National Renewable Energy Laboratory
Innovation for Our Energy Future

Effect of System and Air Contaminants on PEMFC Performance and Durability

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Objectives

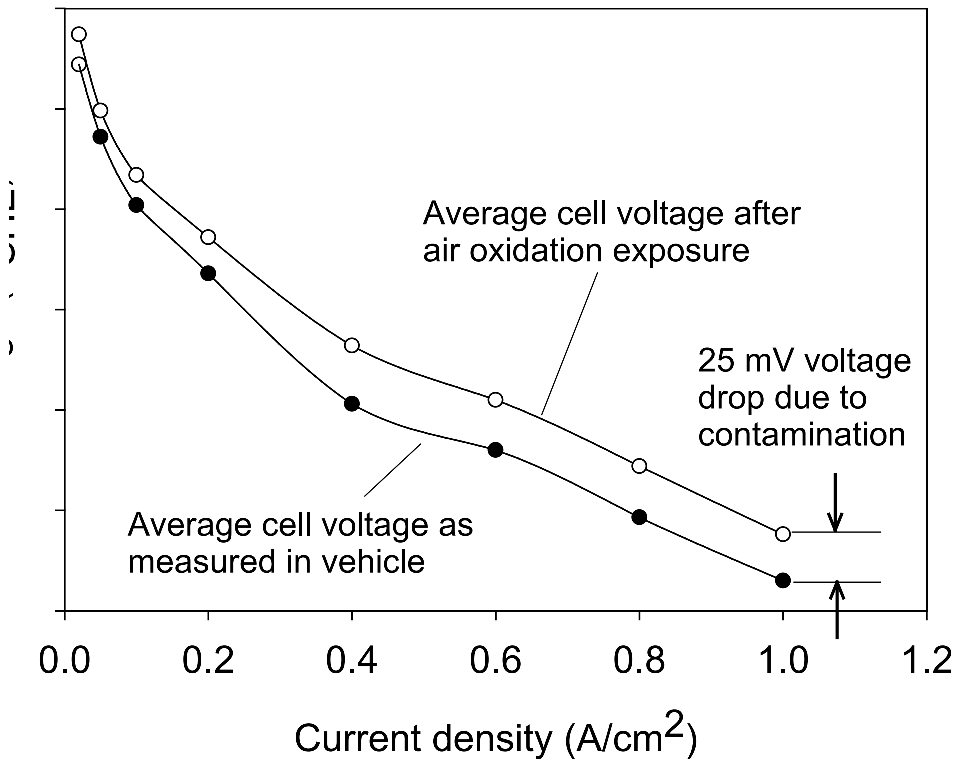
To assist the DOE Fuel Cell Technologies (FCT) Program in meeting cost, durability, and performance targets in the areas of fuel cell systems. The effort is focused on system-derived contaminants, but has a small component addressing "gaps" in the area of air contaminants.

Table 3.4.2 Technical Targets for Automotive Applications: 80-kW$_e$ (net) Integrated Transportation Fuel Cell Power Systems Operating on Direct Hydrogen [a]					
Characteristic	**Units**	**2003 Status**	**2005 Status**	**2010**	**2015**
Cost [d]	\$ / kW$_e$	200	110 [e]	45	30
Durability with cycling	hours	N/A	~1,000 [g]	5,000 [h]	5,000 [h]

Table 3.4.4 Technical Targets [a]: Integrated Stationary PEM Fuel Cell Power Systems (5-250kW) Operating on Reformate				
Characteristic	**Units**	**2003 Status**	**2005 Status**	**2011**
Cost [e]	\$ / kW$_e$	2,500	2,500	750
Durability @ <10% rated power degradation	hours	15,000	20,000	40,000

Premise

System-derived contaminants can have negative effect on fuel cell performance.



Average cell performance of a 90kW fuel cell stack after 850+ hours of use in test vehicle. The cell performance improved after exposure to oxidation. The 25 mV voltage loss is attributed to system-based contaminants because similar stacks run on lab test stands (known to be free from contaminants) did not show such voltage loss.

