V.G.2 Transport in Proton Exchange Membrane Fuel Cells

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- Ballard Material Products, Inc., Lowell, MA
- Virginia Polytechnic and State University (VA Tech), Blacksburg, VA
- University of South Carolina (USC), Columbia, SC

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Overall Objectives

- Design fuel cell components (membranes, gas-diffusion media [GDM], bipolar plates and flow fields) that possess specific transport properties
- Establish a computational fluid dynamics (CFD) model to elucidate the effect of component variables on these transport properties
- Determine sensitivity of fuel cell performance to these component properties to identify limiting components for fuel cell transport loss

Fiscal Year (FY) 2014 Objectives

- Evaluate the performance of VA Tech membrane electrode assemblies (MEAs) and the impact of VA Tech membrane on water transport in operating fuel cells
- Perform CFD modeling of VA Tech membrane for fuel cell performance and water transport using measured water uptake and diffusivity and electro-osmotic drag coefficient
- Design GDM with varying substrate, diffusivity and micro-porous layer (MPL) and characterize their microstructures
- Test the performance of fuel cells using the above MEAs and correlate the microstructures of GDM to the fuel cell performance

Technical Barriers

This project addresses the following technical barriers from the Fuel Cells section of the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan:

(C) Performance

Technical Targets

The goals of this project are not to reach specific technical targets put forth by the DOE (i.e. target catalyst loading, target cost per kilowatt). Instead, this project aims to develop fuel cell components (i.e. membranes, GDM, bipolar plates and flow fields) that possess specific properties (i.e. water transport and conductivity). A CFD model will then be developed to elucidate the effect of certain parameters on these specific properties (i.e., the effect of membrane type and thickness on membrane water transport). Ultimately, the model will be used to determine sensitivity of fuel cell performance to component properties to determine limiting components and guide research.

FY 2014 Accomplishments

- Synthesized large batches of hexafluoro bisphenol a benzonitrile (6FPAEB)-bi phenyl sulfone: H form (BPSH) membranes, nitrile containing block copolymers for 50-cm^2 MEA fabrication
- Achieved good reproducibility of the VA Tech 6FPAEB-BPSH-based MEAs
- Successfully integrated VA Tech MEAs with current distribution board (CDB) to study the impact of VA Tech membranes on water transport in fuel cells
- Obtained 12 custom GDM with varying substrate, diffusivity and MPL and characterized their microstructures

- Tested the above GDM in operating fuel cells and illustrated how the microstructures of GDM impact fuel cell performance and water transport

INTRODUCTION

Many fuel cell component properties that influence water transport and thermal management are not well understood [1,2]. A better understanding of how water transport and thermal management can be controlled would represent a significant step forward in meeting the DOE's stated 2015 targets. This project aims for a better understanding of water transport and thermal management by tailoring fuel cell components to exhibit specific measurable transport properties. These transport properties are then used in a model, which will enable the prediction of the effect of changing component parameters on transport properties.

APPROACH

This project seeks to develop fuel cell components possessing specific transport properties. Membranes will be developed to achieve different ratios of water transport and conductivity. Bulk membrane properties (i.e. diffusivity, water uptake, conductivity) will be evaluated and modeled. Also, GDMs with varying substrate, diffusivity and micro-porous layer will be developed and tailored to illustrate specific differences in porosity, tortuosity and hydrophobicity. The fuel cell performance will be evaluated using these components and compared with the model. The model will be used to predict the effect of changing component parameters (i.e. changing membrane type and thickness, changing flow field configuration) on component transport properties and fuel cell performance.

RESULTS

VA Tech 6FPAEB-BPSH-based MEA was made at Giner and sent to USC for measuring local currents using current distribution board on a 50-cm² serpentine flow field. The experimental results were compared and validated with numerical predictions. Work focused on high humidity toward over saturation conditions, 100/125% relative humidity (RH) and 100/150% RH, as liquid water significantly affects the performance of proton exchange membrane fuel cells. The validation between modeling results and experimental data will give an accuracy level of modeling code for further analysis of water transport in the proton exchange membrane fuel cell single cell and stack.

