Journal of Engineering and Technology
Vol.3 No. 2 July - December 2015

Numerical Investigation on Water Transport in Polymer Electrolyte Fuel Cells in Different Flow Field Configurations

Patcharawat Charoen-amornkitt[1], Nuttapol Limjeerajarus[2]

Research Center for Advanced Energy Technology, Faculty of Engineering, Thai-Nichi Institute of Technology
1771/1 Pattanakarn Rd., Suan Luang, Suan Luang, Bangkok, Thailand, 10250
[1] ch.patcharawat_st@tni.ac.th
[2] nuttapol@tni.ac.th

***Abstract*— Water management in a membrane electrode assembly (MEA) is one of the crucial problems which prevents a polymer electrolyte fuel cell (PEFC) from a wide-scale commercialization due to its consequent effect on cell durability and degradation. One of the main components of PEFC which directly deals with the water management problems is the reactants gas flow channel (GFC). A well designed GFC must provide a uniform distribution of water concentration which reduces flooding in catalyst layer and gas diffusion layer as well as drying of the membrane. This work highlights the water transport inside the PEFC, including membrane water content and water saturation of three different commercial flow fields, namely single channel serpentine, three channel parallel in series and z-type parallel by using finite volume method via ANSYS FLUENT software. The results indicated that, for a small-scale PEFC, the single channel serpentine was the best flow field among the studied flow fields with the recommended operating voltage of 0.6.**

***Keywords*— PEFC, CFD, Multiphase flow, Water Transport, Fuel cell modeling**

I. INTRODUCTION

Polymer electrolyte fuel cell (PEFC) is a device which converts chemical energy into electrical energy directly by releasing heat and water as a by-product. However, there are several technological barriers needed to be overcome before competing in the global energy market such as heat and water management problems. Water management problems can be classified into 2 main categories, i.e., the drying problem and the flooding problem. The drying out of the membrane leads to a high protonic resistivity, resulting in the increase of local hot spots. The increased hot spot accelerates the drying further and thus the lower cell performance and the membrane lifetime. A PEFC, typically, operates under low temperatures and therefore the water may condense and form liquid water blocking the gas diffusion passage, resulting in the flooding in the electrodes, which prevent the reactants to reach the reaction site and hence the reduction of the cell performance. In the membrane, generally, there are 2 kinds of the water transport involved, which are the electro-osmotic drag (EOD) and the back diffusion (BD), as depicted in Fig.1. The water flooding mentioned earlier is likely to occur in the cathode catalyst layer (CL) since the water is produced on this side due to the electrochemical reaction and the water also migrates from the anode by the EOD. While the cathode side of the membrane electrode assembly (MEA) has to deal heavily with the water flooding problem, the anode side has a problem of the membrane drying out caused by the EOD. However, when the water concentration at the cathode is higher, the water diffuses back to the anode by the BD. To keep the membrane in the hydration state and avoid the flooding in the electrodes, the effects of those 2 types of water transport are needed to be in balance.

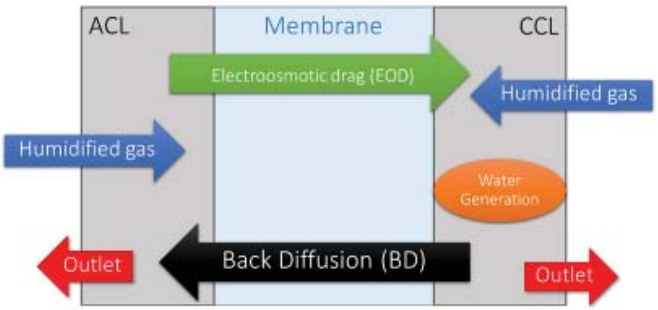

Fig. 1 Schematic of the water transport in the PEFC

Among several components of a PEFC, the gas flow channel (GFC) on the bipolar plates (BPs), which performs several functions affecting PEFC performance and its lifetime, directly relates to the water management. After the reactants are fed into the GFC, the reactants are consumed non-uniformly along the GFC and hence the maldistribution of temperature and water production. Besides its function of distributing the reactants to the reaction site, the GFC is also used to remove the surplus water out through the channel. Therefore, the design of the GFC plays an important role on PEFC performance and stability. The computational fluid dynamics (CFD) has been accepted so far as a powerful tool for PEFC performance evaluation and parametric design optimization. There are several studies using the CFD techniques to investigate the effect of different GFC designs on the PEFC performance [1 – 3].

