2018 DOE H_2 and Fuel Cell Annual Merit Review Meeting

Innovative Bilayer Microporous Layer for PEM Fuel Cells

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Newton, MA

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Project#
FC193

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Project Overview

Timeline

- Project Start Date: 4/9/2018

  Project End Date: 1/8/2019

Budget

- Total Project Value
  - Phase I: $149,973.00
  - Spent: $0 (as of 4/17/18, project not started yet)

Project Nature

- DOE Small Business Innovation Research (SBIR)

Barriers

- Mass transport and water management in PEM fuel cell
- Balance to alleviate flooding issue as well as to prevent drying out of the membrane

Partners

- University of South Carolina (USC): Dr. Sirivatch Shimpalee

Giner Researchers

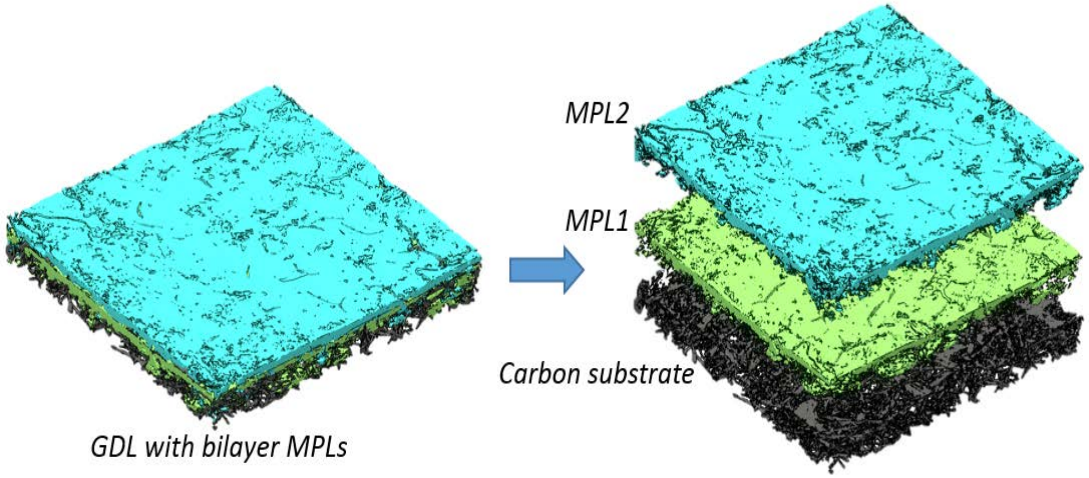
- Magali Spinetta, Zach Green, and Tom McCallum

Relevance

Objectives:

- Design bilayer microporous layer (MPL) - based gas diffusion media (GDM) with controllable pore size gradient and hydrophilic/hydrophobic gradient; and achieve properties better than commercial GDLs/GDMs, including thermal conductivity, electrical conductivity and mass transport
- Identify key design parameters for bilayer MPL using macro-scale PEMFC model and micro-scale transport model to support design and fabrication
- Demonstrate improved water management and better performance from in-situ testing under both wet and dry conditions, targeting performance improvement of 20% at current densities higher than 1.0 A/cm^2
- Conduct preliminary cost analysis of manufacturing scale-up of bilayer MPL-based GDMs

Technical Approach



Pore Size	Hydrophobicity
small	hydrophilic
↓	↓
large	hydrophobic

- Commercially available hydrophobic polymer binders will replace PTFE for the MPL1 hydrophobization → eliminates the use of surfactant, avoid the very high temperature heat treatment

- Non-aqueous ionomer with short side chain & low equivalent weight (EW) to provide hydrophilicity in MPL2 → improved ink rheology for casting, more hydrophilic than Nafion to provide desirable hydrophilicity with reduced content in the layer.

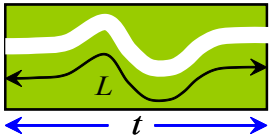
GDL Background

The gas diffusion layer (GDL) is one the most important components in the fuel cell. It transports gas, water, heat, and electrons.

