test at 800 mA/cm^2 for 100 Hours Under Standard Conditions
- Durability Test at 800 mA/cm^2 for 100 Hours Under Standard Conditions – except with TBD Conc.[1] contaminant in hydrogen.

1) 5% - 100 PPM – 50 PPM

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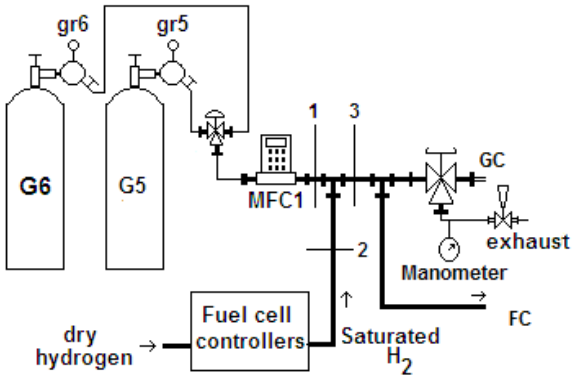
Hydrogen Fuel Preparation/Mixing

Hydrocarbons and Halogenated Compounds

Gases and High Vapor Pressure Oxygenated Compounds
Eg. Methane, Ethane, Acetaldehyde, Formaldehyde

Mixing of H_2 and high vapor pressure oxygenated contaminants

Certified mixtures H_2 and the contaminant G6 and G5

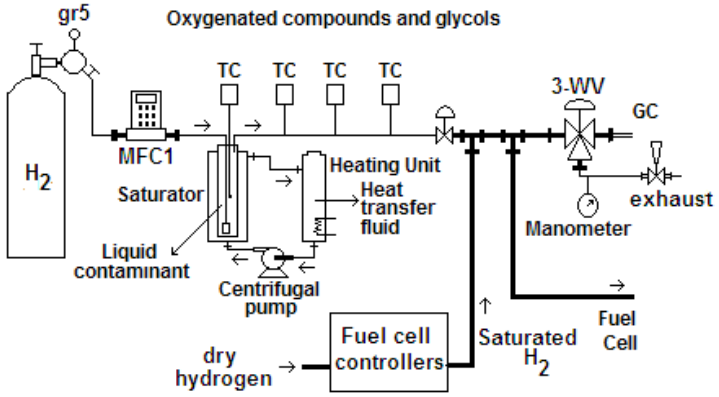


Non-Gaseous Impurities
Eg. Formic Acid, Acetic Acid, Ethanol, Methanol, Propylene Glycol, Ethylene Glycol

Mixing of H_2 and Non-gaseous contaminant

Saturation of a flow of H_2 with a liquid contaminant

Oxygenated compounds and glycols



Contaminant	Maximum Concentration	Limiting the Factor
Acetaldehyde	100 ppm	MFC1
Formic acid	1 % molar	MFC1 and Saturator
Ethylene glycol	200 ppm	MFC1 and energy balances
Propylene glycol	300 ppm	MFC1 and energy balances
Ethanol	0.8 % mol	Saturator
Methanol	1.0 % mol	Saturator

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Impurity Analysis

Hydrocarbons and Halogenated Compounds

Gas Chromatography (GC) of Anode Inlet/Outlet

- Quantitative Analytical Method for Impurities
- On Line Analysis, Simultaneous and Continuous Sampling
- Quantify Species Fed

NMR Evaluation of Condensate

- Anode and Cathode Side
- Periodic Sampling
  - Quantify Species Fed
  - 1H NMR, Protons in Different Chemical Environments Experience Different Shielding and Have Unique Shifts.
  - 13C NMR, Extension to Proton Spectra; Different Carbon Atoms Absorb in a Distinct Range.

In-Situ Contaminant Testing

Hydrocarbons and Halogenated Compounds

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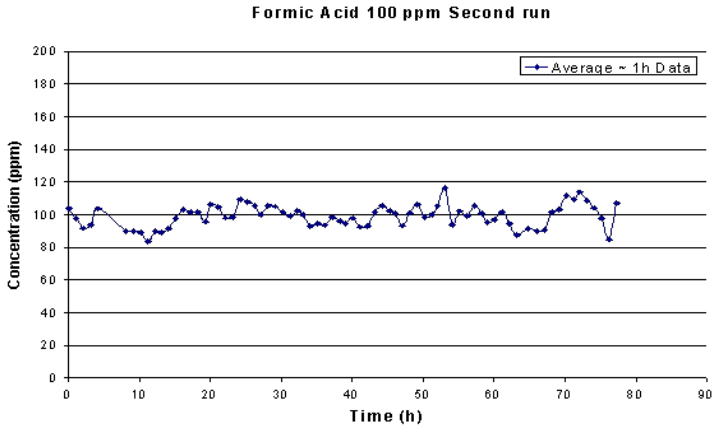
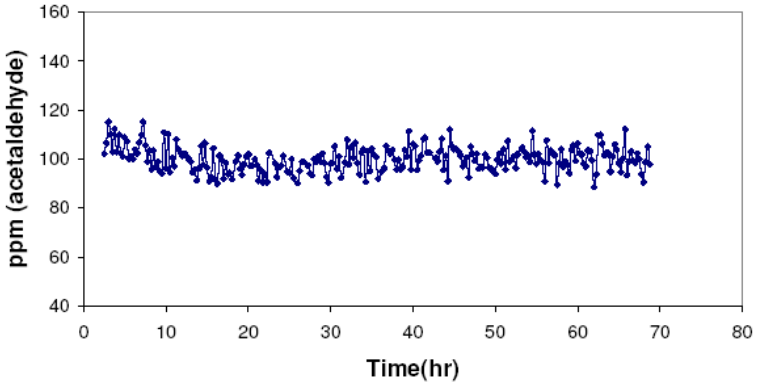
Formic Acid



Acetaldehyde
100 ppm

Acetaldehyde



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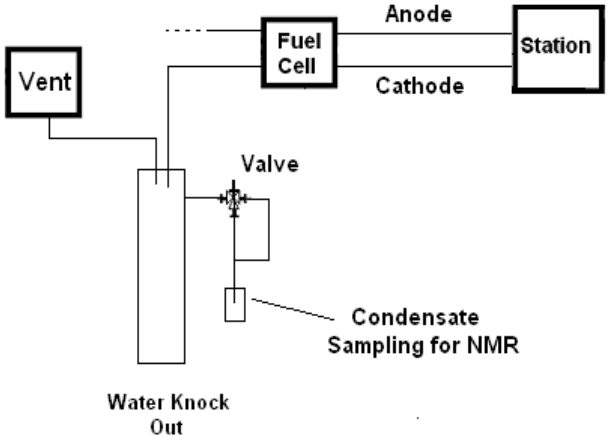
NMR Analysis of Condensate
Hydrocarbons and Halogenated Compounds

NMR Analysis

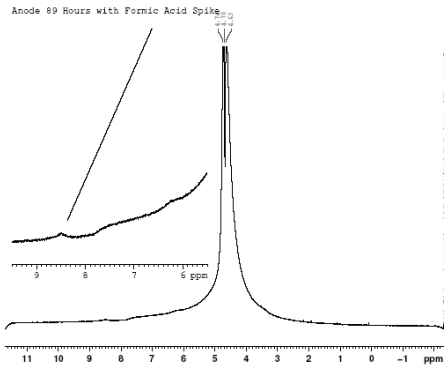
Set up Characteristics:

- Online Collection of Condensate - Anode and Cathode Side (About Every 25 Hours Sample Collected)
- No Perturbation of Cell Operating Conditions

