# Effects of Impurities on Fuel Cell Performance and Durability

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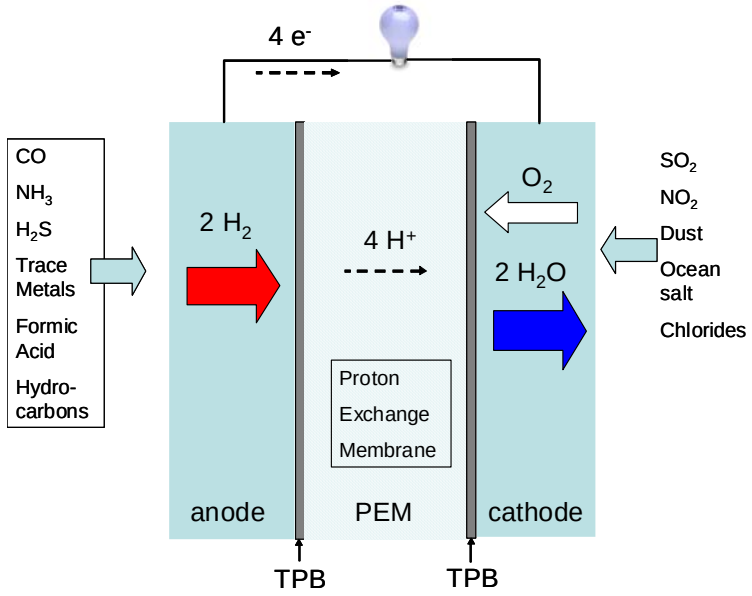
# Agenda

- Introduction
- Background/Technical Concept
- Project Objectives
- Project Work Plan/Deliverables
- Project Timetable
- Roles of Participants
- Facilities and Equipment
- Summary

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# Introduction

- **Cost and Durability of Fuel Cells are Important Barriers to Commercialization**
- **Contamination of Fuel Cells From Fuels/Oxidants Affects Both Cost And Durability**
- **General Effects of Certain Contaminants on Fuel Cell Performance and Durability are Known, But Empirical Relationships and Specific Performance Models are Not Well-Established**

| Contaminant Category | Examples | Fate of Contaminant | General Performance Effects |
|---|---|---|---|
| Large Cations | Fe, Cr, Ni | Broad Distribution Throughout Membrane | Increases Ionic Resistance |
| | Cu | Movement to Cathode/Membrane Interface During Operation | Contributes to Electrode Overvoltage |
| | Mg, Ca | Tends to Agglomerate in Membrane (Forms Rocks) | Increases Ionic Resistance, Causes Pinholing |
| Small Cations | Na+, Li+ | Broad Distribution Throughout Membrane, Move to Cathode During Operation | Increases Ionic Resistance, Reduces Water Content at Cathode Surface |
| Anions | Cl-, SO2-- | Movement to Anode | Sometimes No Effect |
| Organics | HCOOH, | Some Adsorbs on Catalyst Surface | Reduces Catalyst Activity |
| Inerts | N2, Ar | Some Adsorbs on Catalyst Surface | Functions as Diluent for Reactants |

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# Background/Technical Concept

- Initiate Studies by Leveraging Existing Database From Prior Work
  - DOE Sponsored Activity
  - USFCC Data
  - Prior Electrolysis Product Experience
- 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

| Contaminant | Affected Area | Contaminant Source |
|---|---|---|
| Stainless Steel<br>• Cr<br>• Ni<br>• Fe | Membrane Electrode Assembly (MEA) | Gas Diffusion Layer (GDL) Screen and Bipolar Plates |
| Silicon | Pt Catalyst Formed Under Pt Oxides | Gasket and Cooling Fluid |
| Sulfur | Pt Catalyst | Vulcanized Carbon in Catalyst |
| Sodium | Membrane | Membrane Impurities |
| Copper Chloride | Membrane Conductivity | Coating for Aluminum Bipolar Plate |
| $Ca^{2+}$ | Membrane | Membrane Impurity |
| Carbon Monoxide | Pt Catalyst | Gas Reactants |
| Sulfur Dioxide | Membrane | Air Near Battlefield |
| Benzene | Membrane | Air Near Battlefield |
| Ammonia | Membrane | Air Pollution |
| $SO_2$ | Catalyst | Air Pollution |
| HCN | Catalyst | Air Near Battlefield |
| CNCl | Catalyst | Air Near Battlefield |
| Sarin | Catalyst | Air Near Battlefield |
| Sulfur Mustard | Catalyst | Air Near Battlefield |
| Acetaldehyde | Catalyst | Byproduct of Ethanol Fuel Source |

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# Project Objectives

| 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.<br>• Experimental design of analytical studies.<br>• Novel *in situ* detection methods. |
| **3.0 Contaminant Studies** | • Develop contaminant analytical models that explain these effects.<br>• 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<br>• 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. |

