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Transport Water and Performance of Proton Exchange Membrane Fuel Cell

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Abstract: A two-dimensional, steady state model for proton exchange membrane fuel cell (PEMFC) is presented. The model is used to describe the effect of membrane thickness on the water distribution in the membrane, and performance of PEMFC. Simulations with a numerical code for FORTRAN 6.6, the simulation results show that the distribution of water of membrane increases with decreasing the thickness of membrane, and water content gradient across the membrane is high for thick membrane. It seems that the thinner the membrane to be chosen as electrolyte, the better the cell performance.

Keywords:

Proton exchange membrane fuel cell, Water transport, Mathematical mode, Performance.

1. Introduction

Proton exchange membrane fuel cells (PEMFCs) directly convert the chemical energy of fuels into electrical energy without the combustion process that is vital for the operation of the heat-engine cycle [1]-[3]. For automobile applications of PEMFCs, pure hydrogen is supplied to the anode of the cell from a high-pressure tank, whereas hydrogen reformed from town gas is supplied for on-site power generation. As an oxidant, ambient air is supplied to the cathode of the cell after purification to remove contaminants such as SO_2, NO_2, and NH_3, which can cause a severe degradation in the performance of the cell.

The PEMFC has a layered structure, as shown in Fig. 1. The polymer electrolyte membrane (PEM) plays the role of an electrolyte, allowing transport of ions (H^+) from the anode to the cathode. The catalyst layer, which contains the electrodes, is sandwiched between an electrically conductive porous diffusion medium and the membrane.

However, there are still many problematic issues that must be overcome for this technology to be efficient and practical. One major problem is water management, which requires careful attention during operation of a state-of-the-art PEMFC. At low humidity, the proton exchange membrane and electrode assembly (MEA) lose water, which leads to a rapid increase in ohmic resistance. Conversely, if too much liquid water is present in the cell, then the pores in the electrodes are filled with water and the passage of reactant gases becomes obstructed. Therefore, the cell operation conditions and MEA components have to be well matched in order to avoid membrane dehydration and cathode flooding. In addition to experimental approaches, water management models are useful to achieve understanding of the processes that govern water transport to assist optimization of the fuel cell operating conditions and relevant electrode structures [4].

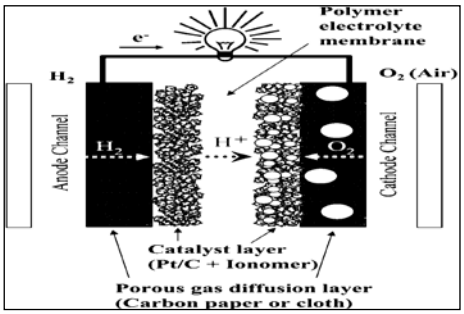

Figure 1: Schematic of a proton exchange membrane fuel cell [5].

The aim of the present work was to develop a model that describes, in steady state, the water transport in the membrane and the fuel cell performance, at different value of membrane thickness. The model includes the porous media of membrane electrode assembly (MEA) in the PEMFC.

2. Analysis

The schematic diagram of the physical system under consideration is shown in Fig. 2, in which the PEMFC consists of a proton exchange membrane in the middle, two gas diffuser layers, and two catalyst layers are considered as interface. To simplify the analysis in the present study, the following assumptions are invoked: (1) stationery model; (2) single phase model; (3) the gas diffuser layers, catalyst layers, and the membrane are considered to be isotropic porous media; (4) the membrane is considered impermeable for the gas phase; and (5) catalyst layers as reactive boundaries.

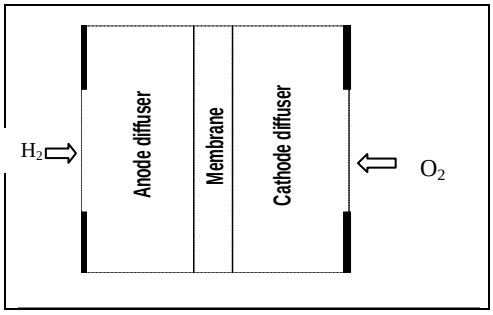

Figure 2: Schematic diagram of 2D PEMFC model.

With the above assumptions, the gas transport equations for the two-dimensional PEM fuel cell can be described as follows.