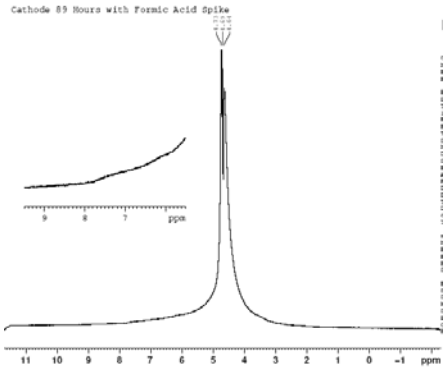


Formic Acid 100 ppm First Run

- Anode Side: Signal for Formic Acid at About 8.5 ppm



- Cathode Side: No signal for Formic Acid



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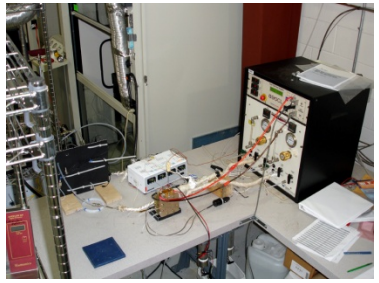
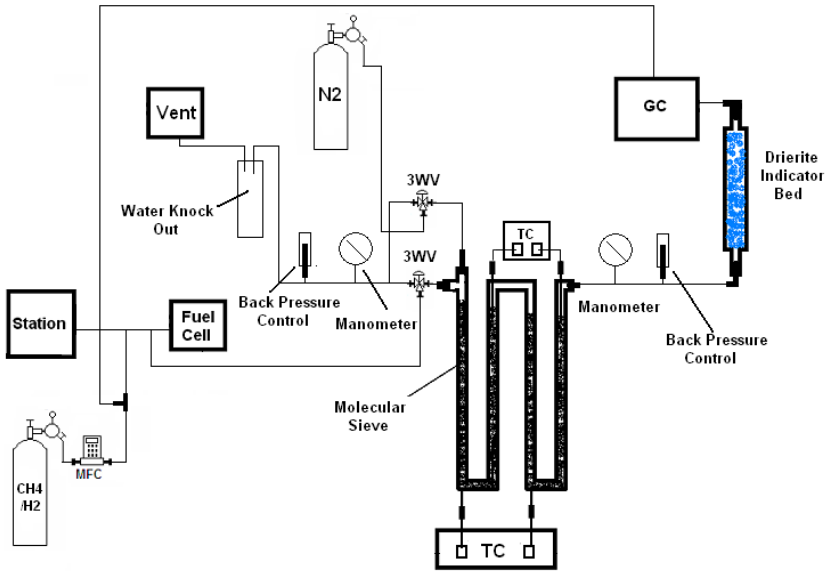
In-Situ Impurity Testing

Hydrocarbons and Halogenated Compounds

- Lab Test Stand Configured for Impurities Testing
- GC Set Up for Impurity Analysis
- Second and Third Lab Test Stands Utilized for Break-In, Some Impurity Testing





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Test Summary

Hydrocarbons and Halogenated Compounds

MEA: Ion-Power Inc. N212®, A/C: 0.4/0.4 mgPt/ cm^2
Cell Hardware: Fuel Cell Technologies Inc.
Active Area: 25 cm^2
Test Station: Teledyne MEDUSA

Cell #	Impurity	Current Density	RH (A/C)	Cell Temp	Flow Rates A/C	Description
1	100 ppm CH4	200 mA/cm2	100%/100%	80 ° C	58.5/214 sccm	No Significant Degradation
2	100 ppm CH4	600 mA/cm2	100%/100%	80 ° C	175/642 sccm	No Significant Degradation
3	5 % CH4 or 5% N2	600 mA/cm2	100%/100%	80 ° C	175/642 sccm	No Significant Degradation
4	100 ppm CH4	800 mA/cm2	100%/100%	80 ° C	234/857 sccm	No Significant Degradation
6	5% C2H6	600 mA/cm2	100%/100%	80 ° C	175/642 sccm	No Significant Degradation
7	5% C2H4	800 mA/cm2	100%/100%	80 ° C	234/857 sccm	No Significant Degradation
11	30 ppm CH3CHO	800 mA/cm2	100%/100%	80 ° C	181/664 sccm	No Significant Degradation
31	100 ppm CH3CHO	800 mA/cm2	100%/75%	80 ° C	278/664 sccm	No Significant Degradation
35	100 ppm HCOOH	800mA/cm2	100%/75%	80 ° C	278/664 sccm	Significant Degradation
38	50 ppm HCOOH	800mA/cm2	100%/75%	80 ° C	278/664 sccm	Some Degradation

Test Summary

Hydrocarbons and Halogenated Compounds

Acetaldehyde (CH_3CHO) *100 ppm*

Stability Test (100 hours with/without CH_3CHO, 100 ppm)

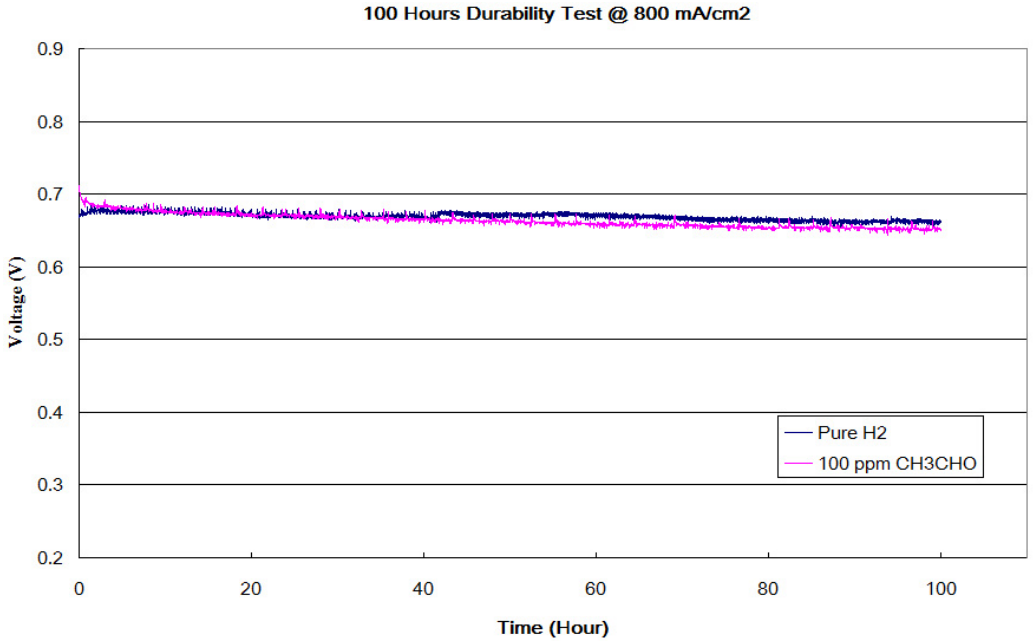
CELL#31 Operating Conditions:

Current Control: 800 mA/cm^2

Pressure-Anode/Cathode: 25/25 psig

Temperature-Cell/Anode/Cathode: 80/80/73ºC

Flow Rate-Anode/Cathode: 278/664 sccm (stoich. 2/2 at 800 mA/cm^2)



No obvious performance impact was evident during testing at the 100 ppm level.

