Proceedings of The Canadian Society for Mechanical Engineering International Congress 2018
CSME International Congress 2018
May 27-30, 2018, Toronto, On, Canada

Numerical Simulation of Gas-Liquid Phenomena in the Cathode of a Stirred Tank Reactor Proton Exchange Membrane Fuel Cell

Xichen Wang, Biao Zhou[1], Mengcheng Jiang
Department of Mechanical, Automotive and Materials Engineering
University of Windsor
Windsor, ON, Canada, N9B 3P4

Abstract—Liquid water management is still a critical issue in the improvement of proton exchange membrane fuel cell (PEMFC) performance. In this work, for the first time, the liquid water behavior and transport inside the cathode of a PEMFC with a stirred tank reactor (STR) design, rather than the conventional PEMFC flow channel design, are numerically studied. The volume of fluid (VOF) method is employed in the simulation to track the gas-liquid interface. The capability of STR-PEMFC to reduce the liquid water flooding is also investigated and verified from the simulation, showing the potential of this channel-less type fuel cell in the further development.

Keywords-proton exchange membrane fuel cell; water management; volume of fluid; stirred tank reactor.

I. INTRODUCTION

Generally, fuel cells can be classified into five major types according to the electrolyte used: the phosphoric acid fuel cell (PAFC), the solid-oxide fuel cell (SOFC), the alkaline fuel cell (AFC), the molten carbonate fuel cell (MCFC), and the proton exchange membrane fuel cell (PEMFC) [1]. Among these types of fuel cells, PEMFC has been considered as one of the best potential candidates for vehicle and distributed power applications, mainly because of their low operating temperature, high power density, and good start-stop cycling durability. However, PEMFCs suffer from a water management problem that may cause a decrease in power output. Because the operating temperature of a PEMFC is under 100°C (usually 50–100°C), water generated from the electrochemical reaction easily condenses into liquid water and accumulates in the cathode.

Channels in the bipolar plate of the PEMFC can distribute the gas flow and remove excess liquid water, which is an effective way to improve the water management [2]. Many different types of flow field channel designs have been developed so far and most of them can be classified into three categories: parallel, serpentine, and interdigitated. In 2004, an innovative PEMFC with a porous layer connected to a stirred tank reactor (STR) rather than conventional gas flow channels was developed by Benziger et al. [3]. This STR PEMFC provides ideally suitable approaches to examine the fuel cell dynamics in the reaction and transport processes. The further experiments and analysis of the operating STR fuel cell were also reported by Hogarth and Benziger [4]. The results showed that compared to the conventional PEMFC with serpentine channels under humidified feeds or dry feeds, the STR fuel cell with dry feeds can provide higher power density and voltage at high current density. The features of this channel-less PEMFC include "dry-feeding, auto-humidification and self-draining" [4]. These research works by Benziger et al. [3, 4] not only revealed a simplified method for the PEMFC design, operation and control, but also indicated the remarkable advantages of auto-humidification in the commercialization of PEMFCs. However, no research to date has investigated the liquid water behavior and transport inside the STR PEMFC.

Comparing with other numerical models applied in the simulation of water management in PEMFCs such as the two-fluid model [5–7] and the mixture model [8–10], the volume of fluid (VOF) model [11] has the advantage of simulating the liquid water removal process by tracking the interface between the liquid and gaseous phases. In recent years, VOF method has been recognized as the most popular approach in the simulation of gas-liquid two-phase flow in PEMFCs [12] and a series of numerical studies have been reported in this area [13-19].

In this study, a three-dimensional, two-phase flow model is developed to study the gas-liquid dynamics in the cathode of a PEMFC with STR flow field design. The corresponding simulations are conducted by using the VOF method. The liquid water general transport and emerging process are presented and discussed.

II. NUMERICAL MODEL DESCRIPTION

A. Computational Domain and Boundary Conditions

The numerical simulation domain (Fig. 1) is an STR PEMFC cathode, having similar dimensions to Hogarth and Benziger's model [4], consisting of a porous layer connected to a stirred tank reactor rather than conventional gas flow channels.

The porous layer is 0.019 m × 0.019 m × 0.0003 m (in the X, Y and Z direction respectively). The attached STR is 0.015 m × 0.015 m × 0.0017 m and has an open rectangular plenum

[1] Corresponding Author and Principal Investigator: Dr. Biao Zhou, bzhou@uwindsor.ca, 1-519-253-3000 ext. 2630

as the gas flow field, minus four distributed pillars at intervals of 0.003 m in the X-Y plane. The dimension of these pillars is 0.003 m × 0.003 m × 0.0017 m. A gas inlet channel and an outlet channel with the same dimensions as the pillars are connected to the STR and distributed on the diagonal corners. Gravity acts along the diagonal of the plenum connecting the gas inlet and outlet channels and is directed toward the outlet. The porosity of the porous layer is 0.3.