Local polarization curves from CDB measurements and CFD modeling results are shown in Figure 1**:** (a) 100/125% RH; (b) 100/150% RH. The numbers 1 to 10 represent the segments associated to the flow direction. Both conditions reveal similar local performance profiles but 100/125% RH gives higher performance than 100/150% RH. To compare the experimental results with model predictions, the contour plot pattern was used. The experimental data were imported to plotting software for a contour plot. The comparison of current density between experiment and model predictions for two inlet humidity conditions is illustrated in Figure 1c and 1d. It can be seen that the model predictions agree with experimental data for very high humidity conditions. There is a significant drop in local performance around the middle toward the exit of the cell observed in both experiment and modeling results. This is because of the high flooding in those areas.

Figure 2 shows the prediction of liquid water film thickness on the cathode membrane surface for both conditions. It shows that the thickness of liquid water is higher with the inlet humidity of the cathode side is increased. As expected, the thicker the liquid water, the lower local performance is in those areas. It also presents that with this over saturated humidity condition on the cathode, the condensation of water vapor starts from the entrance event though there is a heat generated due to the high electrochemical reaction (data not shown).

Twelve custom GDMs from AvCarb have been tested under selected humidity conditions. There are three different carbon substrates. They are EP40, P50, and P75. All of them have differences in thickness and properties (e.g., bulk density, permeability, porosity, tortuosity, etc.). These substrates were modified by adding two MPLs. Each of these was then treated with two different methods to provide two different values of diffusivity (i.e. <0.15 cm^2/s and >0.35 cm^2/s). Moreover, two MPLs have been constructed with two different sizes of carbon particles (i.e. small and large). Table 1 shows a list of samples for experiment and comparison in this report using seven custom GDMs. In this table the measurement of MacNullin number from those GDMs is also provided.

The pore distribution and microstructures of these GDMs are shown in Figure 3. The pore size distribution in both accumulative pore volume and differential pore volume of the baseline GDM compared to custom GDMs is shown in Figure 3a. Adding two different MPLs greatly reduces the volume of large pores. The scanning electron microscope images on the EP 40 substrate surfaces and cross section of custom GDMs compared to baseline GDM are shown in Figure 3b.

The fuel cell performance measurements and predictions of three main substrate-based GDMs are shown in Figure 4 (i.e. P50, P75, and EP40, with large carbon particle in MP1 and small carbon particle in MP2). As shown in Figure 4a, EP40 exhibits the best performance compared with other types especially at dryer humidity conditions. When inlet humidity increases, the performance of those three GDMs