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Test Summary

Hydrocarbons and Halogenated Compounds

Formic Acid (HCOOH) *100 ppm*

Stability Test (100 hours with/without HCOOH, 100 ppm)

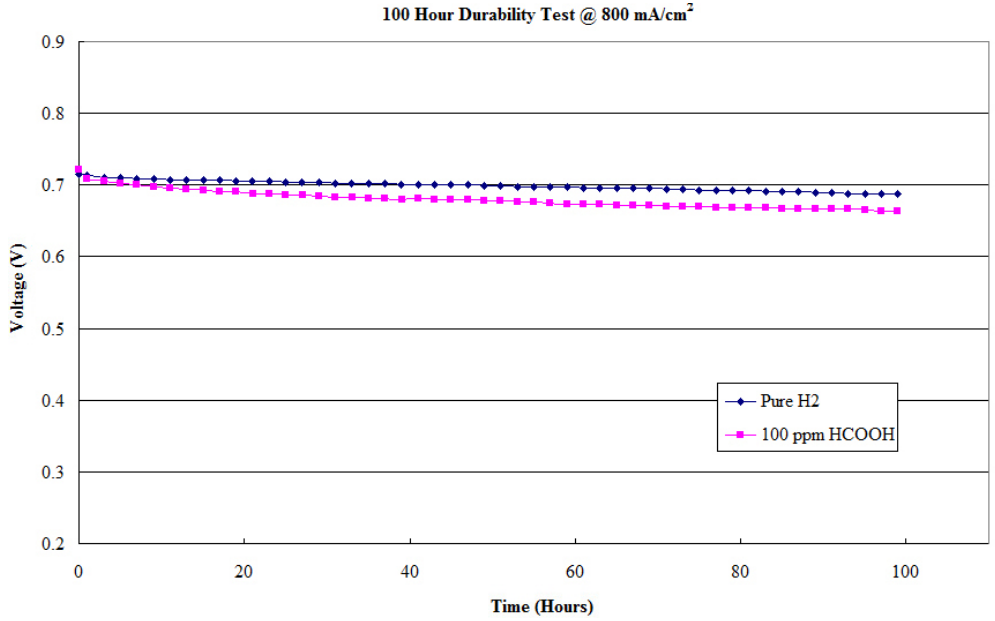
CELL#35 Operating Conditions:

Current Control: 800 mA/cm^2

Pressure-Anode/Cathode: 25/25 psig

Temperature-Cell/Anode/Cathode: 80/80/73ºC

Flow Rate-Anode/Cathode: 278/664 sccm (stoich. 2/2 at 800 mA/cm^2)



100 ppm formic acid in the H_2 fuel stream shows some effect on fuel cell performance

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Test Summary

Hydrocarbons and Halogenated Compounds

Formic Acid (HCOOH) *50 ppm*

Stability Test (100 hours with/without HCOOH, 50 ppm)

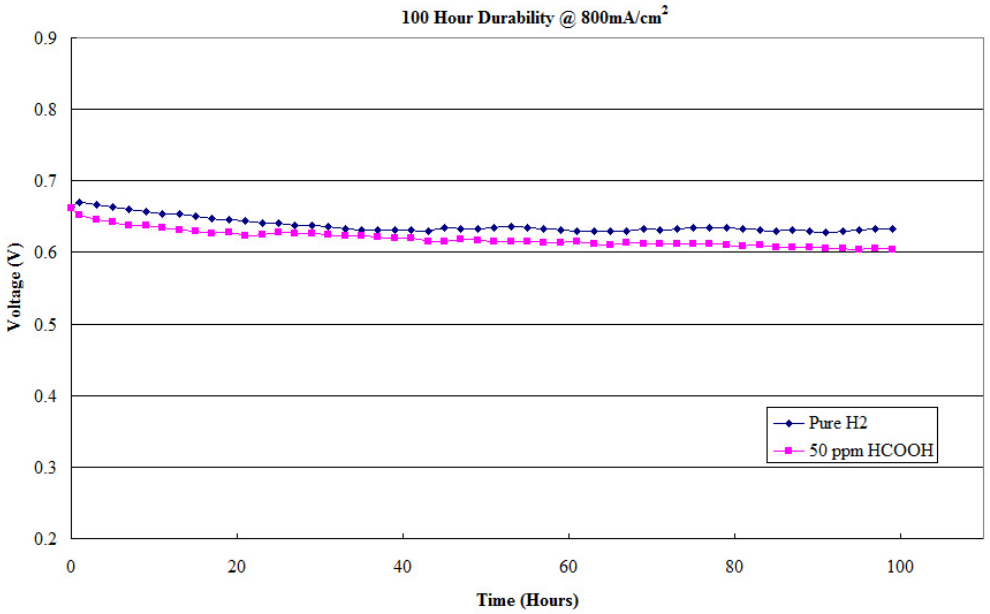
CELL#38 Operating Conditions:

Current Control: 800 mA/cm^2

Pressure-Anode/Cathode: 25/25 psig

Temperature-Cell/Anode/Cathode: 80/80/73ºC

Flow Rate-Anode/Cathode: 278/664 sccm (stoich. 2/2 at 800 mA/cm^2)



50 ppm formic acid in the H_2 fuel stream shows some effect on fuel cell performance, but less pronounced than 100 ppm.

Test Summary

Hydrocarbons and Halogenated Compounds

Formic Acid (HCOOH) *100 ppm*

"Hot"Cyclic Voltammetry During Contamination

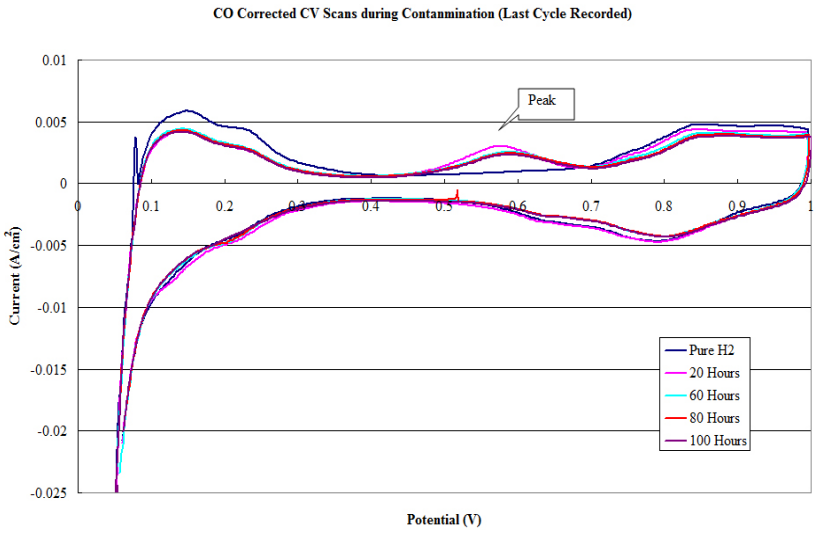
-Record the last CV cycles at each time step