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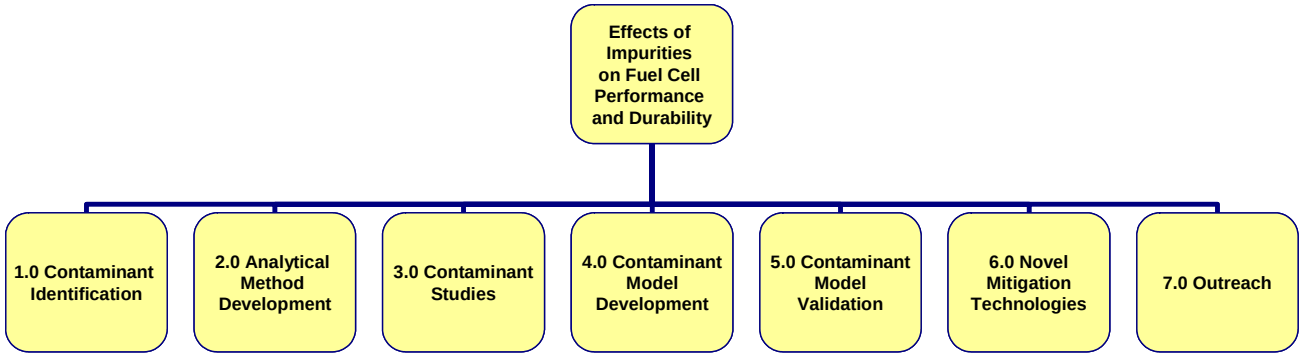
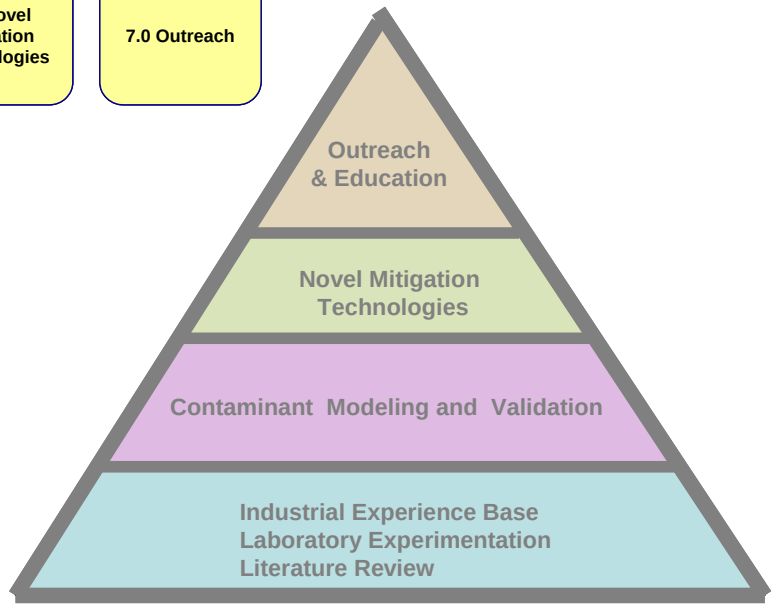
# Project Work Plan/Deliverables




Deliverables

- Validated Contaminant Models
- New Mitigation Technologies

Outreach: Papers, Workshops, Technical Interchange, Etc.

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# Project Timetable

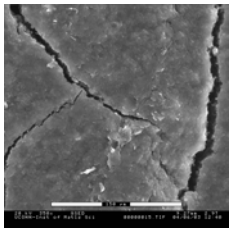
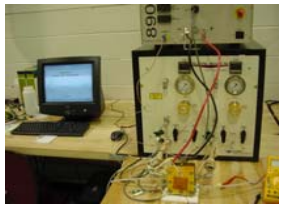
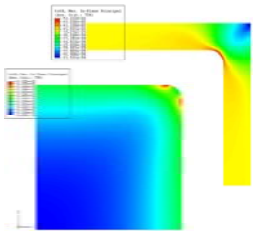
| | Yr 1 | | | | Yr 2 | | | | Yr 3 | | | | Yr 4 | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Task** | **Q1** | **Q2** | **Q3** | **Q4** | **Q1** | **Q2** | **Q3** | **Q4** | **Q1** | **Q2** | **Q3** | **Q4** | **Q1** | **Q2** | **Q3** | **Q4** |
| **1.0 Contaminant Identification** | ■ | ■ | | | | | | | | | | | | | | |
| **2.0 Analytical Method Devt.** | | ■ | ■ | ■ | | | | | | | | | | | | |
| **3.0 Contaminant Studies** | | | | ■ | ■ | ■ | ■ | ■ | | | | | | | | |
| **4.0 Contaminant Model Devt.** | | | | | | | ■ | ■ | ■ | ■ | ■ | ■ | | | | |
| **5.0 Contaminant Model Validation** | | | | | | | | | ■ | ■ | ■ | ■ | ■ | | | |
| **6.0 Novel Mitigation Tech.** | | | | | | | | | | | | | ■ | ■ | ■ | ■ |
| **7.0 Outreach** | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ |
| **8.0 Project Management and Reporting** | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ |