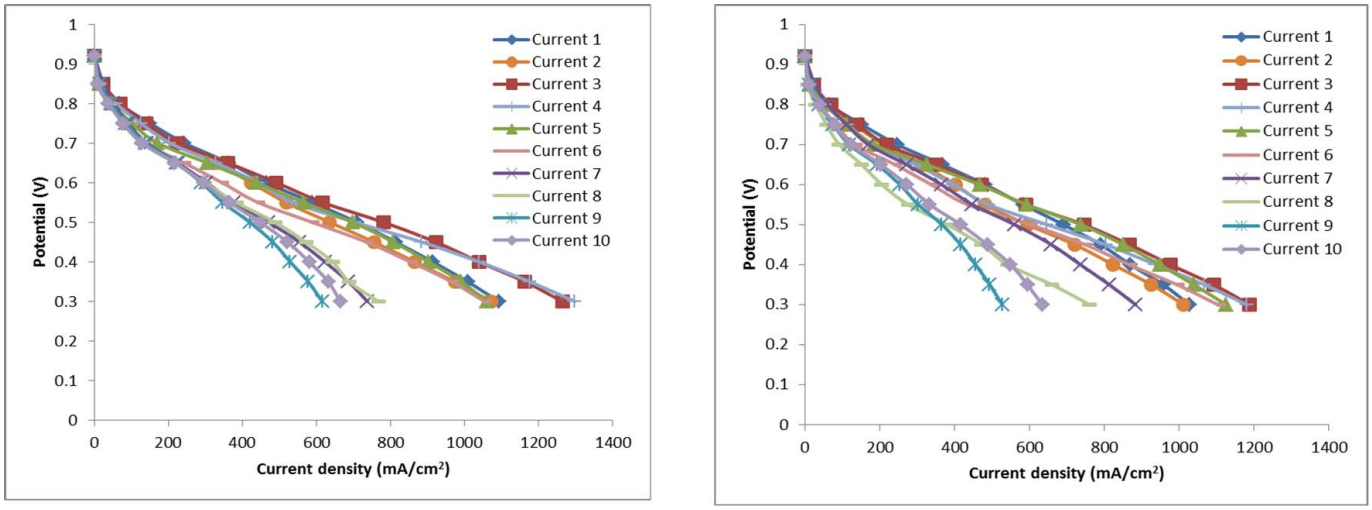

FIGURE 1. Local polarization curves of 6FPAEB-BPSH membrane from CDB measurements and CFD modeling for H_2 (anode)/air (cathode).

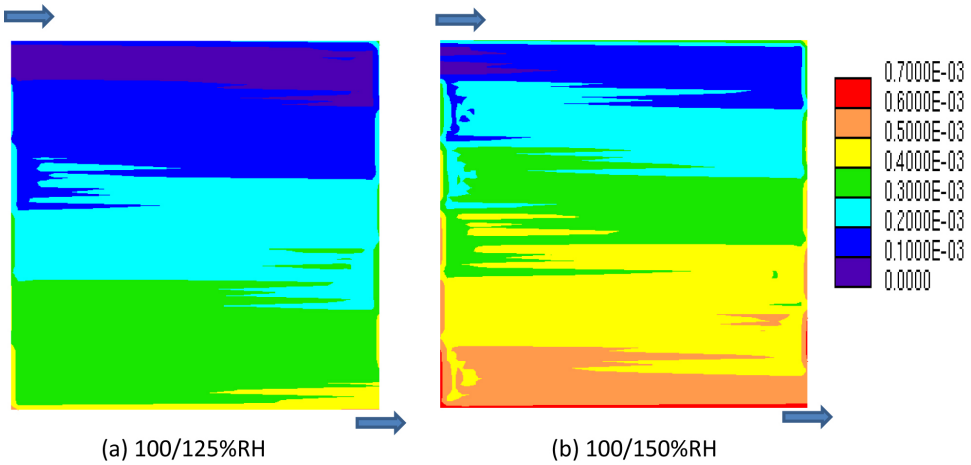

FIGURE 2. Predictions of liquid water film thickness on the cathode 6FPAEB-BPSH membrane surface for both RH conditions.

TABLE 1. GDM Design Matrix

Substrate	Diffusivity	MPL1	MPL2	MacMullin No.	Status
P50T				3.09	Done
P50	Low	Large	Small	2.63	Done
P50	High	Large	Small	2.18	Done
P50	Low	Small	Large	4.04	Done
P50	High	Small	Large	2.73	Done
P75T				4.43	Done
P75	Low	Large	Small	2.14	Done
P75	High	Large	Small	1.92	Done
P75	Low	Small	Large	11.11	Done
P75	High	Small	Large	2.63	Done
EP40T				3.70	Done
EP40	Low	Large	Small	5.18	Done
EP40	High	Large	Small	2.34	Done
EP40	Low	Small	Large	3.18	Done
EP40	High	Small	Large	2.62	Done