The no-slip boundary condition is applied to the walls in STR model. The liquid mass flow rate is set as 1.331×10^{-4} kgs^{-1} and the gas mass flow rate is set as 6.615×10^{-5} kgs^{-1}. The pressure outlet boundary condition is applied at the outlet. The contact angle for the side walls of plenum, upper walls of plenum and walls of porous layer are 53°, 43° and 130° respectively.

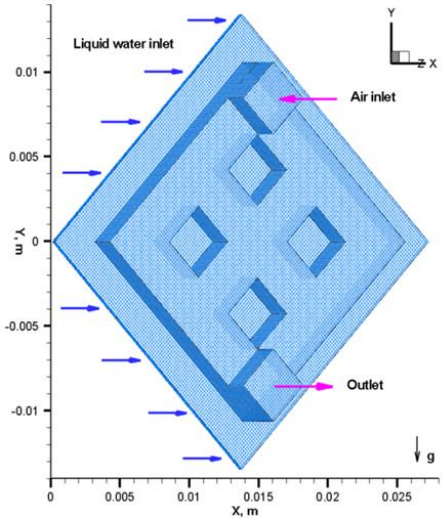

Figure 1. Computational domain of STR model.

B. Computational Methodology

The VOF method is employed in the present study to track the gas-liquid flow interface. Air is considered as the gaseous phase and liquid water is considered as the liquid phase. The fluid flow is laminar because of the low flow velocity and the small size of the channels. Heat transfer and phase changes are not considered in this study to reduce the computation time. The simulations are conducted using the commercial software package ANSYS Fluent. The governing equations for VOF method are the same as those employed in our previous work by Wang and Zhou [15].

C. Grid Independency

The computational domain of the STR model is meshed by 167,400 cells with a total volume of 4.602×10^{-7} m^3. The cell size is approximately 1.67×10^{-4} m in the X and Y directions, whereas the dimensions in the Z-direction are 1.4×10^{-4} m in the plenum domain and 5×10^{-5} m in the porous layer domain. This grid size has been validated for PEMFC-related simulations by Le et al. [14], and the grid independency check is achieved by increasing and decreasing certain percentages of grid cells.