Scan Rate: 20 mV/sec, Scan Range: 0.05 – 1.0 V,

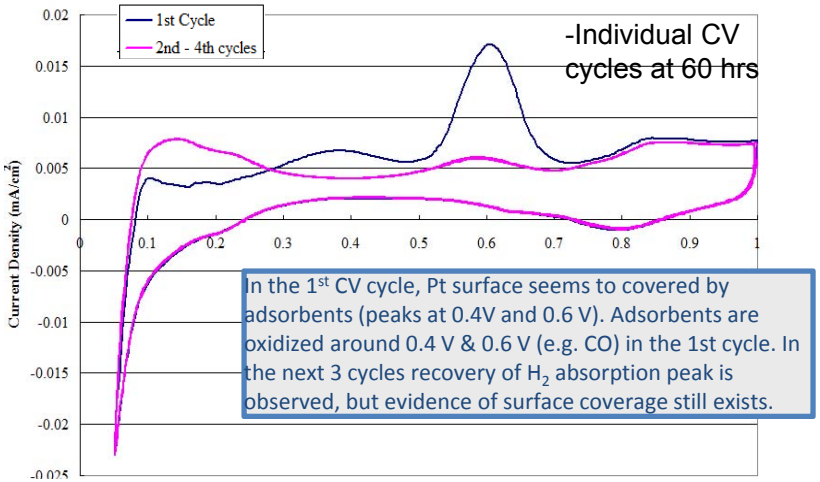
Pressure-Anode/Cathode: 25/25 psig

Temperature-Cell/Anode/Cathode: 80/80/73ºC

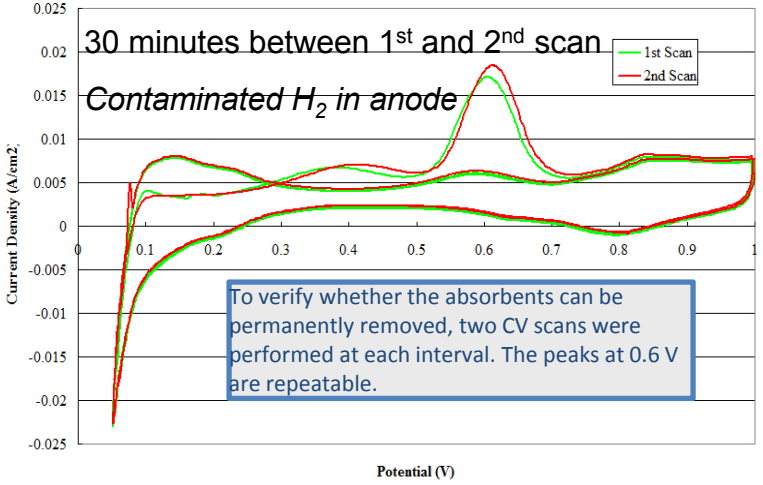
Flow Rate-Anode/Cathode: 250/250 sccm



CVs were performed every 20 hours to characterize cathode poisoning. Last cycle of each scan is shown above. CVs show a decrease in H2 adsorption peaks and an oxidation peak at 0.6 V →Impurities present on Pt surface?



In the 1st CV cycle, Pt surface seems to covered by adsorbents (peaks at 0.4V and 0.6 V). Adsorbents are oxidized around 0.4 V & 0.6 V (e.g. CO) in the 1st cycle. In the next 3 cycles recovery of H_2 absorption peak is observed, but evidence of surface coverage still exists.



To verify whether the absorbents can be permanently removed, two CV scans were performed at each interval. The peaks at 0.6 V are repeatable.

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Test Summary

Hydrocarbons and Halogenated Compounds

Recovery After Contamination

"Hot" Cyclic Voltammetry During Recovery

-Record last CV cycles at each time step

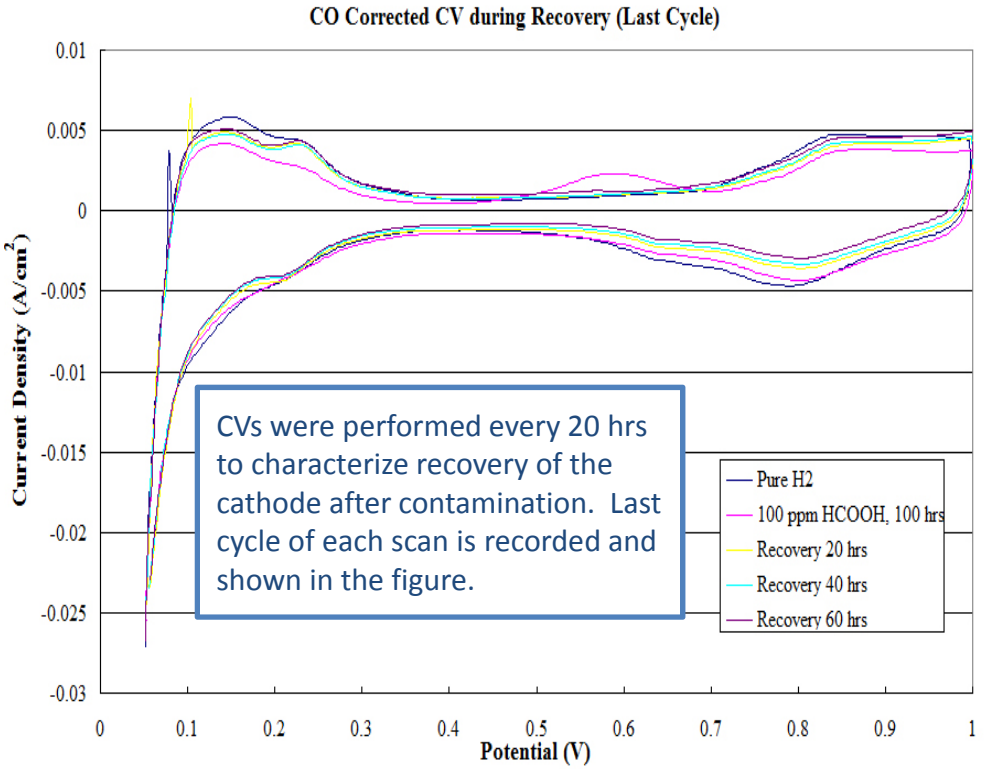
Scan Rate: 20 mV/sec, Scan Range: 0.05 – 1.0 V,

Pressure-Anode/Cathode: 25/25 psig

Temperature-Cell/Anode/Cathode: 80/80/73ºC

Flow Rate-Anode/Cathode: 250/250 sccm

After recovery with pure H_2 for 20 hours, hydrogen adsorption peaks are partially recovered. Further operation (up to 100 hrs) with pure H_2 does not result in additional recovery.



Contamination of HCOOH on the cathode is not fully recoverable just by purging pure H_2 through the anode.

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Cell & System Hygiene Management

Hydrocarbons and Halogenated Compounds

How Do We Know That The System is Clean at the Start of a Test? Hydrocarbons are "Sticky" – Sometimes Difficult to Remove.

- **New "Wetted" Cell Components**
- **Cleaning Procedure Adopted For Other System Components Plus Endplates, etc.**

Cleaning Procedure After Contaminant Evaluation

- Acetone through tubing
- N_2 purge
- Step ramping to evaporate remaining solvent
  - 40° C, 80°C, 120°C
- N_2 purge

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MEA Characterization

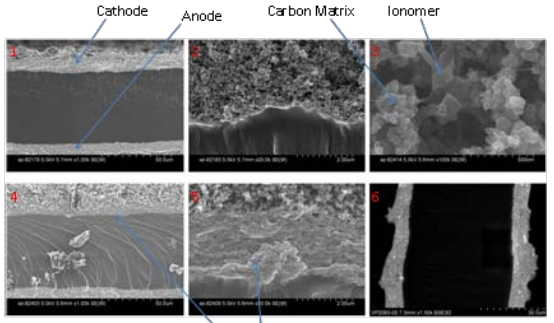
- Materials Characterization Techniques Used to Support Impurity Testing
- Baseline and Aged MEA's Cation Impurity Distribution
- Collaborating With ORNL

Scanning Electron Microscopy :

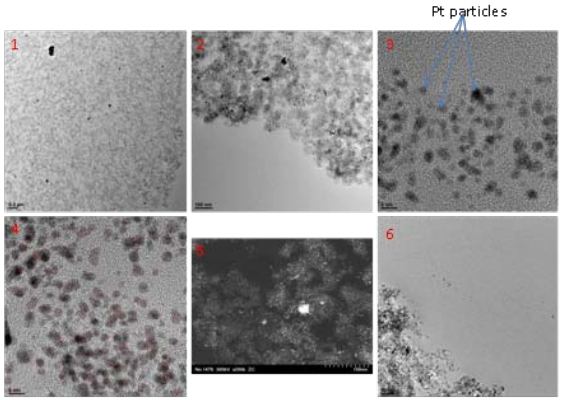
- Interface bonding
- Edge effect or appearance
- Electrode thickness
- Membrane thickness
- Electrode Porosity
- Ionomer Distribution
- Spectral Imaging (EDXS)
- Any noticeable physical change

Transmission Electron Microscopy:

- Distribution of the catalyst
- Porosity of electrodes
- Membrane/electrode interface
- Ionomer distribution
- Chemical composition of membrane and electrodes
- Pt particles sizes and distribution
- STEM : (HA-ADF) and EDXS mapping (at ORNL)



Baseline MEA: 1) Cross Section, 2) Membrane/electrode interface,3) High mag. image of ionomer and carbon matrix 6) BSE image . Aged MEA: 4) Cross section 5) Membrane/electrode interface



Baseline MEA 1) General View, 2) Membrane/Electrode interface ,3-4) Pt particles 5) STEM image of electrode, 6) Membrane adjacent cathode.

