Iranica Journal of Energy & Environment 4 (2): 126-129, 2013
ISSN 2079-2115
IJEE an Official Peer Reviewed Journal of Babol Noshirvani University of Technology
DOI: 10.5829/idosi.ijee.2012.04.02.08

BUT

A Numerical Study of the Influence of Gas Diffusion Layer Porosity on Cell Performance of Counter Flow Proton Exchange Membrane Fuel Cells

Ali Shokuhfar, Omid Nejadseyfi and Ashkan Zolriasatein

Advanced Materials and Nanotechnology Research Center, Mechanical
Engineering Faculty, K. N. Toosi University of Technology, Iran

(Received: August 10, 2012; Accepted in Revised Form: February 26, 2013)

Abstract: This study characterizes the cell performance of a proton exchange membrane fuel cell (PEMFC) considering the counter flow of hydrogen and air. The effects of porosity of anode and cathode Gas Diffusion Layers (GDL) on current density, power density and mass transfer were investigated. Half-cell model was employed for computational analysis and parallel flow was simulated for process validation. The results showed that the porosity affects the limiting current density especially in low cell voltages. Such condition is achievable in practice by diminishing the oxygen diffusion in the GDL. Also, the simulations confirmed an increase in power density by about 6 percent, when increasing the porosity of GDL by about 20 percent in the counter flow of PEMFC.

Key words: Current Density; Fluent; Gas Diffusion Layer (GDL); Porosity; Proton Exchange Membrane Fuel Cell (PEMFC)

INTRODUCTION

Direct conversion of chemical energy in the fuel, into electrical energy using fuel cells has a lot of advantages; such as obviating the exhausting issues of conventional batteries, continuous electrical energy, as long as the fuel and an oxidant are supplied to the cell, low maintenance, excellent load performance, less heat generation, etc. Among the several types of fuel cells, the proton exchange membrane fuel cell (PEMFC) has attracted more attention in the last decades especially in automotive applications because of low operating temperature and fast response to changes in the power demand [1]. On the other hand, the high cost is the greatest obstacle for commercialization of this kind of fuel cells.

Although there are several reports evaluating the performance of PEMFC experimentally, but it is more convenient to employ numerical methods to better understand the effective parameters in designing and optimizing the functions of fuel cells, in order to improve the fuel cell technology [2].

Gurau et al. [3] developed a two-dimensional PEMFC model that included fluid flow, mass transfer and the electro-kinetics and introduced the computational fluid dynamics into fuel cell modeling.

Kumar et al. [4] investigated the Effects of channel dimensions and shape in the flow-field distributor on the performance of polymer electrolyte membrane fuel cells. They employed different channel dimensions in their simulations and concluded that optimum values exist for channel width, land width and channel depths. Also their simulations for a variety of shapes showed an increase in hydrogen consumption by 9% over the rectangular shaped cross section and they concluded that the use of rectangular channels with optimum dimensions will lead to increased hydrogen consumption at the anode, which will lead to better fuel cell performance.

The simulations are usually implemented on the characterization of parallel flow PEMFC [5], so this study concentrates on the effects of porosity of gas diffusion layer in a single channel, Counter Flow PEMFC.

MODEL DEVELOPMENT

A schematic of a proton exchange membrane fuel cell with a counter flow is illustrated in Figure 1. The dimensions of the fuel cell are 2.8mm, 2.4mm and 100mm in the x, y and z directions respectively. This model represents a repeating channel of larger counter flow PEM fuel cell.

According to Figure 1, the protons migrate across the membrane onto the cathode side and the electrons flow through the outer circuit generating electricity. These protons and electrons react at the cathode with oxygen to produce water. The electrochemical reactions are given by:

***Corresponding Author:** Ali Shokuhfar, Advanced Materials and Nanotechnology Research Center, Mechanical Engineering Faculty, K. N. Toosi University of Technology, Iran E-mail shokuhfar@kntu.ac.ir

In anode:

$$H_2 \rightarrow 2H^+ + 2e^- \qquad (1)$$

In cathode:

$$\frac{1}{2}O_2 + 2H^+ + 2e^- \rightarrow H_2O \qquad (2)$$

The transport equations of model were simplified assuming the steady state and laminar flow, equilibrium of phases, and isotropic solid materials. The basic transport equations including conservation of mass (continuity) and conservation of momentum (Navier–Stokes equation) were written for each of the zones of the domain. Conservation of mass is represented by the following expression:

$$\frac{\partial(°u)}{\partial x} + \frac{\partial(°v)}{\partial y} + \frac{\partial(°w)}{\partial z} = S_m \qquad (3)$$

Where ρ is the density of the fluid and u, v and w are the components of the velocity in x, y, and z-direction, respectively. In this equation the source term, S_m, appears due to the electrochemical reactions.