In this work, the numerical modeling for the water transport investigation in three different commercial flow field configurations, namely single channel serpentine, three channel parallel in series and parallel of 5 cm^2 PEFC which

operates by using air was carried out via CFD techniques. The objective of this study is to explore the effects of different flow configurations on the water transport inside the MEA which greatly affects the PEFC performance and durability. The results would provide an useful information for a design optimization and suggest the flow field with an appropriate operating cell voltage at which the cell can operate with stability.

II. Model Development

The model, in this work, was carried out through ANSYS FLUENT PEMFC add-on module based on the finite volume method by which the phenomena occurring inside the PEFC are numerically solved. The equations used in this model are including the mass conservation equation, the Navier-Stoke's equations, the conservation of energy equation, the multiphase model equation and a set of several equations, which are a combination of theoretical and experimental derived equations [4]. Note that the multiphase model used in this work assumed the liquid water velocity in the GFC to be equal to the reactants velocity and thus flooding in the GFC cannot be predicted by this model. The 3-D geometries, including BPs, GFCs, gas diffusion layers (GDLs), catalyst layers (CLs), and membrane, of 5 cm^2 PEFCs were generated in ANSYS WORKBENCH and imported into ANSYSY ICEMCFD for discretizing the created geometries into small volume elements. Hexahedral cells were chosen to be the computational cell for the sake of quick convergence rate, good solution accuracy and low required computational time. A grid independent analysis on each layer of the MEA (i.e., GDLs, CLs and membrane) was also carried out to ensure the quality of the solution in our previous work [5]. Finally, 5 cells lined in the through-plane direction of each layer were used since the maximum difference of the cell voltage obtained from the different cell numbers was within 1% of the case of 5 cells in each layer but a higher computational time. Therefore, the computational cells of approximately 680,000 hexahedral cells with a maximum aspect ratio of 94 were used for the final simulation.

The realistic properties and parameters obtained from manufacturers' catalogue and experiments conducted in previous studies were used and summarized in our previous work [5] and will not be repeated here. The boundary conditions of this model were selected based on the real application which uses air as the oxidant for a sake of convenience for which the oxidant storage is not required. Therefore, the stoichiometric flow rates of 1.1/1.1 with 90% RH in both H_2/Air were used in this study. The cell and reactants temperature were set to maintain at 60ºC which was the operating temperature. Since the cell operated under the atmospheric pressure, the pressure at outlet of GFCs was set at 1 atm. Finally, galvanostatic boundary conditions were used since they represented the real operation mode of the experimental test station.

III. Results and Discussion

Since the membrane water content reflected both cell lifetime and performance, the simulation results of the average amount of water content in the membrane of each flow field at each current density are shown in Fig. 2. The results revealed that the water content at the low current densities (below 0.2 A cm^{-2}) increased as the current density increased, while it decreased after 0.2 A cm^{-2}. It was also found that the parallel flow field provided the highest average membrane water content among the three flow fields in the entire current density while the single channel serpentine flow field delivered the lowest water content in most parts of the current density. Note that the membrane in the parallel flow field suffered a severe flooding problem and thus its water content after 1.4 A cm^{-2} could not be simulated. This result was confirmed by the I-V polarization curve presented later in Fig. 7.