2.1. Continuity equation

$$\frac{\partial \boldsymbol{\rho\varepsilon} U}{\partial x} + \frac{\partial \boldsymbol{\rho\varepsilon} V}{\partial y} = 0 \qquad (1)$$

2.2. Momentum equations

$$U = -\frac{K_p}{\mu . \varepsilon} \nabla P \qquad (2)$$

$$V = -\frac{K_p}{\mu . \varepsilon} \nabla P \qquad (3)$$

2.3. Species concentration equation

$$U\frac{\partial \varepsilon C_k}{\partial x} + V\frac{\partial \varepsilon C_k}{\partial y} = \frac{\partial}{\partial x}\left(D_k^{eff}\frac{\partial C_k}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_k^{eff}\frac{\partial C_k}{\partial y}\right) + S_k \qquad (4)$$

Table 1: Detailed expressions of the source term in the governing equations.

	S_K	ε
Diffuser layer	0	ε_d
Catalyst layer	H_2: $S_{H_2} = -\frac{1}{2F}J_a$ O_2 : $S_{O_2} = \frac{1}{4F}J_c$ H_2O : $S_{H_2O} = -\frac{1}{2F}J_c$	ε_{cat}
Membrane	0	ε_m

The source term S_k, in the concentration equations and the parameter ε are listed in Table 1. Darcy's law states that the velocity vector is determined by the pressure gradient, the fluid viscosity, and the structure of the porous media represented in equations (2) and (3) in the x- and y-directions, respectively. k_p the permeability, and D_k^{eff} the effective diffusion coefficient of the k composition of fuel reactant. In Eq. (4), S_k is the rate of consumption or production of each species is different reactant gases, e.g. S_k is $-j_a/2FC_{total,a}$ for hydrogen, $-j_c/4FC_{total,c}$ for oxygen, and $-j_c/2FC_{total,c}$ for water vapor. The parameters j_a and j_c indicate the current densities at the anode and cathode sides, respectively, and can be described by the following Butler–Volmer equations:

$$J_a = a\, j_0^{ref}\left(\frac{C_{H_2}}{C_{H_2}^{ref}}\right)\left[e^{\frac{\alpha_a^c F}{RT}\eta_a} - \frac{1}{e^{\frac{\alpha_c^c F}{RT}\eta_a}}\right] \qquad (5)$$

$$J_c = a\, j_0^{ref}\left(\frac{C_{O_2}}{C_{O_2}^{ref}}\right)\left[e^{\frac{\alpha_a^c F}{RT}\eta_c} - \frac{1}{e^{\frac{\alpha_c^c F}{RT}\eta_c}}\right] \qquad (6)$$

2.3. Fuel cell performance

The cell potential is expressed as:

$$V = V_{OC} - \eta_{act} - \eta_{ohm} - \eta_{conc} \qquad (7)$$

Where V_{oc} is the thermodynamic open circuit potential, η_{act} is the cell activation over potential, η_{ohm} Polarisation ohmique and η_{conc} Polarisation de la concentration.
V_{OC} it is equal to zero on the anode but is a function of temperature on the cathode and is calculated using the Nernst law [6]:

$$V_{c,OC} = (0.0025 \times T) + 0.2329 \qquad (8)$$

The cell activation and concentration over potential are calculated as:

$$\eta_{act} = A \ln\left(\frac{i}{i_0}\right) \qquad (9)$$

$$\eta_{conc} = -B \ln\left(1 - \frac{i}{i_l}\right) \qquad (10)$$

Where i_0 is the exchange current density.
The polarisation ohmique is defined as:

$$\eta_{ohm} = i \times R \qquad (11)$$

The membrane resistance is:

$$R = \int_0^{l_m} \frac{1}{\sigma(\lambda)}\, dy \qquad (12)$$

3. Numerical method

The solution to the governing equations is performed by employing a finite volume scheme with the model domain divided into a number of cells as control volumes. The governing equations are numerically integrated over each of these computational cells or control volumes. The method exploits a collocated cell-centered variable arrangement with the local or cell-averaged values of the physical quantities evaluated and stored at each cell center.
The governing equations can be expressed in the form of a generalized type of transport equation:

$$\mathrm{div}\,(\varepsilon \rho u \phi) = \mathrm{div}\big(\Gamma.\mathrm{grad}(\phi)\big) + S_\phi \qquad (13)$$