Approach

Primary focus on the effect of commercially-relevant system-derived contaminants on fuel cell performance and durability. System contaminants have been studied little (compared to H_2 quality or air contaminant effects, although some mechanisms are similar), and have significant sources for potential contamination.

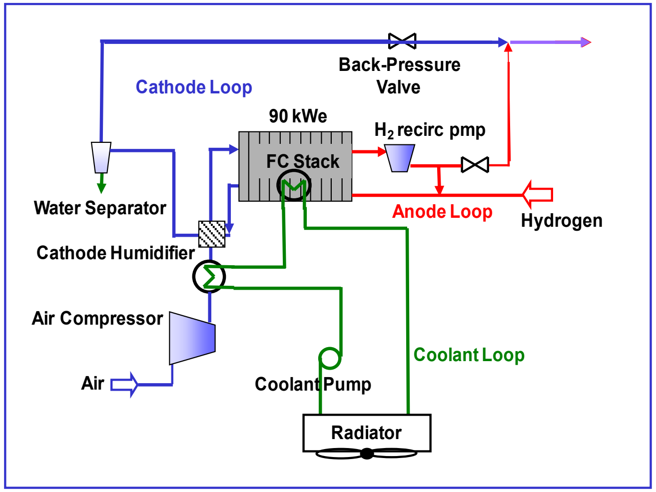


Figure. 1. Typical automotive fuel cell system, which requires the components of Table 1.

Table 1. Typical "gas wetted" components used in a PEMFC system.

Air management	Fuel management	Stack	Integration
Compressor	Gas metering	Bipolar plates	Stack manifolds
Humidifier	Recirculation pump	Seals/sealants	Seals/sealants
Heat exchanger	Valves	Subgaskets	Conduits/hoses
Valves	Sensors	Membrane	
Sensors	Seals/sealants	Electrodes	
Seals/sealants	Conduits/hoses	Insulators and ports	
Conduits/hoses		Seals/sealants	
		Conduits/hoses	

Approach

Many of the system components can be made with different polymers and additives. Proper selection and specification of additives are critical for balancing cost, PEMFC system performance, and durability.

Table 2A. Examples of polymer classes with generalized costs for the system

PSU>PC>PBT>PPS>PPA>PA>PPO>POM>PET>PU>UP>Phenolic>Melamine>ABS>PS>PE>PP>PVC

Higher cost → Lower cost

Table 2B. Examples of common additives in automotive thermoplastics

Glass fiber sizing	Primary antioxidant	Secondary antioxidant	UV stabilizer	Flame retardant	Processing aids	Biocides	Other
Vinyl silane	Hindered phenols	Organophosphates	Hindered amines	Antimony oxide	Calcium stearate	Triclosan	Residual monomer
Amino silane	Organotins	Thio esters	Benzophenones	Borates	Amide wax	Oxy-bisphenoxarsine	Catalysts
Mercapto silane	Mercapto-		Hydroxyphenyl	Bromates	Oligomeric wax		Residual solvents
Epoxy silane	benzoimidizoles		benzotriazoles	Phophates	Fatty acid amides		
					Glycerides		

Background

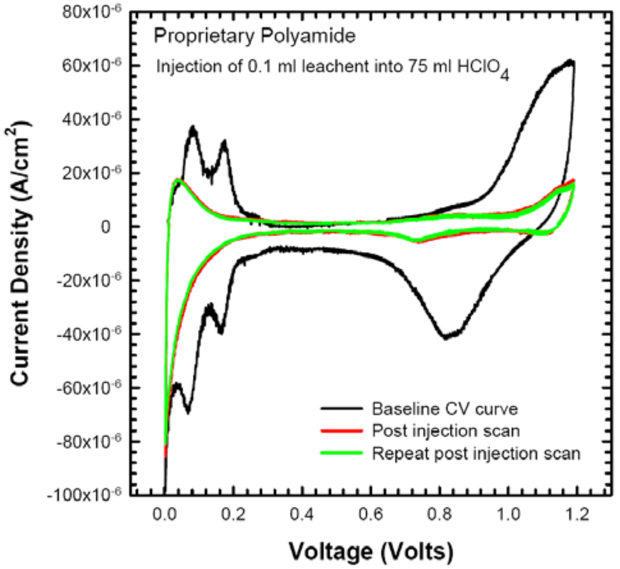
Have begun identifying system-based contaminants and test protocols to study impact of system contaminants on performance.