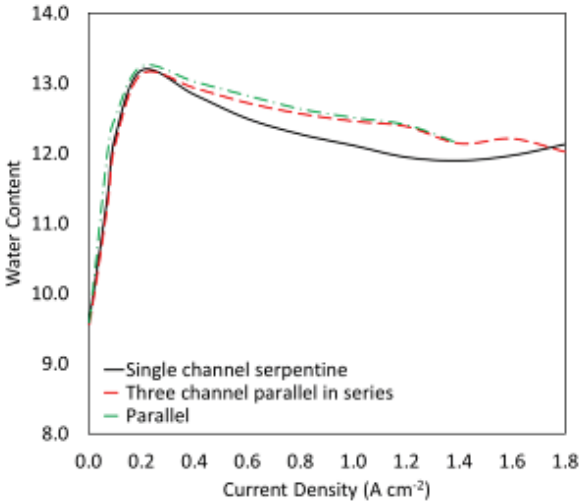

Fig. 2 Average water content at each current density

However, the driving mechanism behind the increasing and decreasing of the water content in each current density were not yet well understood. Fig. 3 shows the amount of transferring water due to the membrane water transport and oxygen reduction reaction (ORR) to clarify those ambiguities. It was clearly seen that the amount of water at the anode side decreased rapidly after 0.2 A cm^{-2} which indicated that the EOD became significantly dominant. Although the EOD increased the amount of water on the cathode side, the much higher amount of water on the cathode side was mainly caused by the water generation via ORR since the increased water on the cathode has to be equal to the decreased water on the anode if the ORR is neglected. From Fig. 3, it could be implied that while the water was being generated at the cathode side and almost no water was being moved from the anode to the cathode via the EOD at the low current densities, the membrane humidification was increased and thus the increasing of the membrane water content. In the region after 0.2 A cm^{-2}, the amount of water at the anode side reduced significantly, resulting in the lower average water content.

Therefore, it can be concluded that although the transportation of proton mainly depends on the water content, the transportation of proton also significantly influenced bi-directionally the water transport in the membrane and thus the water content.

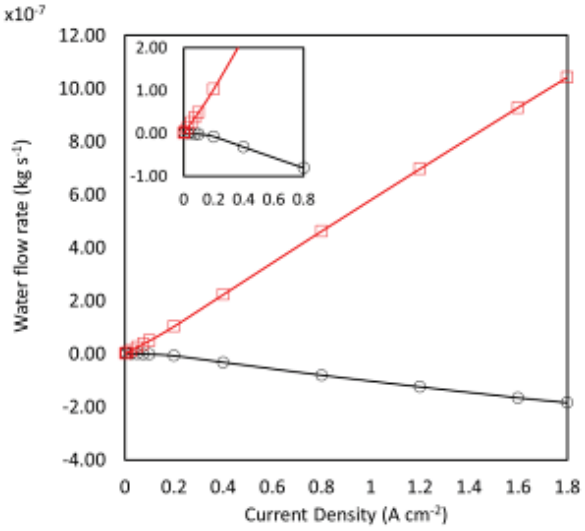

Fig. 3 The amount of transferring water in the electrodes (○) Anode (□) Cathode

In each flow field, there were differences in the water transport since the amount of fed and generated water was the same by the boundary conditions, but the average membrane water content was different and hence the water distribution. To prevent the local hot spots which may lead to the problems of cell degradation and durability, the uniform distribution of the water content is needed. Since the anode side of the membrane has to deal with the drying problem, the investigation on the anode water content distribution at different cell voltages was conducted and presented in Fig. 4.

It was found that the results were in concurrence with the average water content (see Fig. 2) in which the anode side of the membrane was getting drier when the load was increased. Additionally, the parallel flow field was also found providing the highest membrane water content followed by the three channel parallel in series and the single channel serpentine flow field, respectively. The single channel serpentine flow field delivered the most uniform water content distribution among the flow fields, while the parallel provided the worst uniformity. From this uniform distribution, it could be implied that the reaction occurred evenly all over the cell area. The areas at the anode side where the hydrogen oxidation reaction (HOR) did not take places were where the water content areas were high since there were no protons to drag the water from the anode to the cathode side via the EOD. Besides the drying of the membrane at the anode side, the flooding at the cathode side could also bring a direct impact on PEFC durability.