Where φ denotes the general dependent variable, Γ the exchange coefficient, S_φ the source term, u the velocity, and ρ the density. With the discretization of the governing equations expressed in the form of:

$$a_P.\phi_P = a_W.\phi_W + a_E.\phi_E + a_S.\phi_S + a_N.\phi_N + S_\phi \qquad (14)$$

Where ϕ_P is the value of φ at the current point P, $\phi_E \cdots \phi_S$ stand for the values of the grid points adjacent to the point P, and $a_P \cdots a_S$ are known as the link coefficients. Three grid systems shown in Figure. 3 are considered.

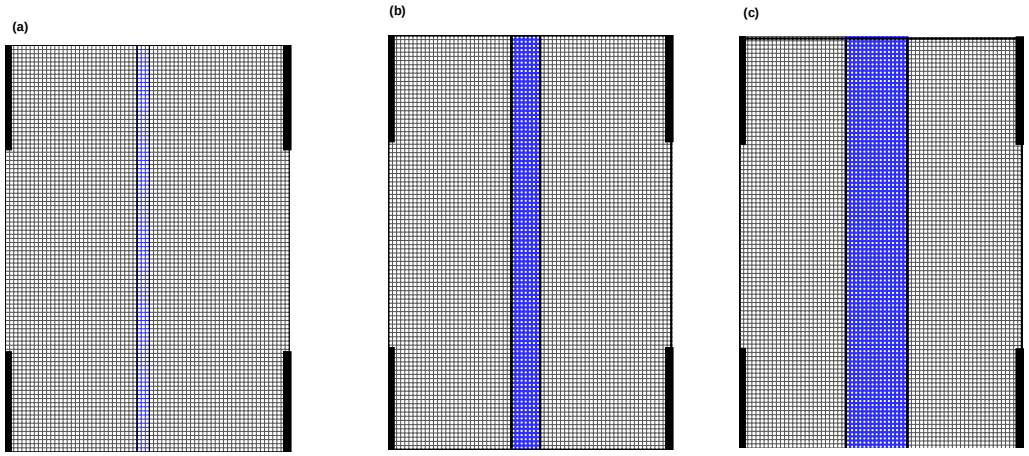

Figure3: Mesh structure of three different thickness of membrane: (a) tm=0.3×10^{-4}, (b)0.7×10^{-4}, (c)1.5×10^{4}(m).

Therefore, the grid system of 70×100 points seems sufficient to resolve the behaviors of the reactant gas transport in the present PEM fuel cell model.

Table 2: Parameter values of electrode and membrane used as the base case.

Parameter	Value
Cell/electrode length, L_y(m)	1×10^{-3}
Anode and Cathode GDL thickness GDL, t_a, t_c(m)	0.3×10^{-3}
Membrane thickness (Nafion 117), t_m(m)	0.1×10^{-3}
Porosity of anode and cathode GDL, $\varepsilon_a, \varepsilon_c$	0.4
Porosity of anode and cathode CL, $\varepsilon_{CLa}, \varepsilon_{CLc}$	0.2
Porosity of membrane, ε_m	0.28
Temperature, T(K)	353
Pressure at gas channel inlet of anode side, P_a(Pa)	3×10^5
Pressure at gas channel inlet of cathode side, P_c(Pa)	3×10^5

4. Results and discussion

Correct water management has been found to be important to maintain high proton conductivity of membrane and achieve high performance for PEMFCs. A mathematical model of PEMFC is very useful and effective tool to optimize cell designs and operation conditions. In this section, this model will be used to investigate the effect of membrane thickness on the performance of a PEMFC. Table 2 lists the important parameters of electrode and membrane used as the base case.

Fig. 4 shows the polarization curves for three thicknesses of membrane. Cell performance increases with decreasing the thickness of membrane in the both modes, due to the higher water content of membrane and shorter distance of proton across the membrane.

Fig. 5 and Fig. 6 show the water concentration profiles for three thicknesses of membrane.

The simulation results show that the distribution of water of membrane increases with decreasing the thickness of membrane, and water content gradient across the membrane is high for thick membrane. It seems that the thinner the membrane to be chosen as electrolyte, the better the cell performance.

