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Modeling of the effect of ionomer volume fraction on water management for proton exchange membrane fuel cell

Pu He^a, Li Chen^a, Yu-Tong Mu^b, Wen-Quan Tao^{a,*}

^a Key Laboratory of Thermo-Fluid Science and Engineering, Ministry of Education, School of Energy & Power Engineering, Xi'an Jiaotong University, Shaanxi, China

^b School of Human Settlements and Civil Engineering, Xi'an Jiaotong University, Shaanxi, China

Abstract

Proton exchange membrane fuel cell (PEMFC) has been recognized as the most promising energy conversion device due to its outstanding merits, such as high energy efficiency, low pollution, low operating temperature and low noise. Due to the complicated process of water production and transportation in porous media, the water concentration can affect the distribution of species and ionic conductivity, thus, the water management has been regarded as one of the most critical issues for PEMFC. In this paper, a three dimensional multiphase non-isothermal model for the PEMFC performance prediction has been developed to study the effect of ionomer volume fraction on the performance of PEMFC. The numerical results show that the ionomer volume fraction of catalyst layer has an appreciable effect on the performance of PEMFC and water distribution in porous electrodes, the higher ionomer volume fraction in catalyst layer can be helpful to avoid the flooding problem in porous electrodes.

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Keywords: proton exchange membrane fuel cell; three dimensional multiphase non-isothermal model; water management; ionomer volume fraction; porous electrode

1. Introduction

Proton exchange membrane fuel cell (PEMFC) has attracted more and more attention during the past two decades because of its outstanding merits, such as high energy efficiency, low operating temperature and environmentally

* Corresponding author. Tel.: +86 29 82663232; fax: +86 29 82663232.

E-mail address: wqtao@mail.xjtu.edu.cn

friendly character. The operating principle of PEMFC is shown in Fig. 1. For PEMFC, water management has been one of the most important problems for the cell performance. Water content in PEMFC is influenced by the inlet gas humidity, the water produced during the reaction, phase change between the different state of water and the electro-osmotic drag (EOD). A lot of studies have been conducted to investigate the water management problems in PEM fuel cell [2-4], and the results reveal that the water management has a great influence on the cost and durability of PEMFC [5]. There are two major ways to reduce the power loss from the water management problem. One is by improving the electrode design, and the other is by optimizing the control strategy. For the electrode design, in order to improve the performance of gas diffusion layer (GDL), PTFE is loaded in the GDL, which is good for the removing liquid water [6-7]. In addition, adding a micro-porous layer (MPL) between the GDL and catalyst layer (CL) is also helpful [8-12]. In this study, a three-dimensional multiphase non-isothermal model is developed to investigate the effect of ionomer volume fraction on the performance of PEMFC.

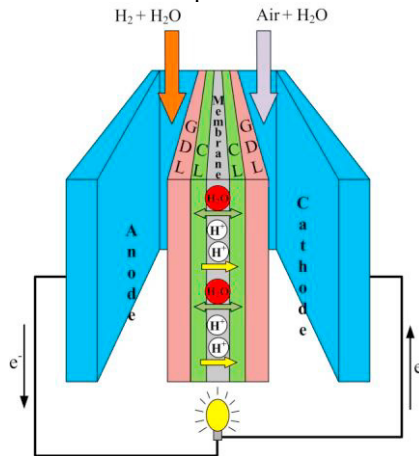


Fig. 1. Operating principle of PEMFC [1]

2. Numerical model

As shown in Fig. 2, the computational domain is consisted of bipolar plates (BPs), flow channels, GDLs, MPLs, CLs and membrane. The GDLs, MPLs, CLs and membrane have 14 mesh layers along the through-plane direction. The geometry and operating conditions are listed in Table 1.

The present model solves twelve conservation equations, including the conservation of mass and momentum of gas mixture, gas species, liquid water, membrane water, energy, electronic potential, ionic potential.