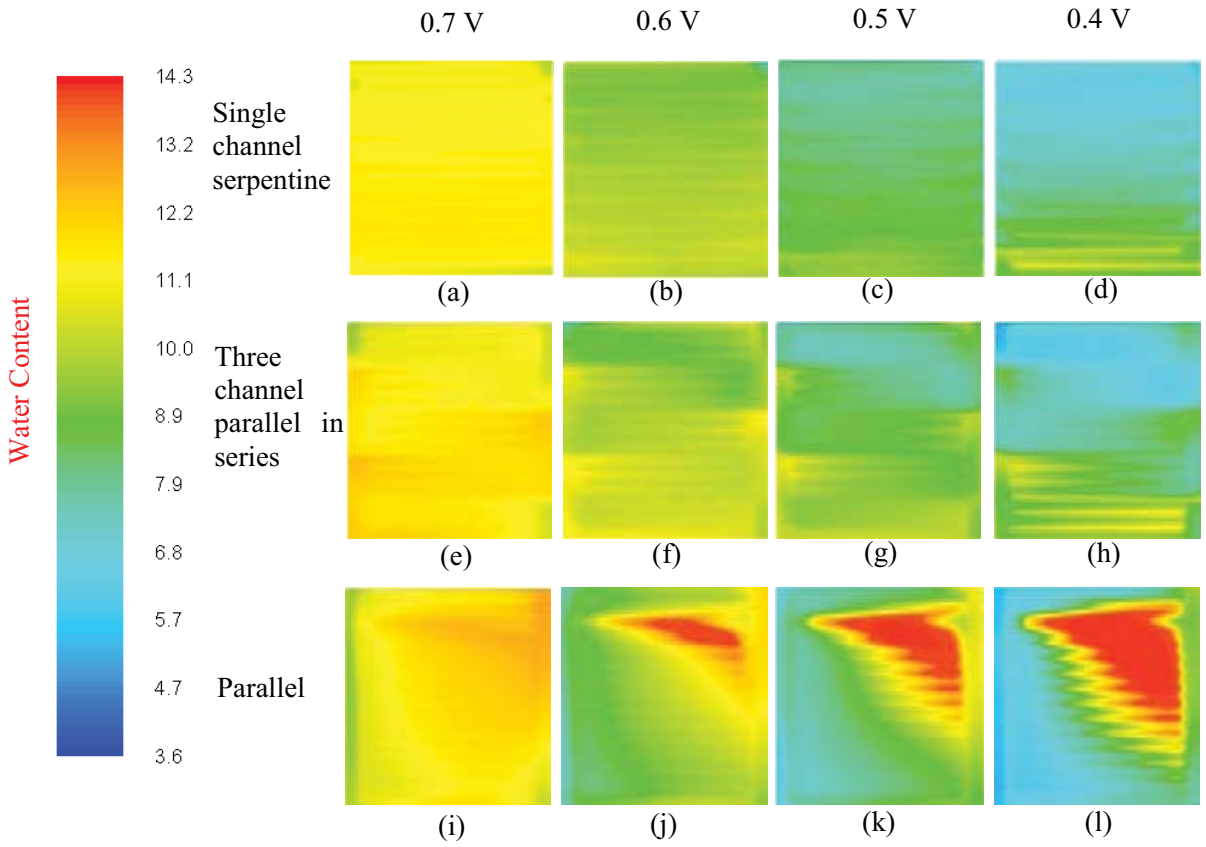

Fig. 4. The anode water content distribution

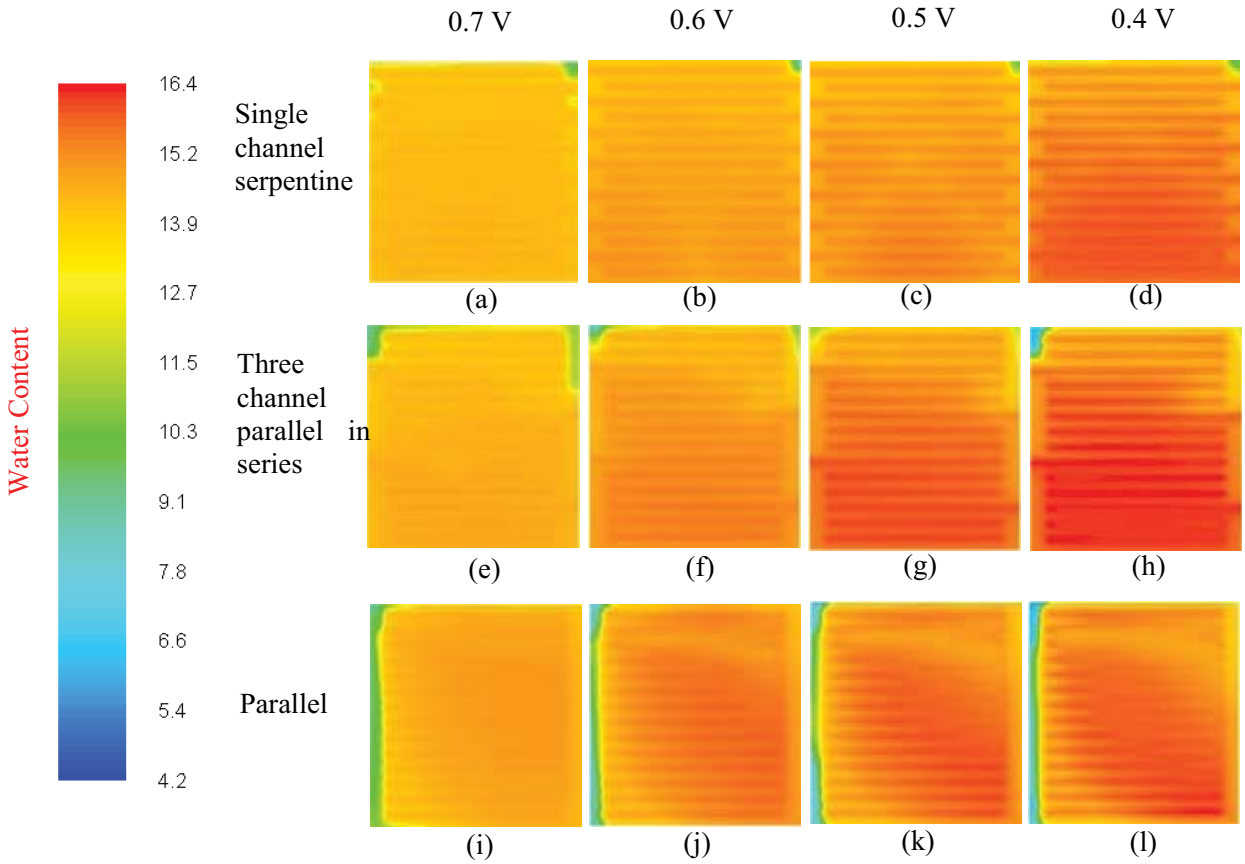

Fig. 5 The cathode water content distribution

Therefore, the cathode membrane water content distribution of each flow field at different cell voltages was also studied and displayed in Fig. 5.

The results coincided with the amount of transferring water in the electrodes in Fig. 5 in which, at the cathode side, the amount of water increased as the increasing of the current density and thus the decreasing of the cell voltage. However, the results of the parallel flow field were found contradictory to the statement mentioned earlier