Table 3A. Table of identified organic leachants from stacks and systems.

Organics
Acetone
2 propanol
Trimethysilanol
3-pentenone
Hexamethylcyclosiloxane
2,2,5,5,tetramethyltetrahydro-3-ketofuran
Styrene
Benzaldehyde
Silicone
2-propyl-1-pentanol
Acetophenone
Dodecamethylcyclopentasiloxane
Dodecamethylcyclohexasiloxane
Ions
K, P, Si, Acetate

Table 3B. Ten most significant organic leachants found in a composite bipolar plate material.

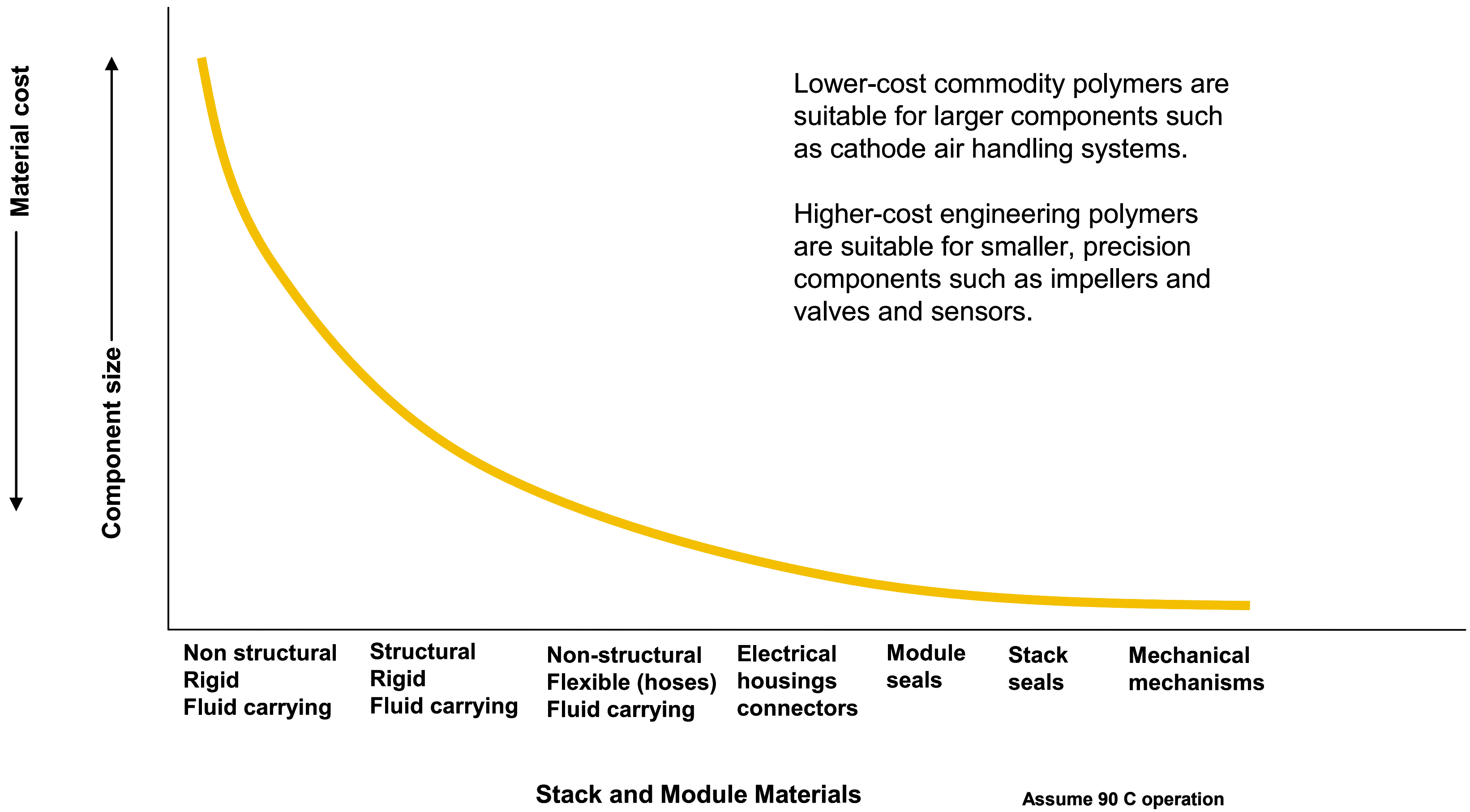
Group	Identified Compound	Tested Model Compound
Group I	2-Methyl-2-Propanol	t-Butyl Alcohol
Group II	Dimethyl Butanedioic Acid	Dimethyl Succinate
	Dimethyl Pentanedioic Acid	Dimethyl Glutarate
	Dimethyl Hexanedioic Acid	Dimethyl Adipate
Group III	2-Propanone	Acetone
Group IV	Ethenylbenzene	Styrene
	Cyclopentacycloheptene	Azulene
Group V	2,2,7,7-Tetramethyloctane	
Group VI	1-Methyl-2-Pyrrolidinone	
	2-Oxazolidinone	



