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The Combined Effects of Water Transport on Proton Exchange Membrane Fuel Cell Performance

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A complete set of equations of two-phase water flow within the cathode, anode and membrane for one-dimensional single cell model are developed. Calculations of integrals are only needed in the membrane and the two-phase region of cathode diffuser. The proposed approach greatly reduces the complexity of the model equations, and only iterations of a single algebraic equation are required to obtain final solutions. The combined effects of water transport on proton exchange membrane fuel cell performance are represented in the polarization curve. The simulation results show that higher amount of water may helpful for membrane hydration, but not good for cathode flooding. Hereby, optimal values of temperature, relative humidity, air stoichiometry and pressure can be obtained.

1. Introduction

Proton exchange membrane fuel cell (PEMFC) is considered as a promising candidate for mobile source due to its advantages such as fast start-up, high power density, and zero/low emission. It works on the principle of separation of the oxidation of a fuel such as hydrogen and reduction of an oxidant such as oxygen from the air, with heat and water as typical by-products. Additionally water is introduced through both anode and cathode gas streams because of the demand of humidification (Ji and Wei, 2009). Water management is of vital importance to ensure stable operation, high efficiency and to maintain the power density of PEM fuel cells in the long run (Chen and Tong, 2017). Poor water management can cause membrane dehydration (Murugesan and Senniappan, 2013) or cathode flooding (Aiyejina and Sastry, 2012). Through the novel application of MRI (Minard et al., 2006) and EIS (Kadyk et al., 2009), valuable information regarding liquid water accumulation and transport behavior has been revealed in operating PEM fuel cells (Chatrattanawet et al., 2016). For future investigations more attention should be paid to the fundamental understanding and systematic data of water transport in each component of the MEA under varied operating conditions (Dai et al., 2009). At present, many transport phenomena during fuel cell operation cannot be directly observed or measured. Thus, inverse modelling has been a powerful tool to gain qualitative insights into the dynamics of liquid water transport and its effect on fuel cell performance. In addition to single phase models (Jeng et al., 2004), several two-phase flow models for the cathode of PEMFC have been proposed to simulate the effects of the gas and liquid water hydrodynamics on cell performance. These models were based on the computational fluid dynamics approach (Xing et al., 2014), obtained by solving transport equations governing conservation of mass, momentum, species, energy, and charge by taking into account a possible liquid–vapor phase-change. In this case, calculations became difficult and numerical resolution was sensitive to different parameters (Xing et al., 2016). To reduce the simulation complexity, the simplified models were proposed by Kang (2015) and Abdollahzadeh et al. (2014).

In previous one-dimensional models the liquid water saturation was usually taken as constant, in fact the degree of liquid water saturation in GDL was closely related to cathode flooding (Li et al., 2008). Otherwise, water was present as vapor, liquid or dissolved in the ionomer. The effects of water in all three phases on pore flooding and membrane dehydration, were investigated (Gerteisen et al., 2009). Furthermore, the effects of

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operating conditions on the performance of PEMFC regarding membrane dehydration and cathode flooding ware studied (Hu et al., 2016).

The effect of operating condition on PEMFC performance has been discussed widely, but it is not fully presented in view of water transport. Especially the combined effects of water transport on membrane hydration and cathode flooding are not explained clearly. In this paper, according to the water transport balance flowing in and out PEMFC, membrane water content is estimated by an improved average relative humidity representing the degree of membrane hydration. And a one-dimensional model is presented to investigate the effect of water transport on cathode oxygen mass transfer representing the degree of cathode flooding, especially the presence of liquid water. The performance of PEMFC under different operating conditions based on water transport is studied.