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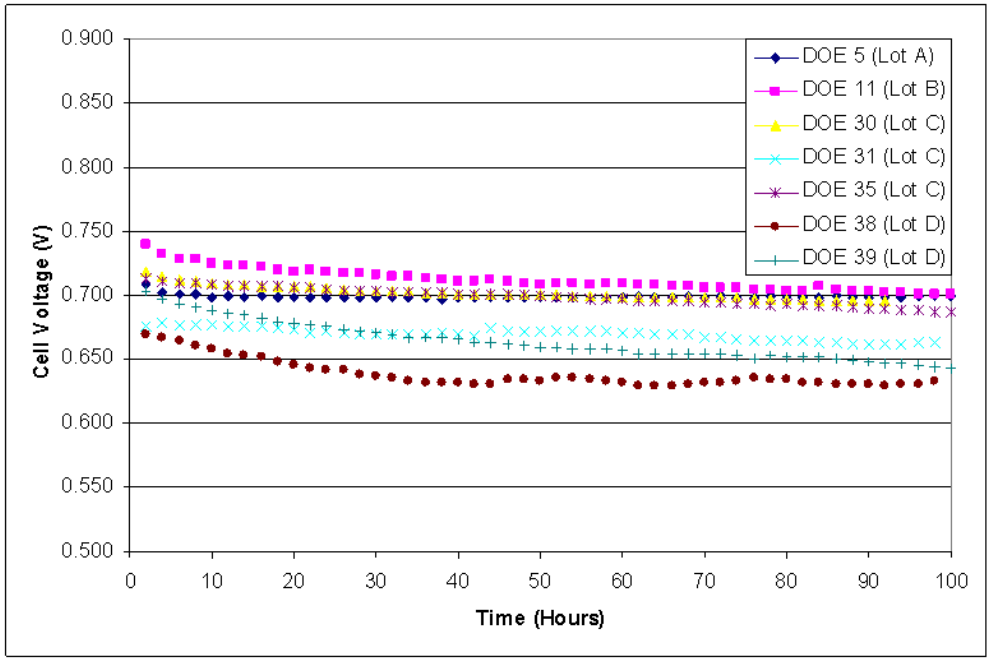
CCM Stability Evaluation



Cell	Loading (A/C)	Stoich	RH (A/C)	Press. (psig)	Temp. (°C)
5	0.4/0.2	1.3/2.0	100%/100%	25	80
11	0.4/0.2	1.3/2.0	100%/100%	25	80
30	0.4/0.4	2.0/2.0	100%/75%	25	80
31	0.4/0.4	2.0/2.0	100%/75%	25	80
35	0.4/0.4	2.0/2.0	100%/75%	25	80
38	0.4/0.4	2.0/2.0	100%/75%	25	80
39	0.4/0.4	2.0/2.0	100%/75%	25	80

- Data Show Significant Spread in Performance/Degradation Rate
- Data Variability Led to a Detailed Investigation of All Potential Contributing Factors
  - Rechecked Test Rig
  - Recalibrated Test Rig
  - Rechecked Procedures
    - Assembly
    - Testing
  - Varied Pressure
  - Varied Flow Rates
  - Varied Relative Humidity
- Data Showed Variation Within and Between Lots of MEA's
- Worked With Manufacturer & Other Labs to Identify Lots That Show More Consistent Performance
- Inter-Lab Effort Underway to Specify Generic, Stable MEA

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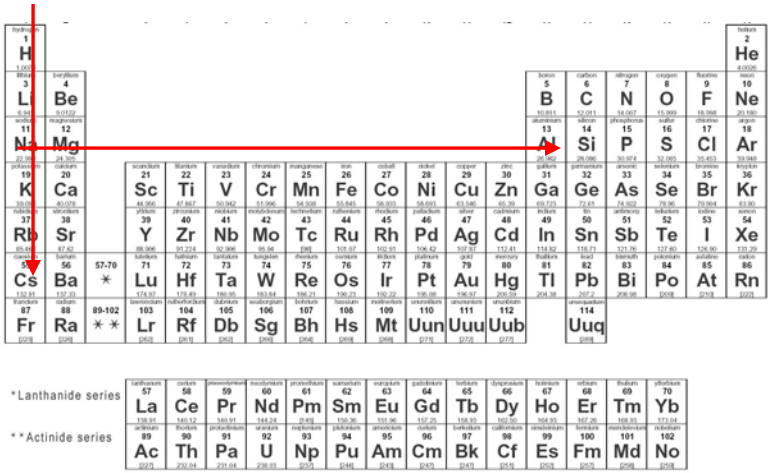
Membrane Studies
Cationic Impurities

- Focus is on Membrane Properties Rather Than Fuel Cell Operational Tests
  - Fluids Permeability
  - Water Content
  - Ion Exchange Capacity
  - Conductivity/Ionic Resistance
  - Mechanical Properties
  - Contaminant Characterization Using SEM/EDX
- Move Down and Across Periodic Table to Examine Mass and Valence Effects of Common Ions



Key Findings

- Membrane Water Content Drops Significantly With Cation Exposure
- Membrane Water Content Decreases Significantly as We Move Down Periodic Table – Largely Due to the Change in Hydration Shell for Each Ion
- Nearly 100% of Ion Exchange Sites Consumed for Most Cation Contaminants, Sites Consumed at Low Concentration
- Permeation Rate Appears to be Linear With Pressure
- Cationic Contaminants Affect Permeability in Different Ways
  - H2, O2, N2 and H2O Reduced
- Yield Strength and Modulus Found to Increase With Contamination
- Tensile Strength and Elongation at Break Found to Decrease With Contamination