The expanded form of Momentum equation is given by equations 4 to 6:

In x direction:

$$u\frac{\partial(°u)}{\partial x} + v\frac{\partial(°u)}{\partial y} + w\frac{\partial(°u)}{\partial z} = -\frac{\partial P}{\partial x} + \frac{\partial}{\partial x}(«\frac{\partial u}{\partial x}) + \frac{\partial}{\partial y}(«\frac{\partial u}{\partial y}) + \frac{\partial}{\partial z}(«\frac{\partial u}{\partial z}) + S_{px} \qquad (4)$$

In y direction:

$$u\frac{\partial(°v)}{\partial x} + v\frac{\partial(°v)}{\partial y} + w\frac{\partial(°v)}{\partial z} = -\frac{\partial P}{\partial x} + \frac{\partial}{\partial x}(«\frac{\partial v}{\partial x}) + \frac{\partial}{\partial y}(«\frac{\partial v}{\partial y}) + \frac{\partial}{\partial z}(«\frac{\partial v}{\partial z}) + S_{py} \qquad (5)$$

In z direction:

$$u\frac{\partial(°w)}{\partial x} + v\frac{\partial(°w)}{\partial y} + w\frac{\partial(°w)}{\partial z} = -\frac{\partial P}{\partial x} + \frac{\partial}{\partial x}(«\frac{\partial w}{\partial x}) + \frac{\partial}{\partial y}(«\frac{\partial w}{\partial y}) + \frac{\partial}{\partial z}(«\frac{\partial w}{\partial z}) + S_{pw} \qquad (6)$$

Similar to conservation of mass, the source terms are appeared in these conservation of momentum equations. The presence of these terms is due to the pressure difference when the fluid passes through a porous medium.

$$S_{px} = -\frac{«u}{x} \qquad (7)$$

$$S_{py} = -\frac{«v}{z} \qquad (8)$$

$$S_{pz} = -\frac{«w}{z} \qquad (9)$$

In these equations, μ is the viscosity of the fluid and β is the permeability of the electrode material which is assumed to be the same in different directions in isotropic materials.

Energy equation can be described as:

$$u\frac{\partial(°CT)}{\partial x} + v\frac{\partial(°CT)}{\partial y} + w\frac{\partial(°CT)}{\partial z} = \frac{\partial}{\partial x}(k\frac{\partial T}{\partial x}) + \frac{\partial}{\partial y}(k\frac{\partial T}{\partial x}) + \frac{\partial}{\partial z}(k\frac{\partial T}{\partial x}) + S_h \qquad (10)$$

The transport equation for oxygen and water in cathode side together with the transport equation for hydrogen and water in anode side, is represented by equations 11 to14.

$$u\frac{\partial(°Y_{O2})}{\partial x} + v\frac{\partial(°Y_{O2})}{\partial y} + w\frac{\partial(°Y_{O2})}{\partial z} = \frac{\partial(J_{X,O2})}{\partial x} + \frac{\partial(J_{Y,O2})}{\partial y} + \frac{\partial(J_{Z,O2})}{\partial z} + S_{O2} \qquad (11)$$

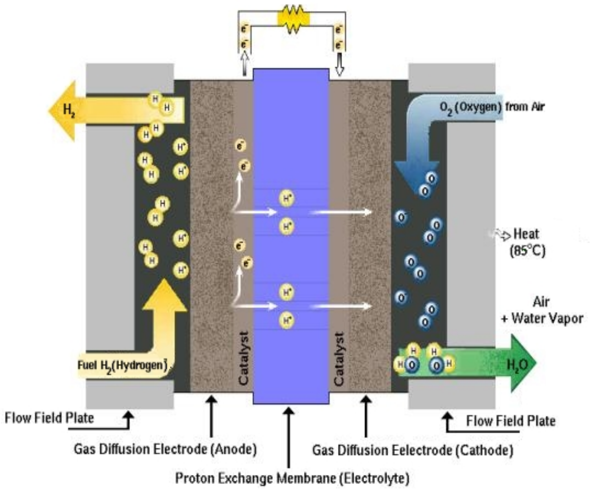

Fig. 1: schematic of a Counter Flow PEMFC.