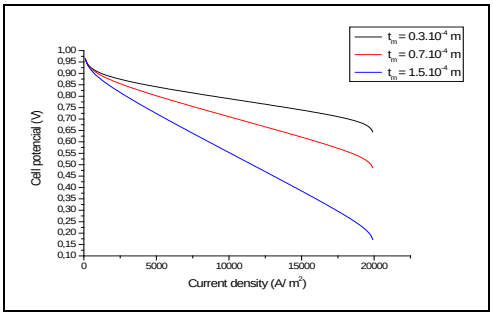

Figure 4: The polarization curves for three thicknesses of membrane.

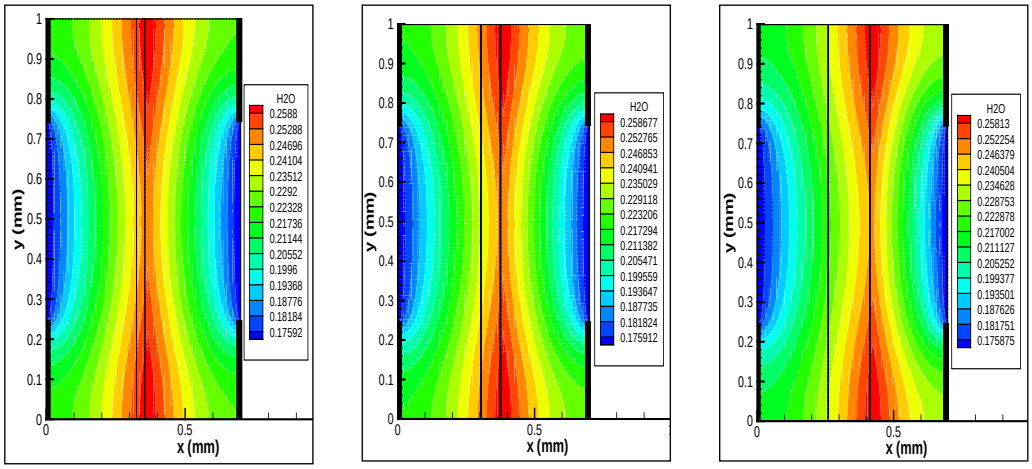

Figure 5: Water concentration distribution in PEM fuel cell for three thicknesses of membrane.

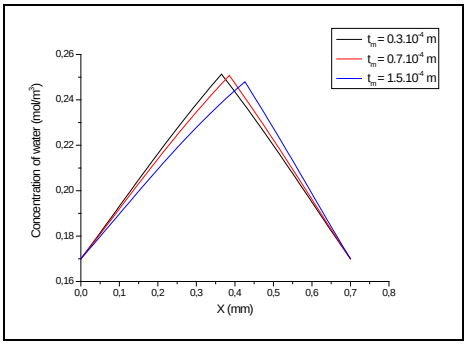

Figure 6: The water concentration profiles for three thicknesses of membrane.

Conclusion

A two-dimensional model for a proton exchange membrane fuel cell was developed. The model is used to investigate the effect membrane thickness on the water transport, and performance of fuel cell.

The results show that the water concentration of membrane and cell performance increases with decrease in the thickness of the membrane. These studies will be useful for the design and operation of practical PEMFC stacks.

Nomenclature

Symbole Nom, *unité*

C concentration, $mol.m^{-3}$
D diffusivité thermique, $m^2.S^{-1}$
F Faraday constant, $C.mol^{-1}$
i current density, $A.m^{-2}$
i_0 Exchange current density, $A.m^{-2}$
J volume density, $A.m^{-3}$
S source terme
T temperature, *K*
P pressure, *Pa*
K permeability, m^{-2}

Symboles grecs

ρ density, $Kg.m^{-3}$
σ membrane conductivity, $S.m^{-1}$
α coefficient of charge transfer, $m^2.S^{-1}$
ε porosity
η electrode overpotential, *V*
λ water content of membrane, mol_{H_2O}/mol_{SO_3}
μ water viscosity, $Kg.m^{-1}.S^{-1}$

Exposant, Indices
a anode
c cathode
cat Catalyst layer of anode and cathode
eff Effective value
g gas
k species
m Membrane

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