- Thermal conductivity
- Electrical conductivity
- Gas permeability
- Hydrophobicity
- Water permeability

•Tortuosity

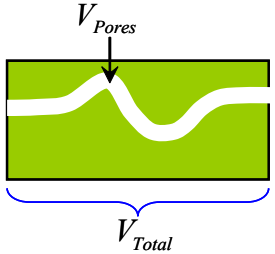
– Ratio of the actual path length through the pores to the shortest linear distance between two points.



$$\tau = \frac{L}{t}$$

•Porosity

– Ratio of void volume (volume of pores) to the total volume.



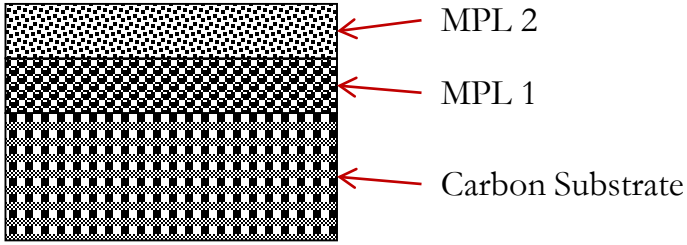
$$\varepsilon = \frac{V_{Pores}}{V_{Total}}$$

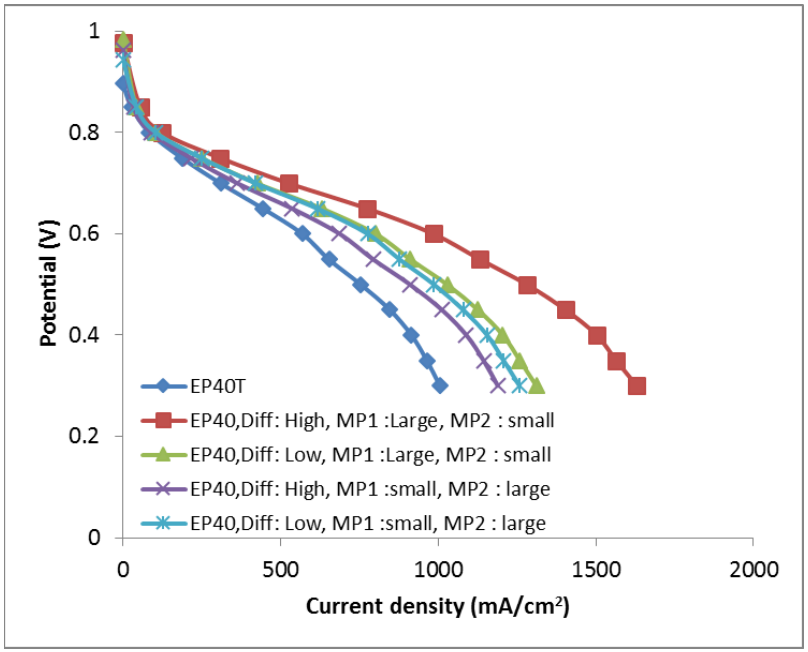
•MacMullin Number

– Function of tortuosity and pososity.