$$u\frac{\partial(°Y_{aw})}{\partial x} + v\frac{\partial(°Y_{aw})}{\partial y} + w\frac{\partial(°Y_{aw})}{\partial z} = \frac{\partial(J_{X,aw})}{\partial x} + \frac{\partial(J_{Y,aw})}{\partial y} + \frac{\partial(J_{Z,aw})}{\partial z} + S_{aw} \qquad (12)$$

$$u\frac{\partial({}^{\circ}Y_{H2})}{\partial x}+v\frac{\partial({}^{\circ}Y_{H2})}{\partial y}+w\frac{\partial({}^{\circ}Y_{H2})}{\partial z} = \frac{\partial(J_{X,H2})}{\partial x}+\frac{\partial(J_{Y,H2})}{\partial y}+\frac{\partial(J_{Z,H2})}{\partial z}+S_{H2} \qquad (13)$$

$$u\frac{\partial({}^{\circ}Y_{cw})}{\partial x}+v\frac{\partial({}^{\circ}Y_{cw})}{\partial y}+w\frac{\partial({}^{\circ}Y_{cw})}{\partial z} = \frac{\partial(J_{X,cw})}{\partial x}+\frac{\partial(J_{Y,cw})}{\partial y}+\frac{\partial(J_{Z,cw})}{\partial z}+S_{cw} \qquad (14)$$

A finite volume code (Fluent) was employed to solve the above mentioned equations. The code includes a module that takes into account the electrochemical effects of the source terms associated with each zone. Only one half of the cell simulated taking advantage of the symmetry condition.

The operating conditions and other assumptions are summarized in Table 1. The model was analyzed under these conditions considering different schemes of meshing and good convergence was observed in simulations. The results of the parallel flow simulations showed excellent accordance with the experimental work of Um et al. [6].

Table 1: Conditions of simulation

Operating pressure	0.2 MPa
Cell operating temperature	358 K (85°C)
Cell Voltage	0.15 V to 1.05 V
Diffusion Layer Porosity	0.3 to 0.7
mass fraction of O_2 (inlet)	0.2
mass fraction of H_2 (inlet)	0.2
Cell Dimension (mm)	2.8 × 1.2 × 100
Mass Flow Rate (inlet)	5.0×10^{-6} kg/s
Permeability (β)	2×10^{-10} m^2

RESULTS AND DISCUSSION

Figure 2 represents the variation of current density versus cell voltage. This figure indicates that the porosity affects the cell voltage especially in high current densities. When the current density passes 4A/m^2, the fluctuations of cell voltage varies for about ±15% by changing the porosity of GDL only for about ±10%.

Figure 3 shows the variation of power density versus current density when the porosity of GDL is exposed to change from 40 to 60%. About 6 to 8% increase in the power density is observed in this figure for high current densities. The exteremum of this curvature implies that achieving higher power densities is possible in the vicinity of 6A/m^2 for current density and 0.6V for cell voltage.

Figure 4 illustrates the oxygen mass fraction in the cathode side GDL. Simulations confirmed that the oxygen diffusion in the GDL is highly coupled to cell voltage. But the variation of the oxygen diffusion with porosity is very low in a certain cell voltage as shown in Figure 3 for V_{cell}=0.55V.

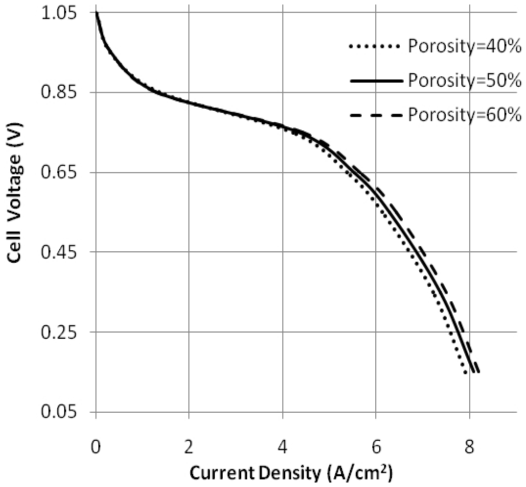

Fig. 2: Variation of current density with cell voltage in different amounts of porosity of gas diffusion layer.

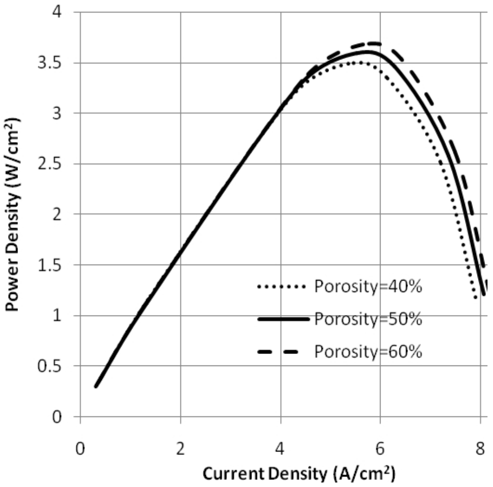

Fig. 3: Influence of the porosity of gas diffusion layer on the power density in a cell