- Current Focus: Trace Contaminant Concentrations

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Other Impurities

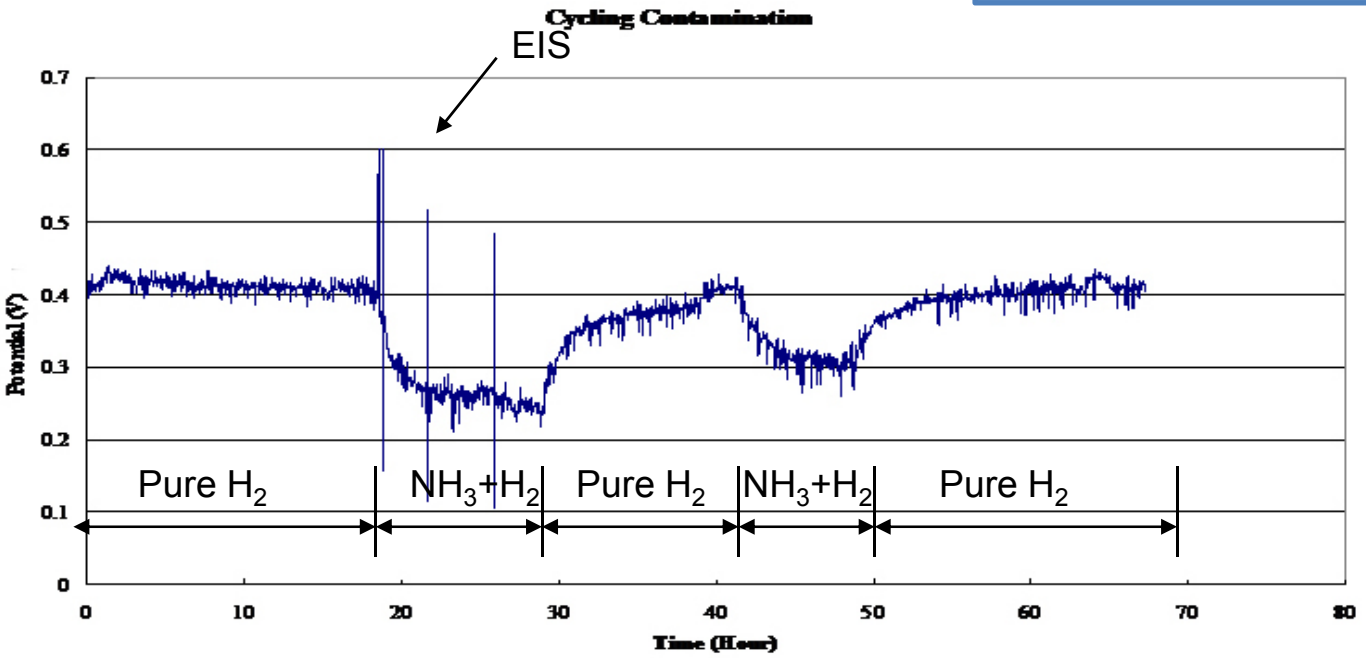
Ammonia (NH_3) Contamination

Current density: 1000 mA/cm^2

Cell: 52 C, Dew Points: 50/50 C

Pressure: Ambient

Early Hydrocarbon Studies Showed No Effects on Fuel Cell Performance. Per Tech Team Suggestion We Tested Ammonia to Evaluate an Impurity That Was Known to Show Some Effect - Ammonia.



25 ppm NH_3 introduced in H_2 causing serious degradation.
Cycling contamination tests showed the cell performance can be recovered.

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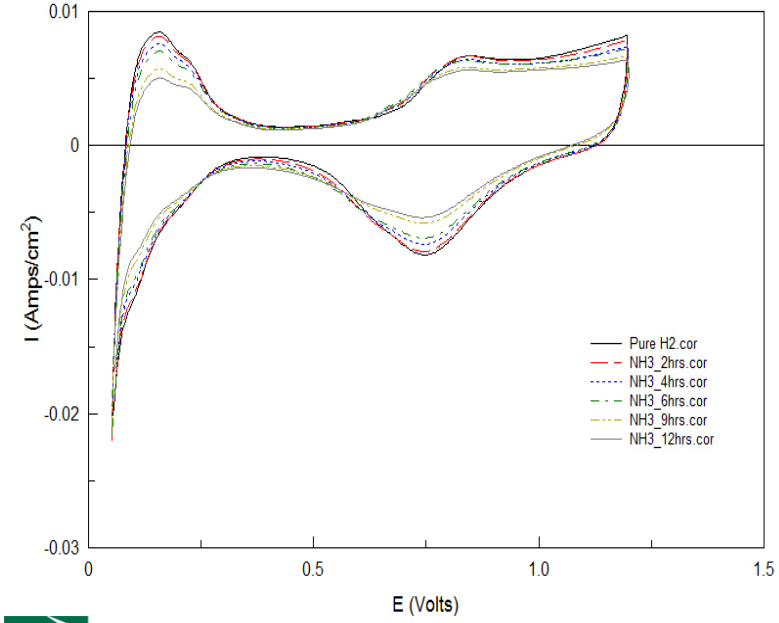
Other Impurities

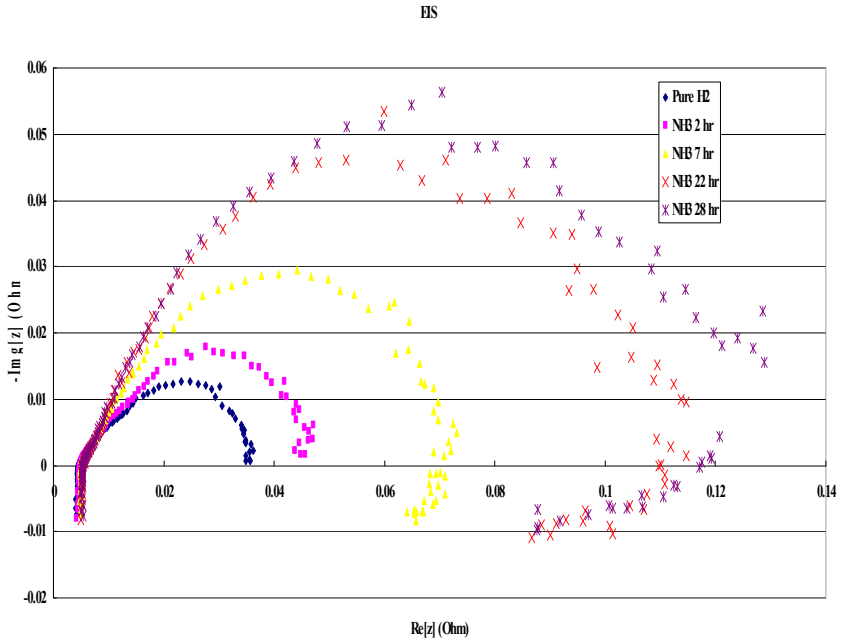
Electrochemical Characterization of the Effect of Ammonia

Cyclic Voltammetry (CV); Electrochemical Impedance Spectroscopy (EIS)

CV scans: 20 mV/s, 0.05 -1.2 V
Anode: 25 ppm NH_3 + H_2 Cathode: N_2
RH: 80%
Brief conclusions: H_2 absorption and Pt oxidation peaks decreased after introducing a trace amount



In-situ EIS scans (shown in the previous slide) show that NH_3 contaminated both Nafion® membrane and the electrodes. Both the membrane and the charge transfer resistances increased.



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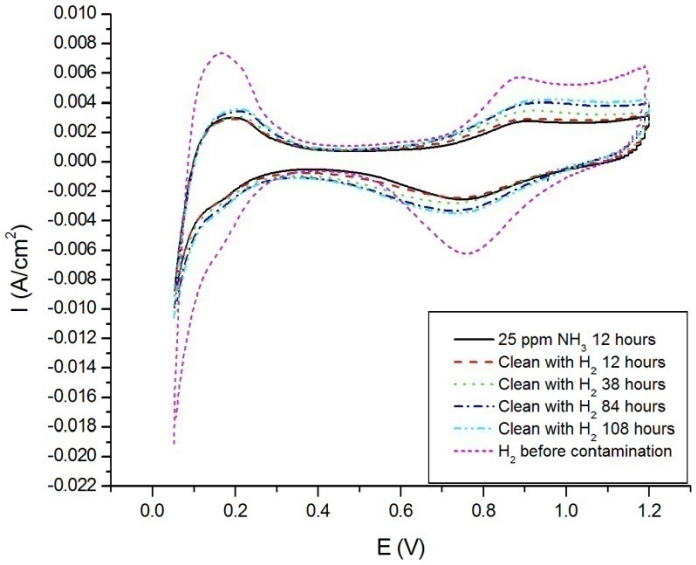
Other Impurities