2. Model development

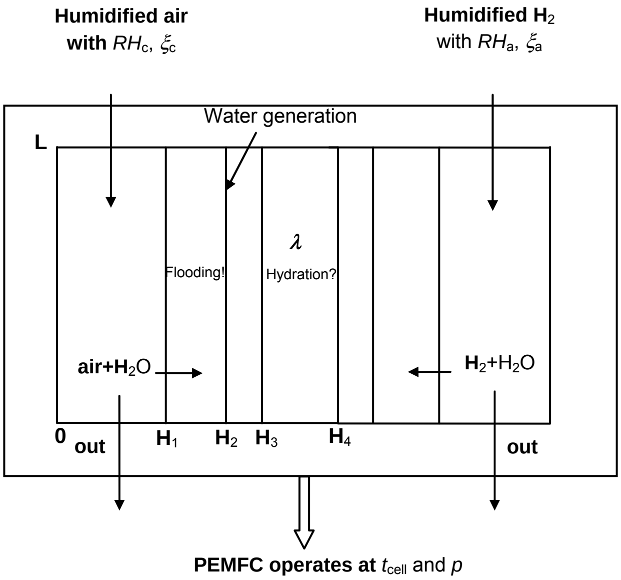


Figure1: The modeling domain for the cathode of PEMFC

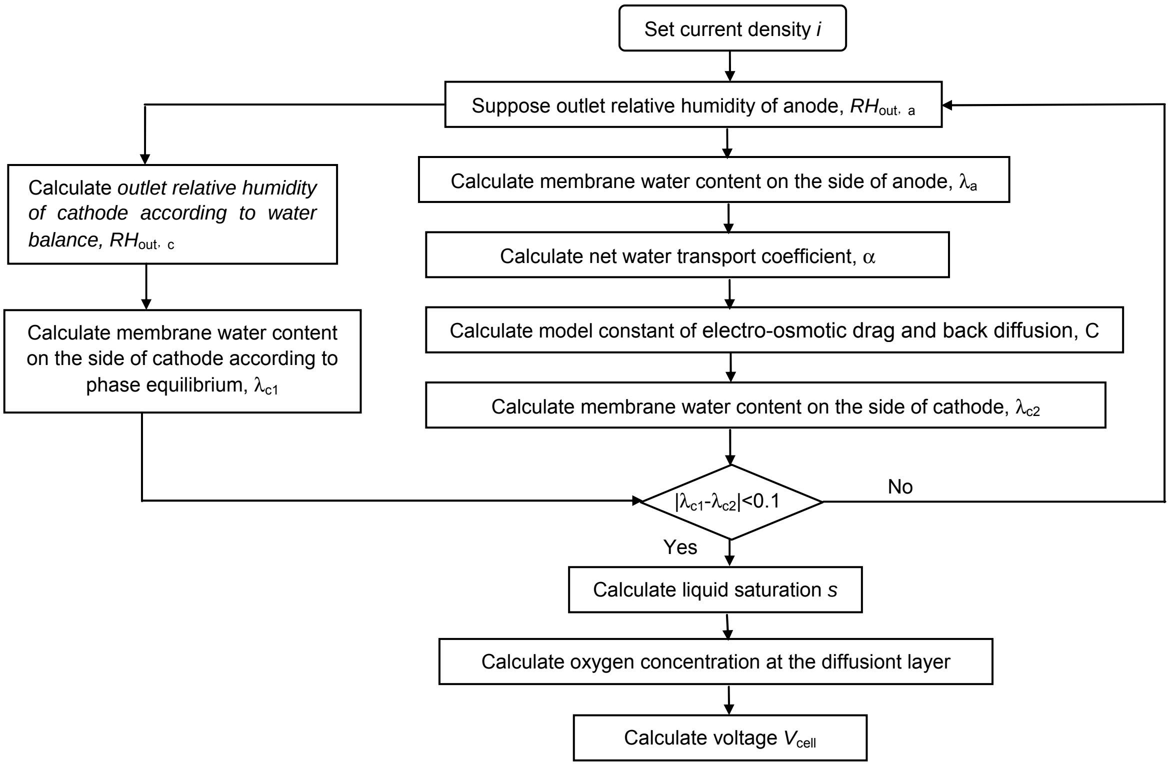


Figure 2: Numerical scheme of water transport on the PEFMC performance

$$m_{in,c} + m_{in,a} + m_{gen} = m_{out,c} + m_{out,a} \tag{1}$$

$$m^{H_2O} = m_{in,a} + m_{in,c} + m_{gen} - m_{out,a}^{sat} - m_{out,c}^{sat} \tag{2}$$

3. Results and discussions

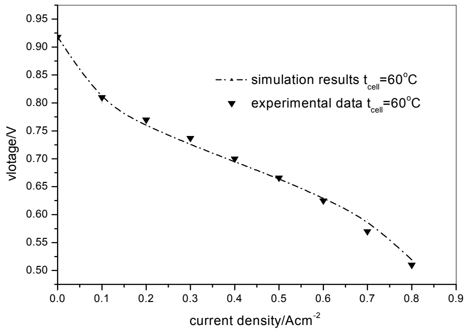


Figure 3: Comparison between the modeling results in this paper and experimental data in Yan et al.

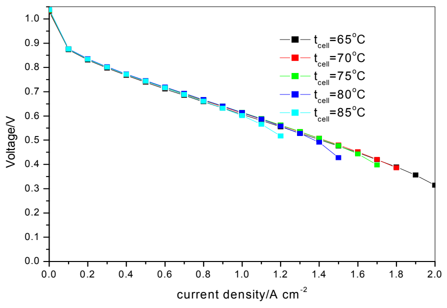


Figure4: Effect of cell temperature on PEMFC Performance

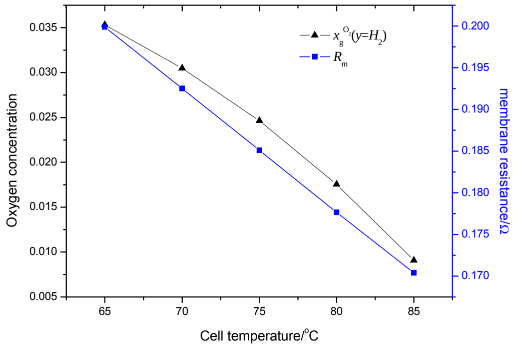


Figure 5: Oxygen concentration and membrane resistance at different cell temperatures

