

# MODELING OF A PROTON EXCHANGE MEMBRANE FUEL CELL

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## INTRODUCTION

Fuel cells are electrochemical devices, which utilize fuel and oxidant to produce electricity and heat [1]. The common electrolyte of a Proton Exchange Membrane Fuel Cell (PEMFC) is a thin layer of proton permeable polymer. In this paper, multiphysics-based numerical simulations were performed on a PEMFC anode/electrolyte/cathode composite using COMSOL [2].

The modeling provides the general cell performance and the fuel/oxidant concentration distributions along the feeding channel. To obtain detailed flow field in the porous gas diffusion layer, a 2D simulation was also performed. Although the simulation did not consider the water flooding effect, the onset of water formation has been identified from the partial pressure of vapor in the feeding channel.

## NUMERICAL MODELING

### Calculation domain

The PEMFC model is a composite consists of an anode flow channel, the anode porous gas diffusion layer, a proton exchange membrane, a cathode diffusion layer, and the cathode side feeding channel. The multi species transportation in the porous electrodes and the coupled electrical current and potential distributions were modeled.

### Anode gas diffusion layer

Darcy's Law is used to describe the flow in the porous structure of anode side. For the fuel, hydrogen, the gas density was calculated using the ideal gas equation.

### Cathode gas diffusion layer

For the mixture of O<sub>2</sub> and H<sub>2</sub>O in the cathode electrode, Maxwell-Stefan diffusion and convection module was used.

$$\frac{\partial \rho \omega_i}{\partial t} + \nabla \cdot \left[ -\rho \omega_i \sum_{j=1}^N D_{ij} \left\{ \frac{M}{M_j} \left( \nabla \omega_j + \omega_j \frac{\nabla M}{M} \right) + (x_j - \omega_j) \frac{\nabla p}{p} \right\} + \left[ \omega_i \rho \bar{u} + D_i^T \frac{\nabla T}{T} \right] \right] = R_i$$

Where, M denotes Molar mass of the mixture.

### Electrolyte:

In the simulation, a DC conductive model is used for the electrolyte layer and the two gas diffusion

layers. The ionic balance was calculated. The mass transfer of species across the anodic and cathodic active layers is related to the local current density according to:

$$-\vec{n} \cdot \vec{n}_{H_2} = -\frac{i_a}{2F} \quad \text{at anode subdomain}$$

$$-\vec{n} \cdot \vec{n}_{O_2} = \frac{i_c}{4F} \quad \text{at cathode subdomain}$$

These two terms also act as source terms in the respective region. At the remaining boundaries, either insulation or symmetry conditions were used.

## Numerical simulations results

In order to compare with the available experimental data, the flow rates of hydrogen was set to be 20, 40, 60, 80, 100 standard cubic centimeter per minute (sccm) in the simulation. And the oxygen flow rate was maintained constant at 46 sccm for all simulation models.

Under the condition of high cell potential, thus light load, less water is formed. Along the hydrogen and air flow directions, the simulations have a more pronounced water formation. Partial pressure of hydrogen also varies accordingly from high to low from the entrance to the exit along the flow direction. Fuel utilization is low for a light load as the high fuel flow rate was fixed in the calculation.

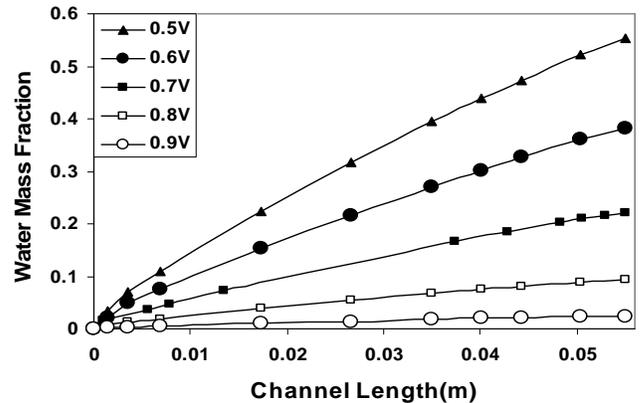


Fig. 1: Water mass fraction along the channel

Figure 1 shows water mass fraction variation along the channel under several cell loadings. This

plot gives a reasonable indication of the amount of water generated from the entrance to the exit of the channel. A small voltage value indicates a high load and thus more water is formed.