- 4 Year Project
- Time Phased Milestones Activities and Expertise

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

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# Task Participants

Program Lead
T. Molter
CGFCC/UConn

Task 1.0 Team Leader
Contaminant Identification and Characterization
Nigel Sammes
CGFCC/UConn

Task 2.0 Team Leader
Analytical Method Development
Steven Suib
IMS/UConn

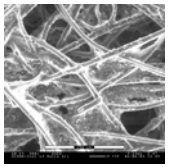
Task 3.0 Team Leader
X. Huang
Contaminant Studies
CGFCC/UConn

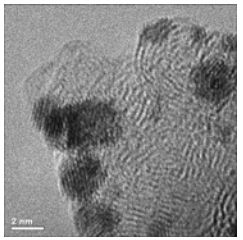
Task 4.0 Team Leader
U. Pasaogullari
Contaminant Model Development
CGFCC/UConn

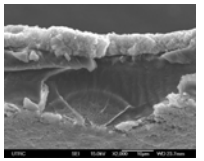
Task 5.0 Team Leader
K. Reifsnider
Contaminant Model Validation
CGFCC/UConn

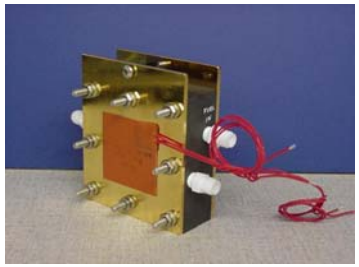
Task 6.0 Team Leader
B. Wilhite
Novel Mitigation Methods
CGFCC/UConn

Task 7.0 Team Leader
T. Molter
OUtreach









# Facilities and Equipment

- **16,000 Ft$^2$ Facility**
- **4 – 24 Foot High Bay Test Areas With Air/Water/Ventilation, Overhead Doors and a 220/480 Electrical Bus**
- **4 Physical Wet-Lab Areas With Air/Water/Ventilation and 110/220 Electrical Service**
- **2 Classrooms**
- **Conference Room**
- **Administrative Offices**
- **Access to Main Campus Facilities Including the Institute for Materials Science**

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# Facilities and Equipment

- **Analytical Capabilities at UConn's Institute for Materials Science Will Be Leveraged to Support This Activity**
  - **Surface Studies**
  - **Gas Analysis**
- **Additional Capabilities at FuelCell Energy/UTC Will Be Leveraged to Support Program Activities As Required**




| Surface | Optical | Catalysis |
|---|---|---|
| Leybold XPS/SIMS/AES/ISS Spectrometer | Nicolet 750 FTIR, Near, Mid and Far Regions | *In Situ* Photoreactors |
| Leybold XPS/ISS/TPD Spectrometer | Spex Raman | Transient Reactor with Nuclide Mass Spec./GC |
| PHI 610 SAM | Spex Fluorolog | Batch and Flow Thermal Reactors |
| PHI Monochromatic XPS | ISA/JY CCD Spectrometer | HP GCMS |
| Nanoscope 4 AFM/STM | Raman Imaging | |
| | | |
| **Structural** | **Thermal** | **Analytical** |
| Scintag XDS 2000 Diffractometer, *in Situ* Heating Stage | DuPont TGA | Inductively Coupled Plasma Mass Spec. |
| In Situ XRD | DSC | Fast Atom Bombardment Mass Spec. |
| Thermo ARL/Anton Parr | Cahn Balance | Energy Dispersive X-Ray Analyzer |
| | Home-Built Temperature Program Desorption/Reduction/Reaction | GCMS |
| **Sorption** | Home-Built Microbalance | TOF Maldi MS |
| Omnisorp and Micromiretics BET | | Atomic Absorption |
| | | |
| **Morphological** | **Magnetic** | **Chromatography** |
| JEOL 2010 FasTEM HRTEM | Varian E-3 EPR | ISCO HPLC System -Single-Pump Ternary Gradient Programmer, Programmable Pump -V $^4$ Variable UV/VIS Detector. |
| Philips EM400T Transmission Electron Microscope | X/Q Band Bruker Spectrometer | HP6890 GC Equipped With TCD and FID Detectors |
| Nikon Optical Metallurgical Microscope | Spin Echo NMR | HP6890 GC With Sulphur Specific PPD |
| AMRAY 1810 D SEM | Vibrating Sample Magnetometer | |
| JEOL 6335F FESEM | | |
| AMRAY 9800 EDX | | |






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# Summary

- **Contaminants Affect Fuel Cell Performance in Many Ways**
- **A Deeper Understanding of the Effects of Specific Contaminants on Fuel Cell Performance is Necessary for Successful Commercialization**
- **Our Experienced Team Will Leverage Existing Knowledge and Will Systematically Investigate Certain Fuel Contaminants of Interest**
- **Empirical and Detailed Analytical Models Will Be Created to Predict the Fate of Specific Contaminants and Their Effect on Fuel Cell Performance**
- **Data Will Be Shared Through Papers, Workshops, Working Groups, Etc.**