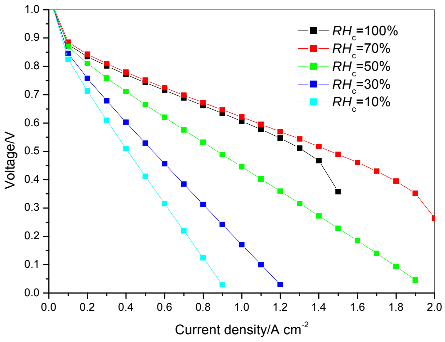
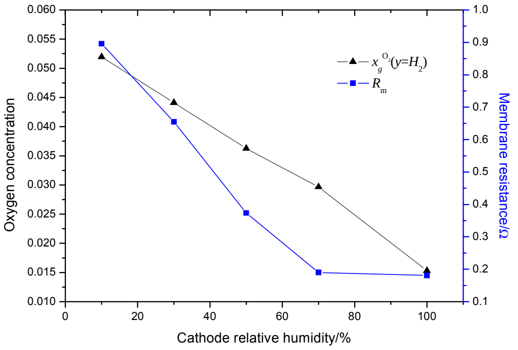


Figure 6: Effect of cathode relative humidity on PEMFC performance

In order to validate the two-dimensional GDL model associated with the thin-film assumption for the catalyst layer and the calculation polarization curve, the fuel cell voltage is calculated, and a comparison is made between the simulation results and experimental data in Huang et al. (2007). The results of the present model shown in Figure 3 are in agreement with experimental data.

As described in Figure 4, the increase of the fuel cell performance with the increase of the cell temperature can be explained by two reasons. First, at high temperature the exchange current density increases, and second, the proton conductivity of Nafion membrane also increases. The membrane resistance decreases slightly in Figure 5 meanwhile the oxygen concentration at the catalyst layer also decreases as shown in Figure 5. Especially when RH_a =100 % and RH_c =100 %, the inlet water mass flow is still high. Therefore, it is difficult to evacuate water with the exhaust cathode flow, and the consequence is that the diffusion layer could become flooded on the cathode side. So the increase of operation temperature leads to a better performance of fuel cell from 65 °C to 80 °C. At 85 °C the performance of fuel cell becomes worse. This behavior could be due to the fact that the positive effect on the membrane conductivity of the combination is not compensated by the negative effect on the oxygen mass transport caused by the flooding. This conclusion is consistent with the result of Yan et al. (2006).



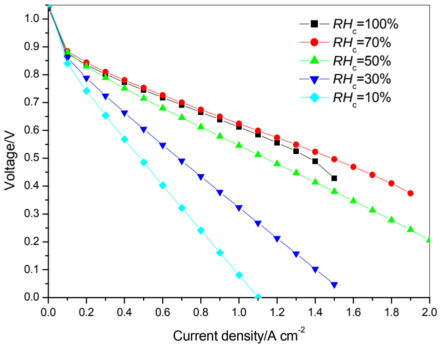
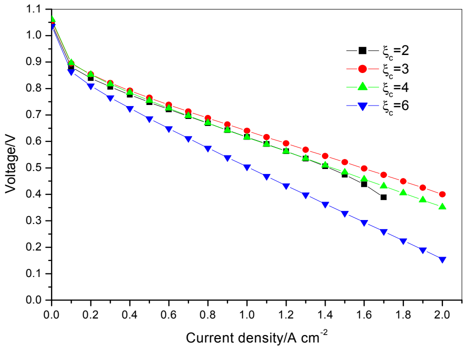


Figure 7: Oxygen concentration and membrane resistance at different cathode relative humidity

Figure 8: Effect of cathode relative humidity on PEMFC performance

In comprehensive consideration, the *i*-V_{cell} curves at different cathode relative humidity are shown in Figure 6. We can see that the cell performance can be improved with the increase of relative humidity because the presence of liquid water is beneficial to membrane hydration shown in Figure 7 and reduces the ohmic overpotential at low relative humidity. But with its further rise, the cell performance becomes worse because excess water will result in the mass transfer limitation. The decrease of the effective porosity of the gas diffusion layers and the decrease of the reactant concentration in Figure 6 may contribute to this phenomenon. When RH_c =100%, the cathode tends to be flooded by excessive water from reaction product and humidified air flow. Therefore, the oxygen transfer is blocked by liquid water in the porous medium so that the concentration of oxygen decreases in the active surface area of catalyst, leading to severe concentration losses.