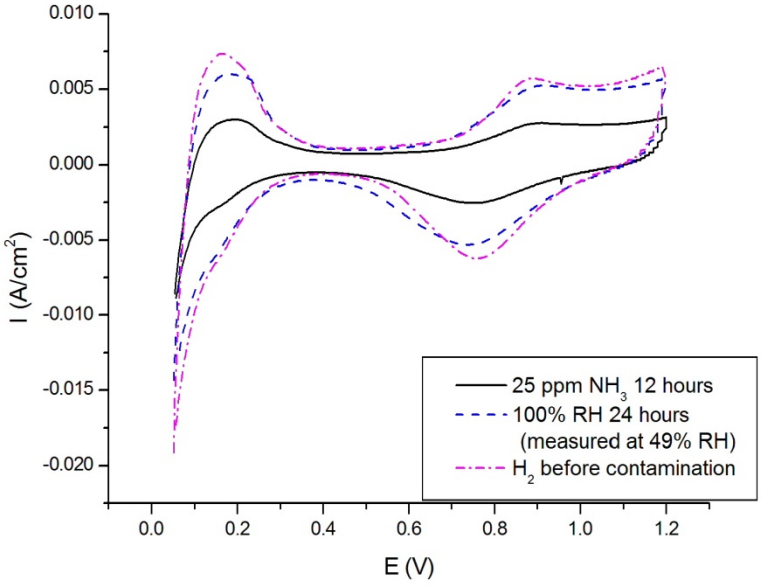
Recovery After Contamination by Ammonia

CV scans: 20 mV/s, 0.05 -1.2 V
Anode: pure H_2, Cathode: N_2
RH=29%, 49%, 80%

CV scans show at low RH (<50%), cell could hardly recover just by purging pure H_2 at the anode.



After staying at RH 100% for 24 hrs, recovery is greatly improved, but still not 100%.



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Impurities Modeling

- Why Modeling?
  - Helps understand the mechanisms via which impurities affect the fuel cell performance.
  - Helps predict the fuel cell behavior under the influence of impurities.
    - How much performance degradation is expected?
      - For how long does the cell generate reasonable current under certain amount of impurities?
    - How is the durability is affected?
  - Assists the experimental design

- Our Strategy
  - Derive the equations which represent the transport of the impurities in the fuel cell
    - i.e. where are the impurities?
  - Derive relations for how the impurities affect the cell behavior
    - i.e. impact of conduction of protons, available catalyst surface for H_2 oxidation
  - Validate these relations and equations
  - Incorporate these equations/relations in our 3D modeling framework

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Cation Transport Across the PEM

- Multi-Component Formulation

- Nernst-Planck Equation

$$\nabla \cdot \left(-D_i \nabla c - z_i u_{m,i} F c_i \nabla \phi \right) = R_i$$

with electro-neutrality condition:

$$\sum z_i c_i = 0$$

results in ionic charge conservation:

$$\sum_{i=1}^{n} \left[F z_i \left(-D_i \nabla c - z_i u_{m,i} F c_i \nabla \phi \right) \right] = \sum_{i=1}^{n} \left(F z_i R_i \right)$$

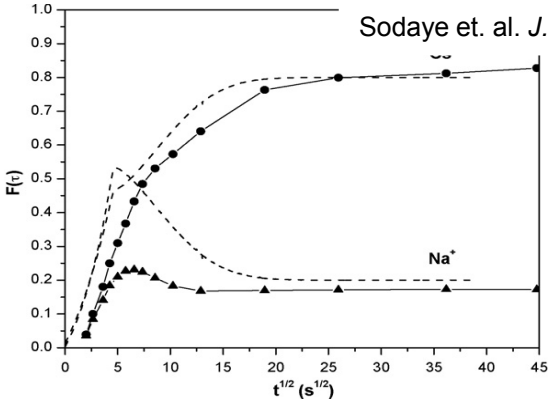
- Multi-component mass balance;

$$-\frac{x_i}{RT} \nabla \mu_i - x_i z_i \frac{F}{RT} \nabla \phi = \sum_{j=1, j \neq i}^{n} \frac{x_j N_i - x_i N_j}{c_{tot} D_{ij}}$$

where $-\frac{x_i}{RT} \nabla \mu = -\sum_{j=1}^{n-1} \Gamma_{ij} \nabla x_i$ *Thermodynamic Correction Factor*

and $\sum_{j=1, j \neq i}^{n} \frac{x_j N_i - x_i N_j}{c_{tot} D_{ij}} \equiv \sum_{j=1}^{n-1} B_{ij} N_i$

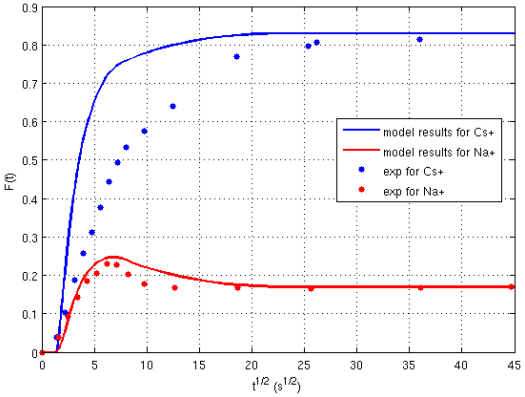
$$-[\Gamma](\nabla x) - \frac{F}{RT}[x][z](\nabla \phi) = [B](N)$$



Sodaye et. al. *J. Membrane Sci.* (2008).

Competitive absorption of Na^+ and Cs^+ into a H^+ form Nafion®

F(τ) is the fractional attainment of equilibrium by each species.



Multi-component mass transport formulation better predicts the competitive absorption.

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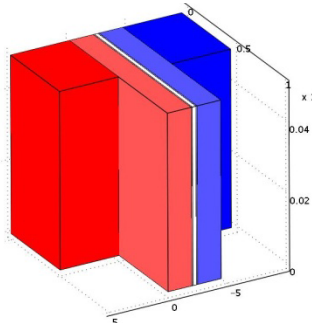
Cationic Impurity in Operating PEFC

-Na^+ in the Cathode

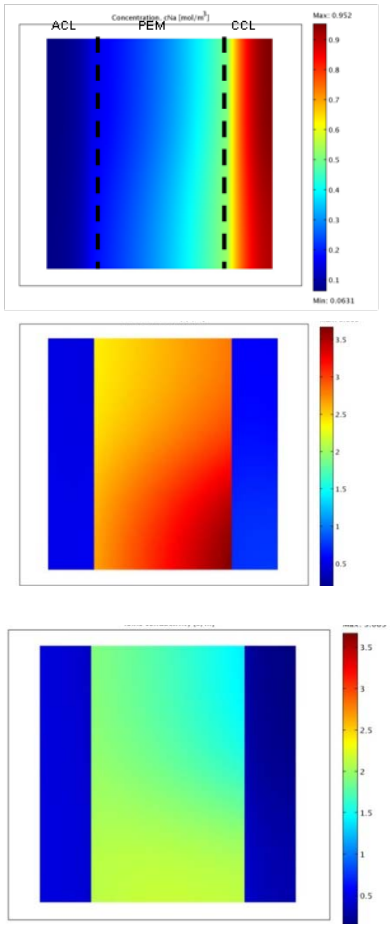
- Multi-physics PEFC Model
  - 3D, transient: COMSOL
  - *Multi-physics:* Mass, momentum, species, energy, charge cons., EC kinetics
  - Solid mechanics: Impact of cations on mechanical stress (durability)



Single-straight channel, 50% RH, 80°C, high stoich.