III. Results and Discussion

A. General Process of Liquid Water Transport in STR Model

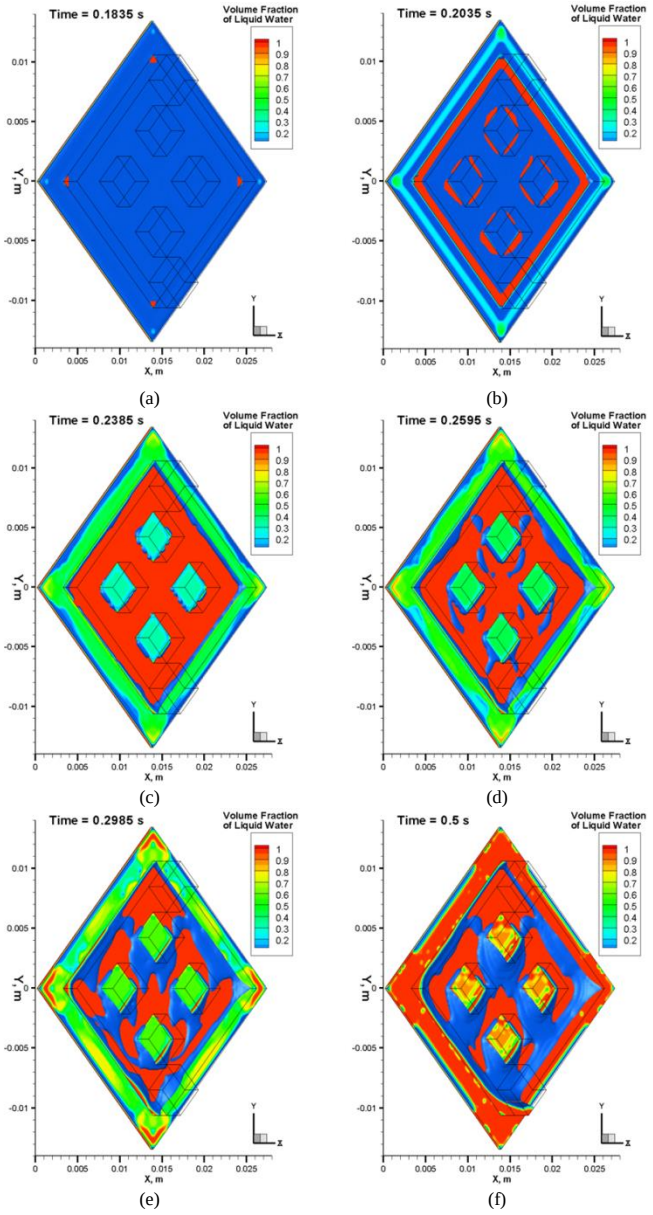

Figure 2. General liquid water transport in the STR model.

Fig. 2 shows the general process of liquid water transport over time at several selected time instants, which can be divided into the following sub-processes:

1) The liquid water generated from the electrochemical reaction is supplied continuously from the liquid inlet boundary, i.e., the back surface of the porous layer.

2) The liquid water migrating through the porous layer reaches the interface between the porous layer and the plenum, first at the four corners (Fig. 2(a)), then at the peripheral edges of the plenum domain and the edges of four pillars (Fig. 2(b)).

3) Liquid water passes through the interface and emerges along the sidewalls of the plenum domain and also at the sidewalls of each pillar (Fig. 2(c)). Some liquid water emerges from the circumjacent areas near the pillars as well (Fig. 2(d)).

4) The liquid water emerging from the peripheral edges of the plenum domain and from the edges of the pillars merge together with the liquid water from the circumjacent areas near the pillars, forming a "tooth shape" (Fig. 2(e)).

5) As more water enters the plenum, the areas below the pillars become flooded. With the force of gravity and the gas flow, the liquid water drains out of the computational domain through the outlet channel (Fig. 2(f)).

B. Liquid Water Distribution in Plenum

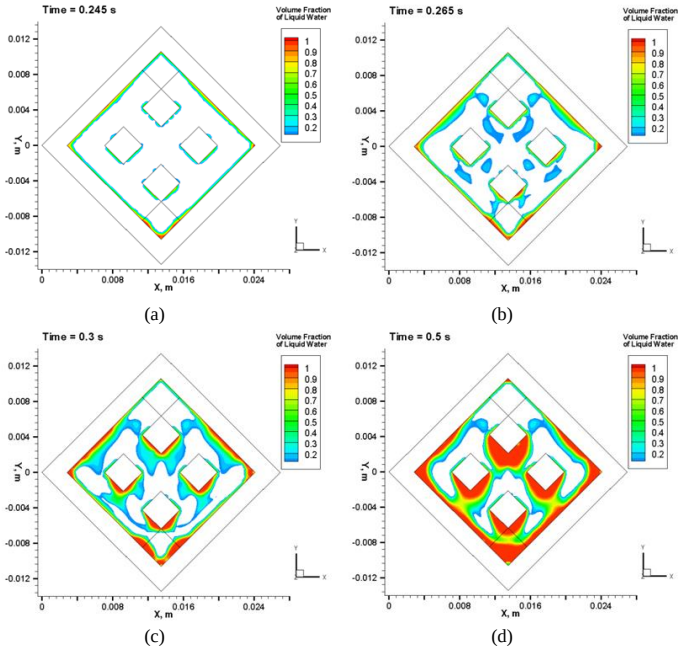

Figure 3. Liquid water distribution on plenum plane near interface (Z = 0.00031 m) in the STR model.

Fig. 3 shows the liquid water distribution on the X-Y plane extracted from the plenum domain at Z = 0.00031 m, which is very close to the interface of the porous layer. At first, liquid water emerges from the peripheral edges of the plenum domain and the edges of pillars (Fig. 3(a)), especially the lower edges. Subsequently, water emerges from the circumjacent areas near the lower sides of the four pillars and also the upper sides of the top pillar and gradually merges with the water from the edges of plenum (Fig. 3(b)), forming tooth-like shapes (Fig. 3(c)). Finally, the lower areas near the pillars become flooded, as well as the areas near the peripheral edges of the plenum (Fig. 4(d)). It can be observed that the liquid water appears mainly in the lower part of the plenum, which is caused by the direction of gravity and the locations of the inlet and outlet channels.

IV. CONCLUSIONS

In this study, the gas-liquid behavior inside an STR PEMFC is numerically investigated through the VOF method. The liquid water general transport process and liquid water distribution in the Plenum are presented and discussed. It is found that a PEMFC cathode with the STR design has a promising capability for water drainage, so that the fluid flow field in the STR model rarely becomes blocked or fully flooded, which weakens the reduction of the power density of fuel cell. These numerical results verify that self-draining liquid water is one of the merits of the STR PEMFC, which has been noted by Hogarth and Benziger [4].