since its water content increased slightly when the cell voltage was decreased, which indicated that the flow field suffered a flooding situation and the voltage fell rapidly. As found earlier, the single channel

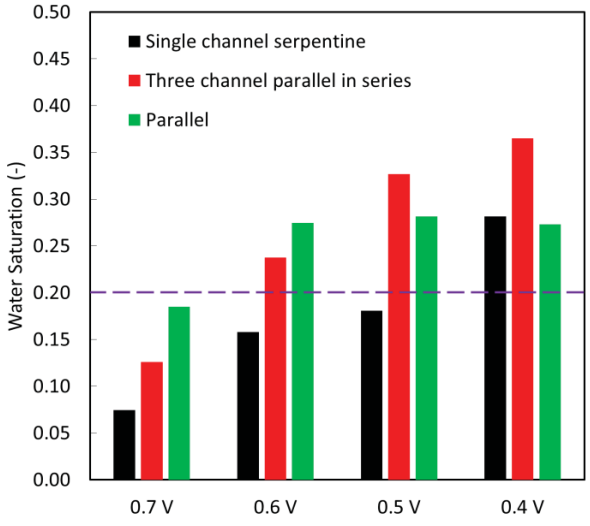

Fig. 6 The average cathode water saturation

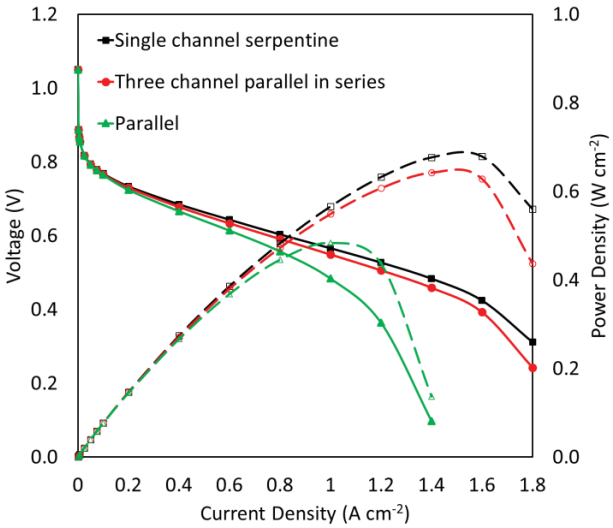

Fig. 7 IV Polarization curve

serpentine flow field provided the best uniformity in the cathode water content distribution, while the parallel contributed the worst. Note that the areas where the water content was higher than 14 was the area that full of liquid water based on the relation suggested by Springer at al. [6].