PEM: 25.4 μm, 1100 EW

NaCl is fed through the air stream.



Na^+ Distribution:

Migration and diffusion fluxes are in reverse direction and almost cancel each other.

Effective Proton Conductivity:

← Uncontaminated

Predicted output:
0.42 A/cm^2 @ 0.7 V

← Contaminated

Predicted output:
0.29 A/cm^2 @ 0.7 V

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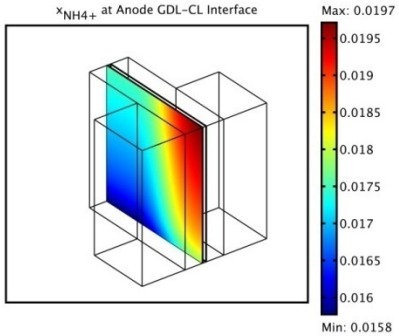
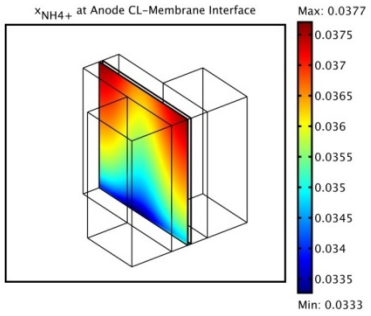
Cationic Impurity in Operating PEFC:

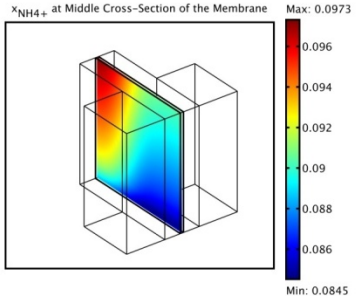
-NH_4^+ Distribution in Steady-State



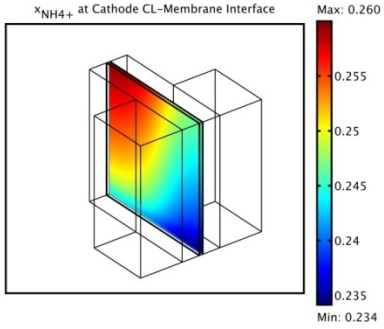
Anode DM-CL interface



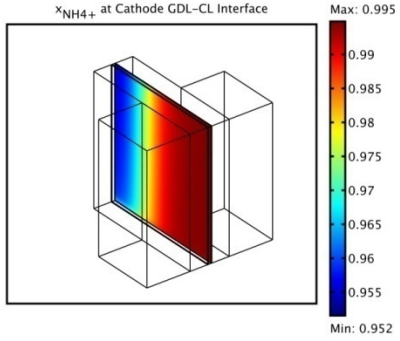
Anode CL-PEM interface



Center of the PEM



PEM-Cathode CL interface



Cathode CL- DM interface

- NH_3 is fed into anode, and is assumed to fully convert into NH_4^+.
- Migration and diffusion of NH_4^+ results in accumulation in the cathode catalyst layer.
- Model predicts a performance drop from 0.63 to 0.43 A/cm^2 at 0.7 V (due to loss of effective proton conductivity)

Transient models are being developed to investigate the recovery.

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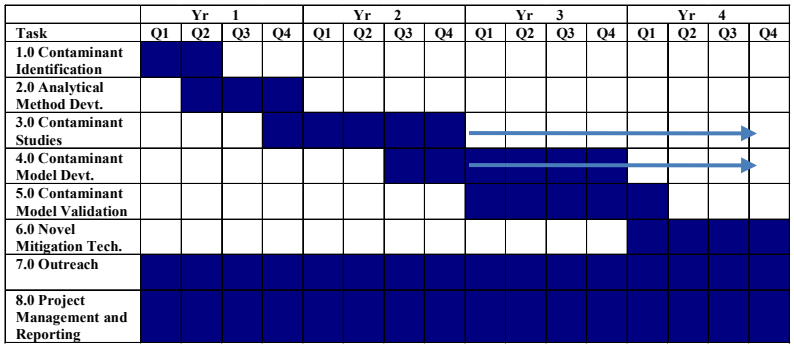
Collaborations

- Active Participant in Fuel Quality Working Group
- Collaborating With Other Test Laboratories on Topics of Mutual Interest (Fluids Mixing, MEA Quality Issues, Testing)
- Collaborating With Karren More (ORNL) on MEA Characterization
- Project Partners (UTC and FCE) Actively Supporting Project
- Working With NRC – Canada On Impurities Research Topics
- Have Visiting Scientist From an Automaker Working on Synergistic Topics

Future Work

- Comprehensive Evaluation of Formic Acid and Formaldehyde to Support ISO Standard Development
  - Continued Testing Using Standard Test Protocols, MEA's
  - Target Low Catalyst Loadings (Reduction From 0.4 mg/cm2 to 0.1 mg/cm2)
  - Develop an Understanding of Mechanism for Performance Impact
  - Modeling of Effects/Sharing of Data
- Extension to Simple Halogenated Compounds
- Continued Study of Effects of Cations on Membrane Properties
  - Application Relevant Contamination Types/Levels
  - Commercially Relevant Membranes
  - Modeling of Effects/Sharing of Data

Task	Milestone	Date Year/Quarter
1.0 Contaminant Identification	• Contaminant Identification Review With DOE Sponsor & Industry Focus Group	Y1/Q2
2.0 Analytical Method Development	• Validate Analytical Methods For Studying Contaminants With Ersatz Gases	Y1/Q4
3.0 Contaminant Studies	• Establish an Understanding of the Major Contamination-Controlled Mechanisms that Cause Material Degradation	**Ongoing**
4.0 Contaminant Model Development	• Determine the Relationship Between Contaminant Mechanisms and the Loss of PEM Performance, Especially Voltage Decay.	**Ongoing**
5.0 Contaminant Model Validation	• Validate Contamination Models Through Single Cell Experimentation Using Standardized Test Protocols and a DOE Approved Test Matrix	Y4/Q1
6.0 Novel Mitigation Technologies	• Demonstrate Novel Technologies for Mitigating the Effects of Contamination on Fuel Cell Performance	Y4/Q4
7.0 Outreach	• Dissemination of Results Through Reports (DOE Approved), Papers and Workshops	Continuous
8.0 Project Management and Reporting	• Program Written Reports and Program Reviews	Continuous



- 4 Year Project
- Time Phased Milestones Activities and Expertise

Project Summary

- Relevance - A Deeper Understanding of the Effects of Specific Contaminants on Fuel Cell Performance is Necessary for Successful Commercialization
- Approach - Our Experienced Team Is:
  - Leveraging Existing Knowledge and Systematically Investigate Certain Fuel Contaminants of Interest
  - Creating Empirical and Detailed Analytical Models to Predict the Fate of Specific Contaminants and Their Effect on Fuel Cell Performance
- Technical Accomplishments and Progress – Screened Several Hydrocarbon Species (Methane, Ethane, Ethylene, Acetaldehyde, Formic Acid) For Effects of Fuel Cell Performance. Developed Methods for Mixing/Analysis. Initiated Modeling. Investigated Effects of Cations on Performance.
- Technology Transfer/Collaborations - Data Shared Through Papers, Workshops, Hydrogen Fuel Quality Working Group, Etc., Active Partnership with UTC and FCE, Collaboration With ORNL on Characterization, Working With NRC-Canada on Impurities Issues, Visiting Scientist From an Automaker
- Proposed Future Research – Support ISO Efforts Through Comprehensive Evaluation of Formic Acid and Formaldehyde, as Well as Simple Halogenated Compounds. Continue Cation Studies Using Commercially Relevant Contaminant Loadings & Membranes.

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