CV of Pt in 75 mL of 0.1 M perchloric acid with and without leachant at 23°C.

Approach

Study fuel cell stack and system components to understand system contaminants through both in-situ and ex-situ testing. Determine test methodologies and materials catalogues that benefit the fuel cell industry in making cost-benefit analyses of system components.

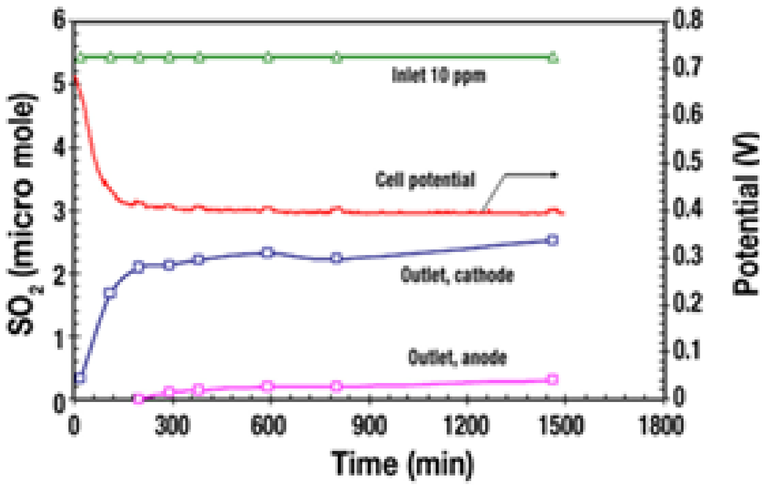


Air contaminants (SO_x & NO_x)

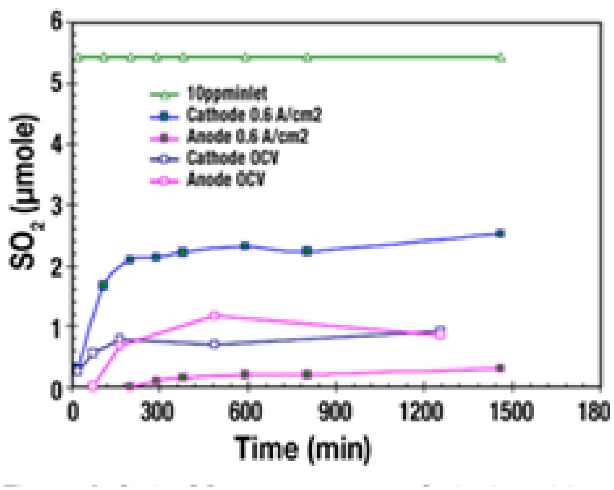
Address data gaps needed for predictive models, including identifying impact of operating conditions and liquid water.