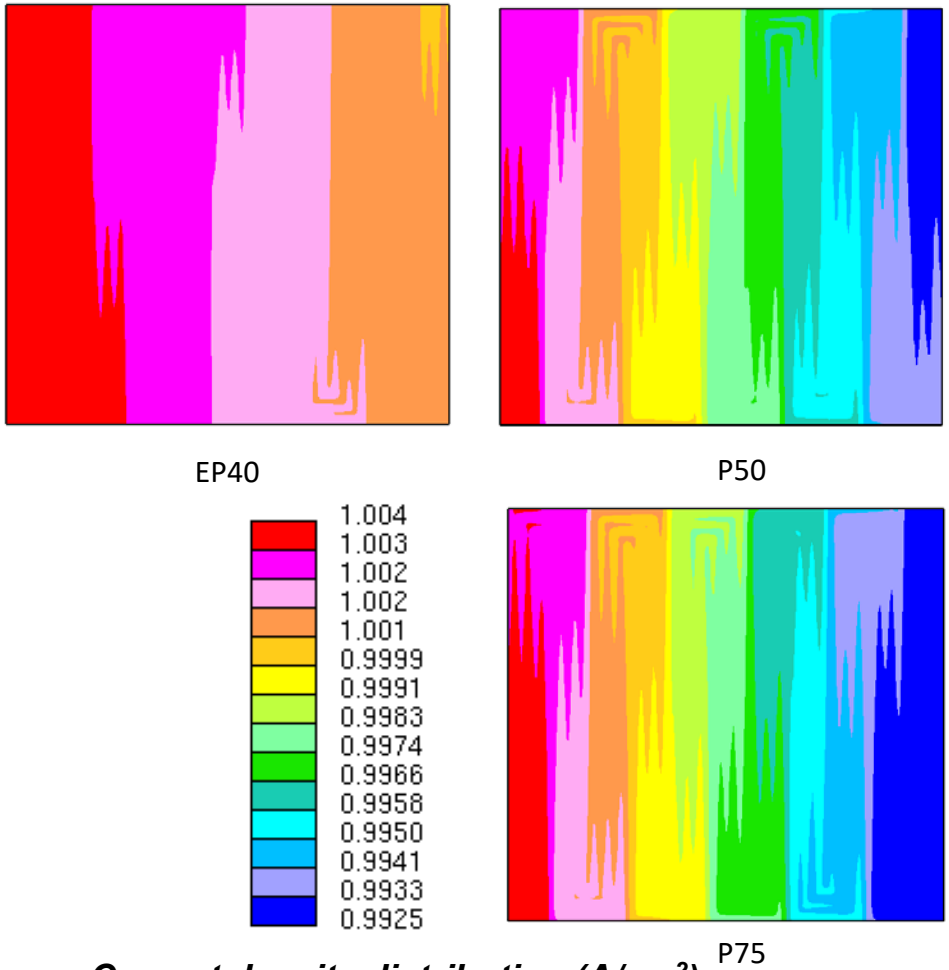
$$N_M = f(\tau, \varepsilon) = \frac{\tau^n}{\varepsilon^m}$$

GDL Background





*The effect of transport properties of GDL and bilayer MPL on local current density distribution. **

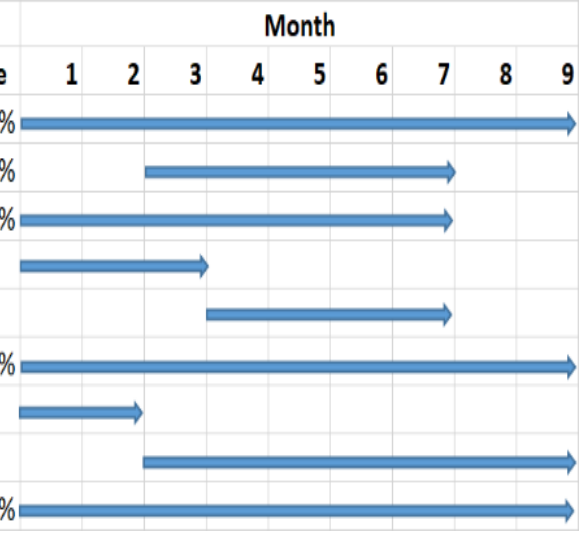


Current density distribution (A/cm²)

* S. Shimpalee, V. Lilavivat, H. Xu, C. K. Mittlesteadt, Y. Khunatorn, "Experimental Investigation and Numerical Determination of Custom Gas Diffusion Layers on PEMFC Performance," Electrochimica Acta, 222, 1210-1219, 2016

Tasks and Milestones

Task Name	% fo time
Task 1: Perform macro scale & micro scale model of transport inside GDMs	20%
Task 2: Fabricate bilayer MPLs with controllable pore sizes and hydrophillic/hydrophobic gradient	30%
Task 3: Ex-situ characterization of these bilayer GDMs	30%
3.1 Develop required tools for ex-situ characterization	
3.2 Measure all the GDMs' ex-situ properties of interests	
Task 4: In-situ performance fuel cell testing under various operating conditions	15%
4.1 Performance using baseline GDMs and GDLs	
4.2 Perofmrance using novel bilayer MPLs	
Task 5: Preliminary cost analysis of manufacturing scale up bilayer GDLs.	5%