Mass of gas mixture (solved in flow channel, GDL, MPL, CL):

$$\nabla \cdot (\rho_g \vec{u}_g) = S_m \quad (1)$$

Momentum of gas mixture (solved in flow channel, GDL, MPL, CL):

$$\begin{aligned} \nabla \cdot \left(\frac{\rho_g \vec{u}_g \vec{u}_g}{\varepsilon^2 (1 - s_{lq})^2} \right) = -\nabla p_g + \mu_g \nabla \cdot \left(\nabla \left(\frac{\vec{u}_g}{\varepsilon (1 - s_{lq})} \right) + \left(\frac{-\vec{u}_g}{\varepsilon (1 - s_{lq})} \right) \right) \\ - \frac{2}{3} \mu_g \nabla \cdot \left(\nabla \cdot \left(\frac{\vec{u}_g}{\varepsilon (1 - s_{lq})} \right) \right) + S_u \end{aligned} \quad (2)$$

Gas species (i : H₂, O₂, H₂O. Solved in flow channel, GDL, MPL, CL):

$$\nabla \cdot (\rho_g \vec{u}_g Y_i) = \nabla \cdot (\rho_g D_i^{\text{eff}} \nabla Y_i) + S_i \quad (3)$$

Liquid pressure (solved in GDL, MPL, CL):

$$\nabla \cdot \left(\rho_l \frac{Kk_l}{\mu_l} \nabla P_l \right) + \dot{m}_l = 0 \tag{4}$$

Membrane water content (solved in membrane, CL):

$$-\frac{\rho_{mem}}{EW} \nabla \cdot (D_{mw}^{eff} \nabla \lambda_{mw}) = S_{mw} \tag{5}$$

Electronic potential (solved in BP, GDL, MPL, CL):

$$0 = \nabla \cdot (\kappa_{ele}^{eff} \nabla \phi_{ele}) + S_{ele} \tag{6}$$

Ionic potential (solved in membrane, CL):

$$0 = \nabla \cdot (\kappa_{ion}^{eff} \nabla \phi_{ion}) + S_{ion} \tag{7}$$

Energy (solved in the entire domains):

$$\nabla \cdot \left((\rho C_p \vec{u}_g)_n^{eff} T \right) = \nabla \cdot (\kappa_{n,sl}^{eff} \nabla T) + S_E \tag{8}$$

The boundary conditions and corresponding source terms for the twelve conservation equations can be referred to [13].

Table 1. Cell properties and operating conditions.

Parameters	Value
Channel length; width; height; rib width	100; 0.5; 1.0; 0.5 mm
Thicknesses of GDL; MPL; CL; Membrane (Nafion 212)	0.25; 0.01; 0.03; 0.0508 mm
Relative humidity of inlet gas	$Ra_a = 0.84; Ra_c = 0.59$
Operating temperature	$T_0 = 353.15$ K
Ionomer volume fraction in CL	$\omega = 0.23, 0.27$
Anode/cathode stoichiometry	2.0; 1.5

3. Numerical procedure

In this study, the conservation equations are solved by Fluent, and the user-defined functions (UDF) coded by C language. In order to ensure the accuracy, a strict convergence criterion of 1.0×10^{-8} is used. The computational domain in Figure 2 includes 80,000 cells. The grid independent study was carried out and the results showed that 80000 cells can get nearly grid-independent solutions.

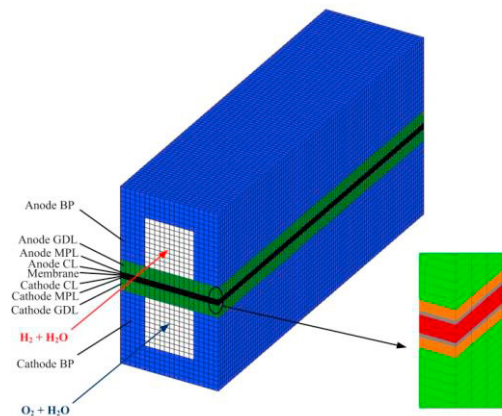


Fig. 2. Computational domain

In order to verify this model and the developed code, the polarization curve presented in [14] is predicted by our code and the results are compared in Fig. 3. The operating conditions and geometry parameters are all the same with [14], and the predicted polarization curve agrees well with the experiment.