Conduct ex-situ and in-situ tests to determine kinetic parameters and rate constants

Develop models to understand the implications of extended operating times, mitigation strategies, and mass transport related aging effects.



SO_2 measurement of cathode and anode exhaust during SO_2 exposure.



Material balance comparison between OCV and 0.6 A/cm^2.

Approach

Parametric studies of the effect of poisons on cell performance and durability

- *Identify fundamental classes of contaminants*
- *Develop and validate test methods*
- *Identify severity of contaminants*
- *Identify impact of operating conditions*

Identification of poisoning mechanisms and recommendations for mitigation

- *Identify poisoning mechanisms*
- *Identify and investigate mitigation strategies*

Models of contaminant effects on cell performance and durability

- *Develop models/predictive capability*
- *Validate models*

Compilation and public dissemination of the data generated during the course of the project

- *Provide guidance on future material selection*
- *Publish papers and participate in working groups*

Overview

Timeline

Start: July 2009

End: September 2013

% complete: 2%

Budget

DOE Cost Share	Recipient Cost Share	TOTAL
$6,000,000	$788,850	$6,788,850*
88%	12%	100%

DOE Budget ($K)

FY 2009	974
FY 2010	620
FY 2011	1438
FY 2012	1476
FY 2013	1492

***Final award amounts are subject to appropriations and award negotiations.**

Partners

General Motors Company (GM)

University of South Carolina (USC)

Los Alamos National Laboratory (LANL)

University of Hawaii (HNEI)

3M

Project Timeline/Structure

Tasks	Y1				Y2				Y3				Y4			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
1. Parametric studies of the effect of poisons on cell performance and durability																
1.1 Identify fundamental classes of contaminants																
Are there system contaminants that do not need further study?								G								
Compile comprehensive list of identified, plausible polymeric and non-polymeric families for fuel cell systems								M								
1.2 Develop & validate test methods																
Establish ex-situ and in-situ test protocols												M				
1.3 Identify (quantify) severity of contaminants																
Report on combined system and fuel impurity studies												M				
1.4 Identify impact of operating conditions																
Is SO2 data set complete to allow fully predictive modeling to be accomplished? If so, then cease SO2								G								
Provide model relevant data on FC performance in pressence of system contaminant, model compound or mixture																M
2. Identification of poisoning mechanisms and recommendation for mitigation																
2.1 Identify poisoning mechanisms																
Determine effect of cation contaminant on performance loss												M				
Correlate between mass transport properties of contaminants in GDLs to performance loss																M
2.2 Identify and investigate mitigation strategies																
Determine fuel cell contaminant tolerance levels								M								
Identify materials that can and cannot be used in fuel cells																M
Are employed remediation methods effective at improving durability?								G								
3. Modeling																
3.1 Develop models and predictive capability																
Does liquid water have significant impact on contaminant related performance losses?								G								
Does the model have good agreement with experimental data?										G						
3.2 Validate Models																
4. Compilation and public dissemination of the data generated																
4.1 Provide guidance on future material selection																M
4.2 Publish papers and participate in working groups																

Project Participants

Contaminant identification (GM, 3M#)

Test method development & validation (NREL, GM, USC)

Contaminant characterization (GM, NREL, USC, LANL, HNEI*)

Poisoning mechanisms identification (NREL, GM, USC, LANL, HNEI*)

Mitigation strategies investigation (NREL, GM, USC)

Model Development (USC)

Model validation (USC, GM, NREL)

Data compilation and public dissemination (NREL, GM, USC, LANL, HNEI)

provide small molecule analogues and degradation products from membranes

* Segmented cell work