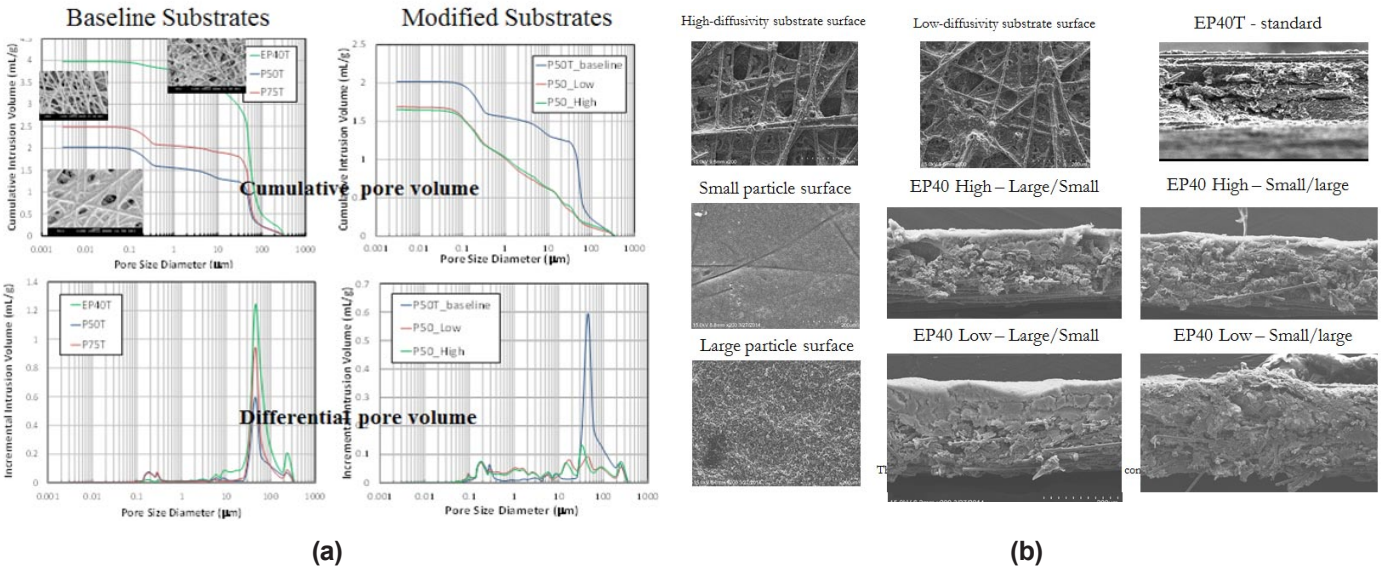

FIGURE 3. Pore distributions and microstructures of designed GDMs. (a) The pore size distribution in both accumulative pore volume and differential pore volume; (b) scanning electron microscope images on the EP40 substrate surfaces and cross section of EP40-based GDL.

are close to each other. GDM P50 and P75 show similar performance at low inlet humidity condition but P50 gives slightly higher performance than P75 at higher inlet humidity conditions. The current density distribution and membrane water content of custom GDMs via CFD simulation are depicted in Figure 4b**.** The simulation is for an average current density of 1 A/cm^2. P75 has the most non-uniform distribution and EP40 shows the most uniform distribution with a high value of membrane water content.

CONCLUSIONS AND FUTURE DIRECTIONS

- Fuel cell performance of hydrocarbon membranes integrated with CDBs has been evaluated and agrees well with the CFD simulations.
- Local distributions of water content in hydrocarbon membranes and liquid have been simulated; hydrocarbon membranes demonstrate more uniform water distribution along the MEA flow fields.
- Custom GDMs with varying substrate, diffusivity and MPLs have been designed and fabricated and their microstructures characterized.