Table 1: The distance to form saturated water, measured from the feeding channel entrance

Voltage (Volt)	The distance for cathode flow to reach saturation from entrance (mm)
0.9	4.5
0.8	0.2852
0.7	0.095
0.6	0.0495
0.5	0.03095

At a temperature of 20 C, saturated vapor pressure is 2.338 KPa [3]. After a certain distance from the entrance of the channel, water vapor will become saturated, and liquid droplets form due to the partial pressure of water is higher than the saturation pressure of water vapor. In the simulation, no water-vapor multi phase model was applied thus the water vapor partial pressure may be well beyond the saturation value. Table 1 shows the location of the onset of saturation from the entrance of the channel under various loads. Increasing the loads, the unsaturated region becomes smaller due to the rapid electrochemical reaction along the flow channel.

Due to the limitation of computing power, the 3D simulation could not reveal the flow details in the gas diffusion layers. A 2D numerical simulation has been conducted to address this issue. Comparing to 3D modeling, the 2D model assumes a uniform distribution of gases, current density, velocity and temperature along the channel width direction. As the flow has a dominate direction along the feeding channel, this is a reasonable assumption.

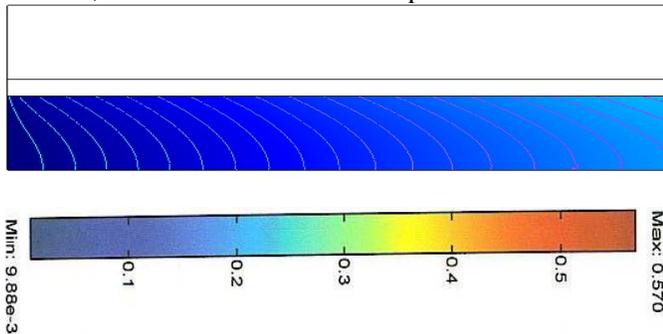


Fig. 2: 2D numerical Simulation of water pattern for 20sccm Hydrogen flow rate at 0.7V with contour lines

It is found that the 2D simulations have the similar water vapor pressure distribution as the 3D

modeling. All the simulations show that with increasing loads water generation increases. Figure 2 shows 2D numerical simulation of water pattern under 20 sccm hydrogen flow rate at a cell voltage of 0.7 volt, where the contour lines indicate the variation of water concentration in the gas diffusion layer. Figure 3 shows 2D numerical simulation of partial pressure of hydrogen under the same condition. As expected, hydrogen pressure decreases along the anode gas diffusion layer flow direction.

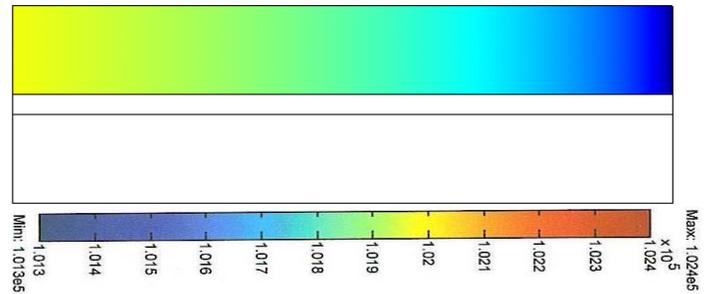


Fig. 3: 2D numerical simulation of partial pressure of hydrogen for 20sccm hydrogen flow rate at 0.7V

### CONCLUSION:

Performance of PEM fuel cell is studied on a single channel configuration using numerical simulation. The cell performance is quantified in terms of polarization curve, power density curve, water pattern by mass fraction, water partial pressure in the feeding channel, fuel utilization rate under different loadings. Both 2D and 3D simulations were performed. The simulation results were compared favorably with the experimental measurements of a single channel PEMFC. It is expected that the methodology of PEMFC simulation could be further extended to other feeding channel designs and provide a useful design tool for the future development of fuel cells.

### REFERENCES

- [1] J. Larminie, A. Dicks, Fuel cell systems explained, Wiley, ISBN: 047084857x, (2003)
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- [3] Sonntag, Borgnakke, & van Wylen, 2003, Fundamentals of Thermodynamics, 6th Edition, Wiley