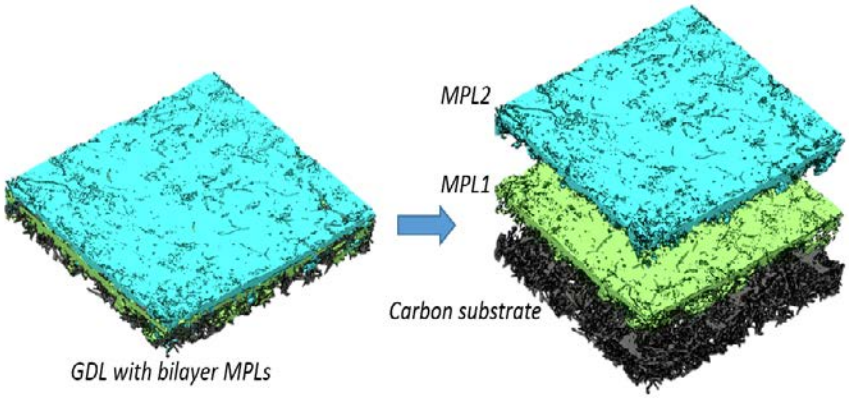
Milestone 1 (M4): Identify key design parameters in bilayer MPL using macro scale PEMFC model, and micro scale of transport model to support and validate bilayer MPL design and fabrication.

Milestone 2 (M7): Design bilayer MPL-based GDMs with controllable pore size gradient and hydrophilic/hydrophobic gradient, and achieve better ex-situ characterization properties compared with commercial GDLs/GDMs, including the thermal conductivity, electrical conductivity and mass transport properties etc.

Milestone 3 (M9): Demonstrate improved water management and better performance from in-situ testing under both wet and dry conditions, targeting at performance improvement by 20% at current densities higher than 1.0 A/cm^2.

Macro scale PEMFC model & micro scale of transport model

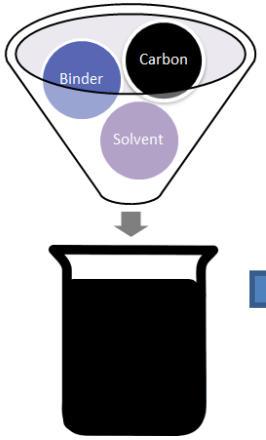
- To use a macro-scale conventional computational fluid dynamics (CFD) model with PEMFC submodel to gain understanding of overall performance and local distributions of PEMFC with standard GDL and GDL with proposed bilayer MPL → **To provide guidance in choosing baseline substrate and standard MPL before producing bilayer MPL samples.**

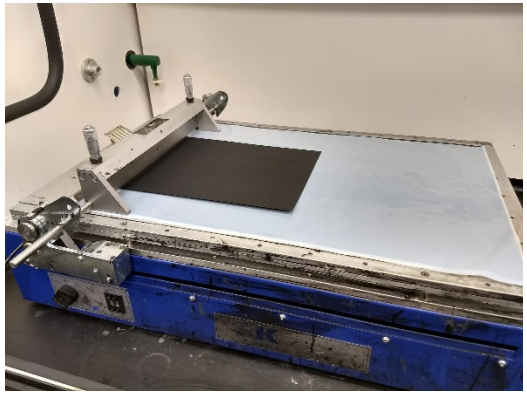


Three dimensional images showing the structure of GDL and bilayer MPL from 3D-XRay and SEM and the transport properties of bilayer MPLs from characterization methods.

- A Lattice Boltzmann Method (LBM) will be introduced to represent condensed water flow and understand the process by which water permeates through the GDL and bilayer MPL → **The outcome of this subtask will guide us in improving and engineering the bilayer MPL and confirm the feasibility of this project.**