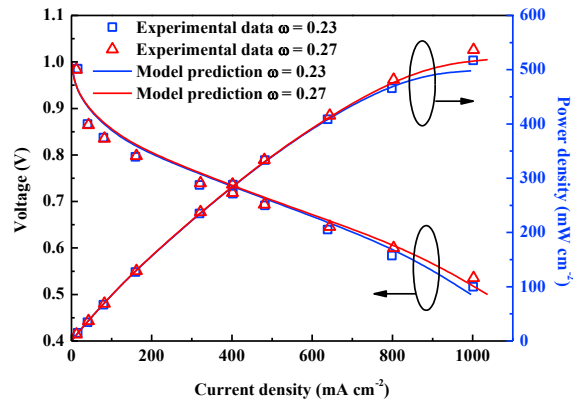


Fig. 3. Comparison of model prediction and experimental data [14]

4. Results and discussion

Based on this model, two different ionomer volume fractions of CL (0.23 and 0.27) are considered.

The effect of the ionomer volume fraction of CL on the variation of voltage loss is shown in Fig. 4. It can be found that except for the ohmic loss, the activation loss and concentration loss are higher for the low ionomer volume fraction of CL, which is much more significant under higher current density. Moreover, with the increase of current density, the activation loss and concentration loss increase nonlinearly, while the ohmic loss increases linearly.

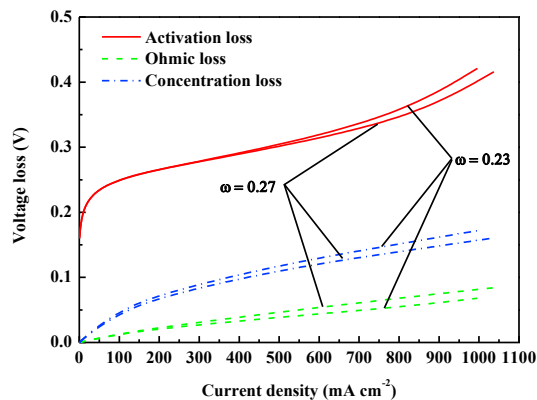


Fig. 4. Variation of voltage loss with current density at two ionomer volume fraction

In this study, the continuous of liquid pressure between two different porous electrodes is considered. Due to the different properties of the porous electrode, such as the contact angle, porosity, permeability, the liquid saturation between two porous electrodes is uncontinuous during the water transport. As shown in Fig. 5, it can be found that there exist liquid saturation jump between two different porous electrodes, and the liquid saturation in the cathode CL is much higher than the liquid saturation in the anode porous electrodes. Comparing with two different ionomer volume fractions of CL, there exists more liquid water in porous electrodes for the lower ionomer volume fraction of

CL especially in the cathode. This suggests that the higher ionomer volume fraction in CL is better for the avoidance of flooding problem in porous electrodes.

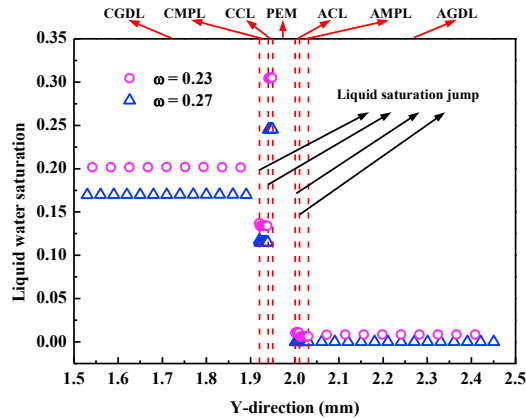


Fig. 5. Liquid distribution in porous electrode membrane at 0.6 V

Fig. 6 shows the variation of membrane water content with current density. It can be found that the membrane water in anode CL is higher than the membrane and cathode CL at low current density due to the better humidification in anode, and with the increase of current density, there is much more water generated in cathode CL, adding the effect of electro-osmotic drag, the membrane water in cathode CL accumulates rapidly, which caused the membrane water content in cathode CL increases sharply with the increase of current density. On the other hand, comparing with the two different ionomer volume fraction in CL, the membrane water content for the higher ω maintains lower membrane water content.