When the anode relative humidity increases to 100%, the cell performance becomes better in Figure 8. The increase of anode relative humidity is beneficial to membrane hydration but has no effect on the cathode oxygen transport. Overall, the best performance occurred at low air relative humidity and high hydrogen relative humidity. The same tendency can be found in Yan et al. (2006), Hung et al. (2007) and Wang et al. (2003).



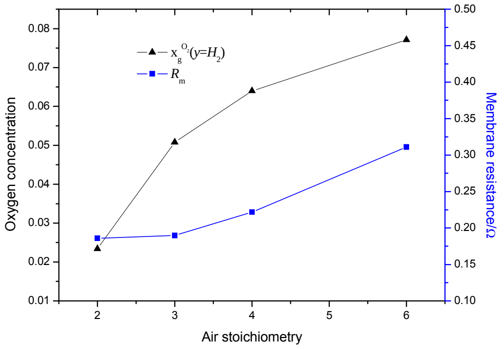
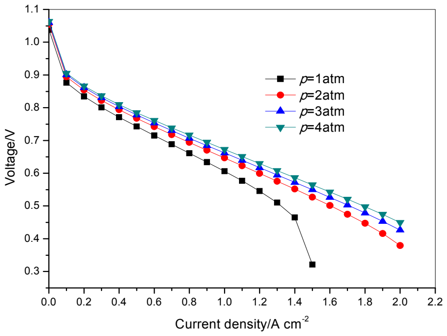


Figure 9: Effect of air stoichiometry on PEMFC Performance

Figure 10: Oxygen concentration and membrane resistance at different air stoichiometry

It is evident from Figure 9 that as the air stoichiometry increases, the fuel cell performance is improved gradually. The air stoichiometry influences both the availability of oxygen as well as the humidity of the membrane. A high air flow rate increases the rate of water removal that causes drying of the membrane in Figure 10. However, the high air flow rate increases the availability of oxygen at the cathode catalyst layer in Figure 9 which improves the performance of the fuel cell. The improvement is not apparent from ξ_c=3 and the cell performance becomes bad for ξ_c=4 because a distinct increase of ohmic overpotential from ξc=3 to ξc=4 can be seen due to the increase of water discharge. So the increased gas flow rate is beneficial to fuel cell operation if the positive effect of increased availability of oxygen offsets the negative effects of membrane dehydration. The same result can be found in Yan et al. (2006), but the decreasing tendency doesn't occur in Huang et al. (2007) and Jang et al. (2008) because the air stoichiometry is not high enough in their experimental conditions.



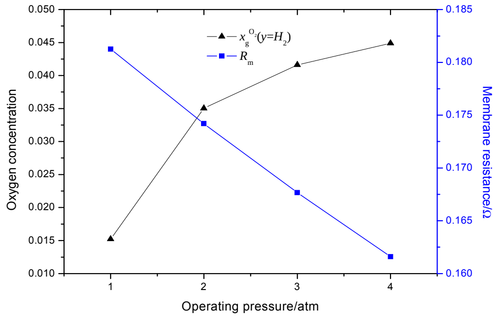


Figure11: Effect of operating pressure on PEMFC Performance

Figure 12: Oxygen concentration and membrane resistance at different operating pressure

The performance of the fuel cell improves with the increase of air pressure as shown in Figure 11. The higher open circuit voltage at the higher pressures can be explained by the Nernst equation. Another reason for the improved performance is that the oxygen concentration increases in Figure 12 with increasing operating pressure. At the same time, the membrane resistance in Figure12 shows a decline due to the presence of liquid water. The same result is presented in Yan et al. (2006), Huang et al. (2007), Jang et al. (2008) and Wang et al. (2003).

4. Conclusions

The cell performance is predicted based on water transport balance flowing in and out PEMFC. Simulation results show good agreement with experimental data. The presence of water has positive effect on membrane hydration and negative effect on cathode flooding. So the operating conditions have an optimal value to sustain the better cell performance in this study.

1) The cell temperature should not be too high or too low for optimal cell performance, and the optimal value is about 80°C in this paper. At high relative humidity, the increase of cell temperature creates cathode flooding, and at low relative humidity, the increase of cell temperature leads to membrane dehydration due to water evaporation.
2) The best cell performance occurs at moderate air relative humidity (70%) and high hydrogen relative humidity (100%). That is due to the fact that the positive effect on the membrane conductivity of the combination is not compensated by the negative effect on the oxygen mass transport associated with the flooding.
3) Air stoichiometry is 3 for better cell performance in this paper because the negative effects of membrane dehydration offset the positive effects of increased availability of oxygen if it is increased further.
4) The performance of the fuel cell improves with the increase of air pressure. But the effect is not obvious with its further increase such as from *p*=3atm to 4atm.

Acknowledgments

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