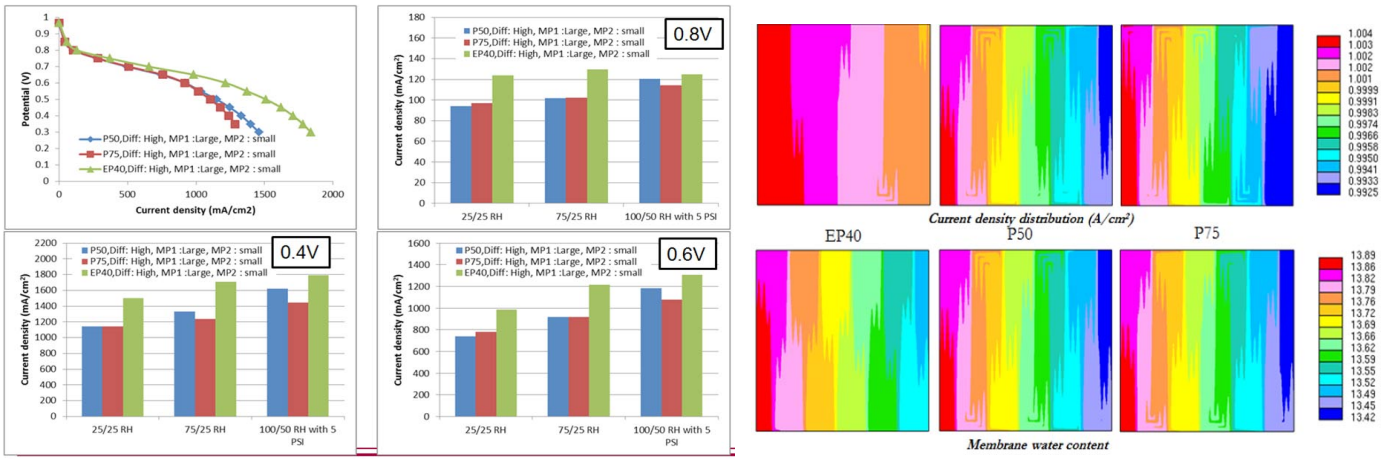

FIGURE 4. Fuel cell performance measurements and predictions of three main substrate-based GDLs. (a) Performance of different types of substrate, P50, P75, and EP40, with high diffusivity, large carbon particle of MP1 and small carbon particle of MP2. Conditions: 80°C; Stoichiometry # 1.5 (anode)/2.0 (cathode); RH (%): 25/25, 75/25 (voltage-current curves are shown), and 100/50 ; pressure: 5 psig. (b) Current density distribution and membrane water content of custom GDLs via CFD simulation.

- The substrate diffusivity and MPL pore structures significantly impacts the performance of MEAs and the GDM optimization has been achieved.
- In the future, the focus will be given to the impact of catalyst layer composition and structure (e.g., hydrocarbon ionomer and advanced catalysts) on fuel cell transport properties.

FY 2014 PUBLICATIONS/PRESENTATIONS

1. "Transport in PEMFC Stacks", Presented by Cortney Mittelsteadt in DOE Hydrogen and Fuel Cell merit review meeting, Arlington, VA, June 2014.

2. "Characterizing Water Transport Properties of Hydrocarbon Block Copolymer Proton Exchange Membranes", presented by Hui Xu in 222th meeting of ECS, Abstract #1344, San Francisco, October 2013.

3. Chen, Yu; Rowlett, Jarrett R.; Lee, Chang Hyun; Lane, Ozma R.; Van Houten, Desmond J.; Zhang, Mingqiang; Moore, Robert B.; McGrath, James E., "Synthesis and characterization of multiblock partially fluorinated hydrophobic poly(arylene ether sulfone)-hydrophilic disulfonated poly(arylene ether sulfone) copolymers for proton exchange membranes", *Journal of Polymer Science, Part A: Polymer Chemistry*, published online: DOI: 10.1002/pola.26618. (2013)

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5. Rowlett, J.R., Chen, Y., Shaver, A.T., Lane, O., Mittelsteadt, C., Xu, H., Zhang, McGrath, J.E., "Multiblock poly(arylene ether nitrile) disulfonated poly(arylene ether sulfone) copolymers for proton exchange membranes: Part 1 synthesis and characterization", *Polymer (United Kingdom)* 54 (23) PP. 6305 – 6313. (2013)

6. V. Lilavivat, S. Shimpalee, H. Xu, J.W. Van Zee, and C.K. Mittelsteadt, "Novel current distribution board for PEMFC," submitted to Intl J. of Hydrogen Energy. (2014).

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