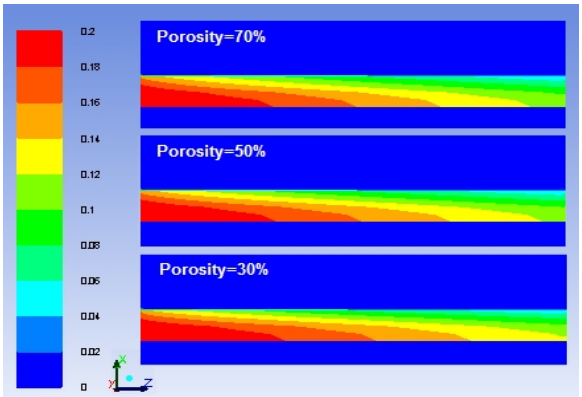

Fig. 4: Contours of oxygen mass fraction along the channel length.

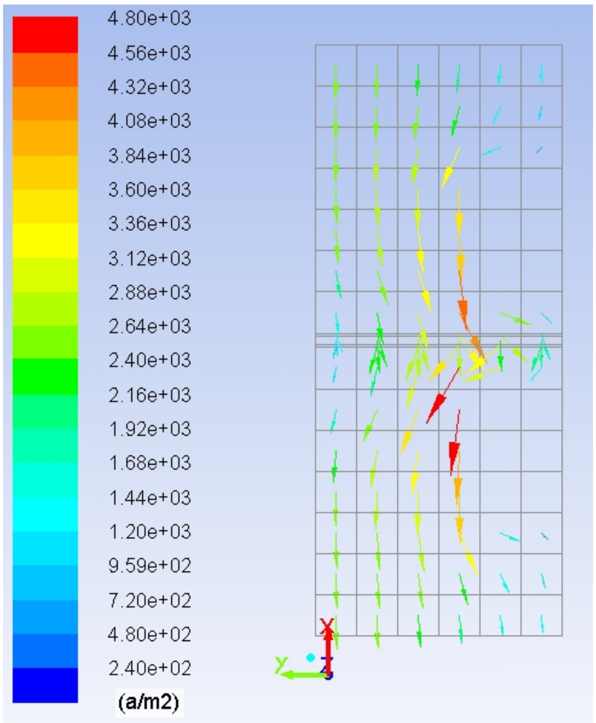

Fig. 5: Magnitude and direction of current flux density (A/m^2) for the case of Porosity=50%, and V$_{cell}$=0.95V

The magnitude and direction of current flux density are presented in Figure 5. The maximum current density occurred somewhere near to the corners of the flow channel in cathode side as expected.

CONCLUSION

Neglecting ohmic losses, simulations showed a slight increase (about 5%) in limiting current density when the porosity of GDL increases 20% in a single channel, Counter Flow PEMFC. Achieving higher power densities is possible in the vicinity of 6A/m^2 for current density and 0.6V for cell voltage in counter flow PEMFC.

Although the oxygen content in the outlet decreases when the porosity of diffusion layer increases; but oxygen mass fraction does not change dramatically and remains above 50% of its initial value. In this way the same voltage is achieved with high current density.

REFERENCES

1. EG &G Services, Parsons Inc., “Fuel Cell Handbook, 5th edition,” US Department of Energy, West Virginia, pp. 1.1–1.37, 2000.
2. S. Dutta, S. Shimpalee, J.W. Van Zee, “Numerical prediction of mass exchange between cathode and anode channels in a PEM fuel cell,” International Journal of Heat and Mass Transfer, vol. 44, pp. 2029–2042, 2001.
3. V. Gurau, H. Liu, S. Kakac, “Two-dimensional model for proton exchange membrane fuel cells,” AIChE Journal, Vol. 44, Issue 11, pp. 2410-2422, 1998.
4. A. Kumar, R. G. Reddy, “Effect of channel dimensions and shape in the flow-field distributor on the performance of polymer electrolyte membrane fuel cells,” Journal of Power Sources, vol. 113, pp. 11-18, 2003.
5. B. Ramos-Alvarado, A. Hernandez-Guerrero, D. Juarez-Robles, P. Li , “Numerical investigation of the performance of symmetric flow distributors as flow channels for PEM fuel cells,” international Journal of hydrogen energy, pp. 1-13, 2011.
6. S. Um, C.Y. Wang, “Three-dimensional analysis of transport and electrochemical reaction in proton exchange membrane fuel cell,” Journal of Power Sources, vol. 125, pp. 40-51, 2004.