MPL Fabrication

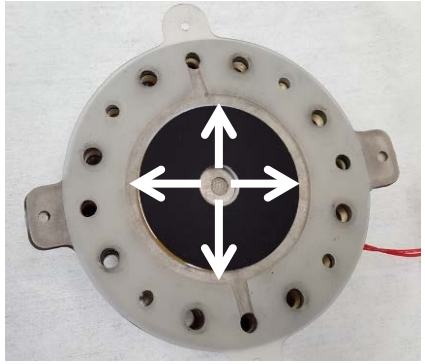




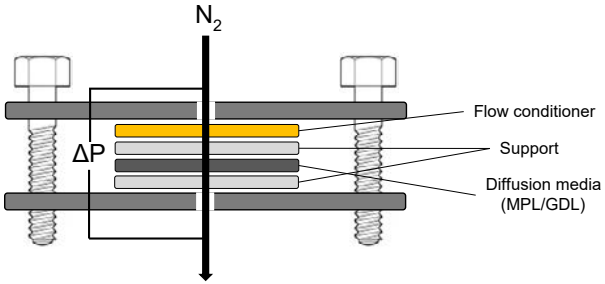
Carbon slurry preparation **Doctor blade coating** **Heat treatment<150°C**

- The introduction of an alternative hydrophobic binder instead of conventional binders (i.e. PTFE) will simplify the GDM fabrication process and greatly lower the GDM manufacturing cost and improve production efficiency..

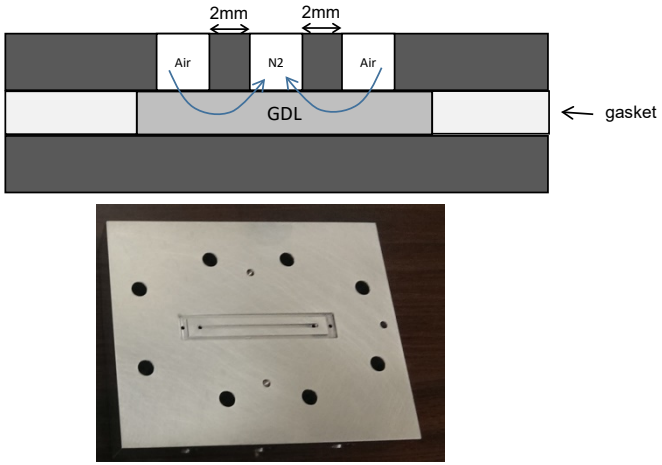
Ex-situ Characterization



In-plane N_2 permeability cell set-up



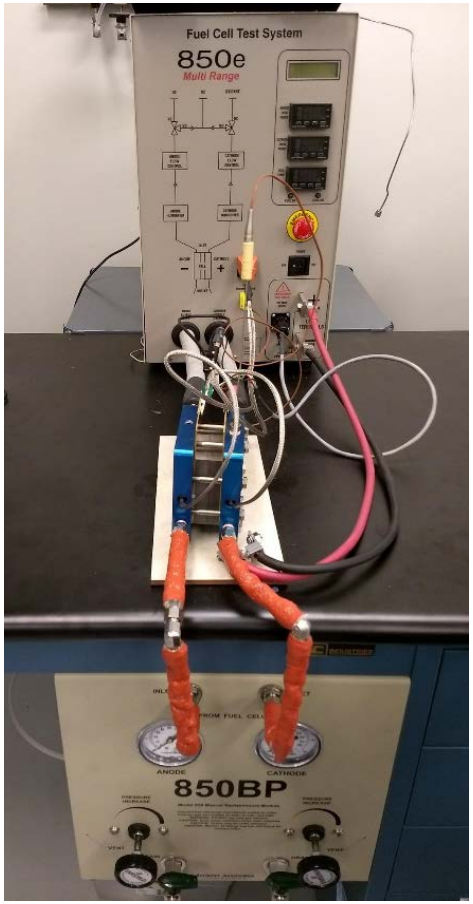
Through-plane N_2 permeability cell set-up



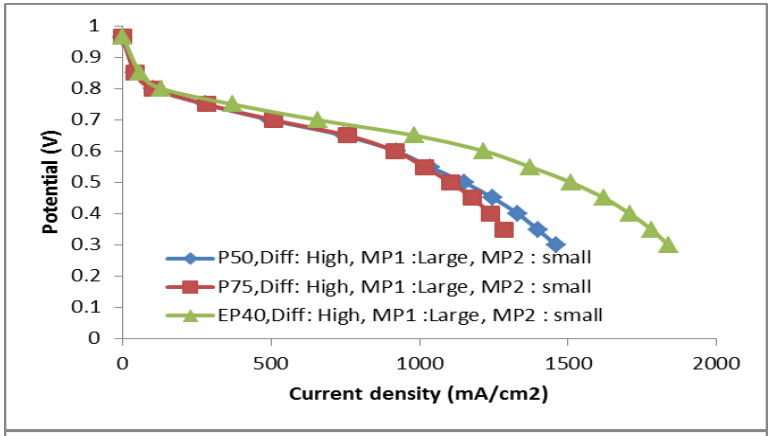
Diffusion media O_2 diffusivity set up (in-plane)