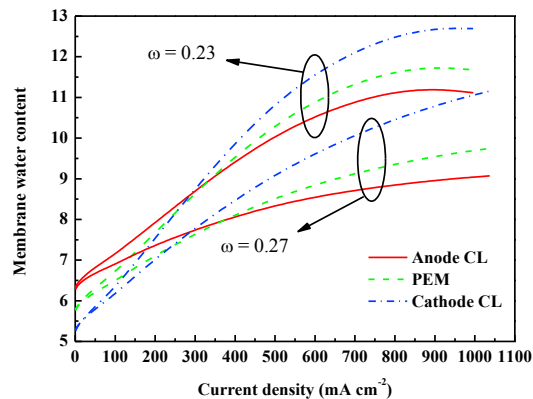


Fig. 6. Variation of membrane water content with current density at two ionomer volume fraction

5. Conclusions

In this study, a three-dimensional multiphase non-isothermal model for PEMFC is developed to investigate the effect of ionomer volume fraction of CL on the water distribution inside the electrode and the cell performance. It can be found that the ionomer volume fraction of CL has an appreciable effect on the performance and water distribution in porous electrodes. With the increase of ionomer volume fraction in CL, the activation loss and concentration loss can be reduced, moreover, the higher ionomer volume fraction in CL can be helpful to avoid the flooding problem in porous electrodes.

Acknowledgements

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References

- [1] Jiao K., He P., Du Q., Yin Y., 2014. “Three-dimensional multiphase modeling of alkaline anion exchange membrane fuel cell”. *International Journal of Hydrogen Energy*, 39, pp. 5981-5995.
- [2] Berning T., Djilali N., 2003. “A 3D, multiphase, multicomponent model of the cathode and anode of a PEM fuel cell”. *Journal of the Electrochemical Society*, 150, pp. 1589-1598.
- [3] Wang Y., 2008. “Modeling of two-phase transport in the diffusion media of polymer electrolyte fuel cells”. *Journal of Power Sources*, 185, pp. 261-271.
- [4] Schmittinger W., Vahidi A., 2008. “A review of the main parameters influencing long-term performance and durability of PEM fuel cells”. *Journal of Power Sources*, 180, pp. 1-14.
- [5] Jiao K., Li X., 2011. “Water transport in polymer electrolyte membrane fuel cells”. *Progress in Energy and Combustion Science*, 37, pp. 221-291.
- [6] Shimpalee S., Beuscher U., Van Zee J.W., 2007. “Analysis of GDL flooding effects on PEMFC performance”. *Electrochimica Acta*, 52(24), pp. 6748-6754.
- [7] Gurau V., Bluemle M.J., De Castro E.S., Tsou T.M., Mann J.A., Zawodzinski T. A., 2006. “Characterization of transport properties in gas diffusion layers for proton exchange membrane fuel cells”. *Journal of Power Sources*, 160(2), pp. 1156-1162.
- [8] Lu Z., Daino M.M., Rath C., Kandlikar S.G., 2010. “Water management studies in PEM fuel cells, part III: dynamic breakthrough and intermittent drainage characteristics from GDLs with and without MPLs”. *International Journal of Hydrogen Energy*, 35(9), pp. 4222-4233.
- [9] Hasan K.A., Kunal K., Brant P., Aaron P., Ela H., Jon P., 2007. “Experimental investigation of the role of a microporous layer on the water transport and performance of a PEM fuel cell”. *Journal of Power Sources*, 170, pp. 111-121.
- [10] Meng H., 2009. “Multi-dimensional liquid water transport in the cathode of a PEM fuel cell with consideration of the micro-porous layer (MPL)”. *International Journal of Hydrogen Energy*, 34, pp. 5488-5497.
- [11] Phengxay D., Takashi S., Shohji T., Shuichiro H., 2013. “Effect of liquid water distribution in gas diffusion media with and without microporous layer on PEM fuel cell performance”. *Electrochemistry Communications*, 34, pp. 239-241.
- [12] Cho J., Oh H., Park J., Min K., Lee E., Jyoung Y., 2014. “Effect of the micro porous layer design on the dynamic performance of a proton exchange membrane fuel cell”. *International Journal of Hydrogen Energy*, 39, pp. 459-468.
- [13] Jiao K., Li X.G., 2009. “Three-dimensional multiphase modeling of cold start processes in polymer electrolyte membrane fuel cells”. *Electrochimica Acta*, 54, pp. 6878-6891.
- [14] Kim K.H., Lee K.Y., Lee S.Y. et al., 2010. “The effects of relative humidity on the performances of PEMFC MEAs with various Nafion ionomer contents”. *International Journal of Hydrogen Energy*, 35(23), pp. 13104-13110.