Fig. 6 displayed the average water saturation (volume fraction of liquid water) over the cathode CL volume. Since Wang and Van Nguyen [7] stated that the cell voltage would not stable if the average water saturation was higher than 0.2 during the operation, all flow fields would operate with stability at approximately 0.7 V. However, the single channel serpentine flow field could also be operated at the lower cell voltage (0.5-0.6 V) which can provide a higher power density as shown in Fig. 7. Although the voltage of 0.5 V was approximately the voltage which provided the highest power density, from the previous study [8], hydrogen peroxide can be formed electrochemically at potentials less than 0.6 V and thus the reduction of membrane durability. Therefore, the operating cell voltage of lower than 0.6 V was not recommended. Considering all studied aspects, the single channel serpentine flow field was suggested to be the best among the studied flow fields due to its higher power density, more uniform water content distribution, and lower amount of liquid water in the cathode CL. The suggested cell operating voltage was 0.6 V since it provided a much higher power density, had no stability problem in an operation, and was not affected by hydrogen peroxide. However, the real PEFC stacks used in a commercial-scale application used much larger cell areas. Therefore, a further study on the transport phenomena, including both heat and water, in much larger cell areas should be carried out and is ongoing in our research group.

IV. Conclusions

The model of PEFC with the different flow fields to investigate the water transports inside the PEFC was successfully developed. The results revealed that the membrane water content increased as an increasing current density at the low current density due to the low effect of electroosmotic drag. While the effect increased significantly after 0.2 A cm^{-2}, the membrane water content increased. Those results were also confirmed by the distribution of the water content at the both sides. However, there were some liquid water inside the MEA indicated by the water content and water saturation which would affect greatly on the cell performance, durability, stability and degradation. The single channel serpentine flow field was suggested to be the optimum designs for using with a small-scale PEFC MEA since it could be operated at the voltage lower than 0.7 V with stability. Since operating with the voltage lower than 0.6 V was found affecting the cell durability, the voltage of 0.6 V was recommended to be the operating cell voltage.

Acknowledgment

The authors would like to express our special thanks for the financial support funded by Thai-Nichi Institute of Technology under the project ID: 1408/A003.

References

[1] E. Birgersson and M. Vynnycky, “A quantitative study of the effect of flow-distributor geometry in the cathode of a PEM fuel cell,” *Journal of Power Sources*, vol. 153, no. 1, pp. 76–88, Jan. 2006.

[2] A. Kumar and R. G. Reddy, “Effect of gas flow-field design in the bipolar/end plates on the steady and transient state performance of polymer electrolyte membrane fuel cells,” *Journal of Power Sources*, vol. 155, no. 2, pp. 264–271, Apr. 2006.

[3] Y. Ferng and A. Su, “A three-dimensional full-cell CFD model used to investigate the effects of different flow channel designs on PEMFC performance,” *International Journal of Hydrogen Energy*, vol. 32, no. 17, pp. 4466–4476, Dec. 2007.

[4] ANSYS, *ANSYS FLUENT Fuel Cell Modules Manual*. USA: ANSYS, 2011.

[5] P. Charoen-amornkitt and N. Limjeerajarus, “Numerical study on the effect of flow field configurations on PEFC performance,” in *Proc. JCREN’14*, 2014.

[6] T. E. Springer, T. A. Zawodzinski, and S. Gottesfeld, “Polymer electrolyte fuel cell model,” *Journal of the Electrochemical Society,* vol. 138, no. 8, pp. 2334–2342, Aug. 1991.

[7] X. Wang and T. V. Nguyen, “An experimental study of the liquid water saturation level in the cathode gas diffusion layer of a PEM fuel cell,” *Journal of Power Sources,* vol. 197, pp. 50 – 56, Jan. 2012.

[8] W. Liu and D. Zuckerbrod, “In Situ Detection of Hydrogen Peroxide in PEM Fuel Cells,” *Journal of the Electrochemical Society*, vol. 152, no. 6, 2005.