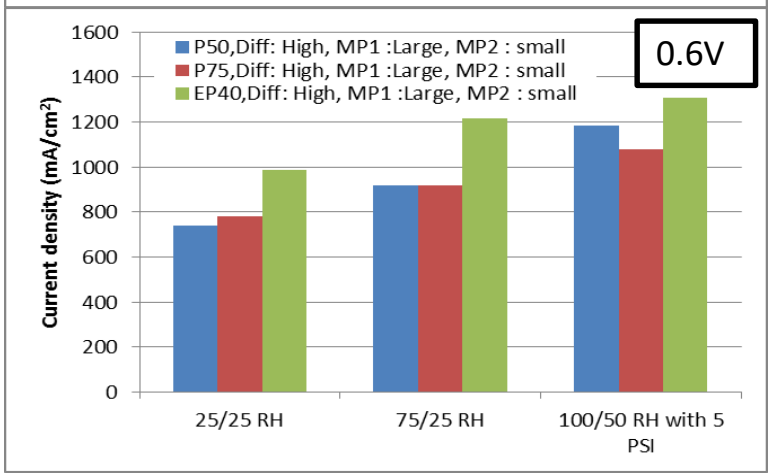
- **Porosity and Pore size distribution** – Hg porosimeter through external service
- **Tortuosity & MacMullin number** – to be developed in-house
- **Thermal conductivity** – to be developed in-house
- **Electrical conductivity** – to be developed in-house
- **In-plane and through-plane N_2 permeability** – developed in-house
- **In-plane O_2 in N_2 diffusion** – developed in-house
- **Water permeability (through-plane) and capillary pressure** – developed in-house

In-situ Performance Test



*Diffusivity: High MPL1: Large MPL2: Small





- Beginning of life (BOL) cell performance under both wet and dry conditions.
- In-situ EIS measurements under high current densities where mass transport dominates.

* Result from DOE Project **DE-PS36-08GO98009**: *Transport Studies and Modeling in PEM Fuel Cells*

Accomplishments and Progress

No progress so far, this is a new project that has not yet started.

Project was not reviewed last year.

Collaborations

- University of South Carolina (USC): Dr. Sirivatch Shimpalee (subcontractor)

  Dr. Shimpalee will be mainly focusing on the macro scale PEMFC model, and micro scale transport model to support and validate bilayer MPL design and fabrication. His team will also be involved in part of the GDL characterizations, i.e. Tortuosity & MacMullin number.

- Future Collaborator: TBD for GDL ex-situ characterization

Proposed Future Work

- Identify key design parameters in bilayer MPL using macro scale PEMFC model, and micro scale of transport model to support and validate bilayer MPL design and fabrication.

- Design bilayer MPL-based GDMs with controllable pore size gradient and hydrophilic/hydrophobic gradient, and achieve better ex-situ characterization properties compared with commercial GDLs/GDMs, including the thermal conductivity, electrical conductivity and mass transport properties etc..

- Demonstrate improved water management and better performance from in-situ testing under both wet and dry conditions, targeting at performance improvement by 20% at current densities higher than 1.0 A/cm^2.

Any proposed future work is subject to change based on funding levels.

Summary

- The goal of this project is to design bilayer microporous layer (MPL) - based gas diffusion media (GDM) with controllable pore size gradient and hydrophilic/hydrophobic gradient; and achieve properties better than commercial GDLs/GDMs, including thermal conductivity, electrical conductivity and mass transport

- Key design parameters for bilayer MPL will be identified using a macro-scale PEMFC model and a micro-scale transport model to support design and fabrication

- It is aimed to demonstrate improved water management and better performance in fuel cell testing under both wet and dry conditions

Technical Back-up Slides