ACKNOWLEDGMENT

The authors are grateful for the support from the Natural Sciences and Engineering Research Council of Canada (NSERC) and the University of Windsor.

REFERENCES

[1] O'hayre R, Cha SW, Prinz FB, Colella W. Fuel cell fundamentals. John Wiley & Sons; 2016 May 2.

[2] Li X, Sabir I. Review of bipolar plates in PEM fuel cells: Flow-field designs. International journal of hydrogen energy. 2005 Mar 31;30(4):359-71.

[3] Benziger J, Chia E, Karnas E, Moxley J, Teuscher C, Kevrekidis IG. The stirred tank reactor polymer electrolyte membrane fuel cell. AIChE Journal. 2004 Aug 1;50(8):1889-900.

[4] Hogarth WH, Benziger JB. Operation of polymer electrolyte membrane fuel cells with dry feeds: Design and operating strategies. Journal of Power Sources. 2006 Sep 22;159(2):968-78.

[5] Ye Q, Van Nguyen T. Three-dimensional simulation of liquid water distribution in a PEMFC with experimentally measured capillary functions. Journal of the Electrochemical Society. 2007 Dec 1;154(12):B1242-51.

[6] Sui PC, Kumar S, Djilali N. Advanced computational tools for PEM fuel cell design: Part 1. Development and base case simulations. Journal of Power Sources. 2008 May 15;180(1):410-22.

[7] Wu H, Berg P, Li X. Steady and unsteady 3D non-isothermal modeling of PEM fuel cells with the effect of non-equilibrium phase transfer. Applied Energy. 2010 Sep 1;87(9):2778-84.

[8] Meng H, Wang CY. Model of two-phase flow and flooding dynamics in polymer electrolyte fuel cells. Journal of the Electrochemical Society. 2005 Sep 1;152(9):A1733-41.

[9] Basu S, Li J, Wang CY. Two-phase flow and maldistribution in gas channels of a polymer electrolyte fuel cell. Journal of Power Sources. 2009 Feb 15;187(2):431-43.

[10] Mukherjee PP, Kang Q, Wang CY. Pore-scale modeling of two-phase transport in polymer electrolyte fuel cells—progress and perspective. Energy & Environmental Science. 2011;4(2):346-69.

[11] Quan P, Zhou B, Sobiesiak A, Liu Z. Water behavior in serpentine micro-channel for proton exchange membrane fuel cell cathode. Journal of Power Sources. 2005 Dec 1;152:131-45.

[12] Ferreira RB, Falcão DS, Oliveira VB, Pinto AM. Numerical simulations of two-phase flow in proton exchange membrane fuel cells using the volume of fluid method–A review. Journal of Power Sources. 2015 Mar 1;277:329-42.

[13] Jiao K, Zhou B. Accelerated numerical test of liquid behavior across gas diffusion layer in proton exchange membrane fuel cell cathode. Journal of Fuel Cell Science and Technology. 2008 Nov 1;5(4):041011.

[14] Le AD, Zhou B, Shiu HR, Lee CI, Chang WC. Numerical simulation and experimental validation of liquid water behaviors in a proton exchange membrane fuel cell cathode with serpentine channels. Journal of Power Sources. 2010 Nov 1;195(21):7302-15.

[15] Wang X, Zhou B. Liquid water flooding process in proton exchange membrane fuel cell cathode with straight parallel channels and porous layer. Journal of Power Sources. 2011 Feb 15;196(4):1776-94.

[16] Kang S, Zhou B. Numerical study of bubble generation and transport in a serpentine channel with a T-junction. International Journal of Hydrogen Energy. 2014 Feb 4;39(5):2325-33.

[17] Kang S, Zhou B, Jiang M. Bubble behaviors in direct methanol fuel cell anode with parallel design. International Journal of Hydrogen Energy. 2017 Aug 3;42(31):20201-15.

[18] Ferreira RB, Falcão DS, Oliveira VB, Pinto AM. Numerical simulations of two-phase flow in an anode gas channel of a proton exchange membrane fuel cell. Energy. 2015 Mar 15;82:619-28.

[19] Ferreira RB, Falcão DS, Oliveira VB, Pinto AM. 1D+ 3D two-phase flow numerical model of a proton exchange membrane fuel cell. Applied Energy. 2017 Oct 1;203:474-95.