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Two-Dimensional PEM Fuel Cells Modeling using COMSOL Multiphysics

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1. Introduction

A fuel cell has been considered as an efficient and clean alternative power source for automobile industry since the energy crisis forced people to find a substitution for fossil fuels. A proton exchange membrane fuel cell, also known as polymer electrolyte membrane fuel cell (PEMFC), becomes a prime candidate for applications in vehicles because of its following features: the PEMFC operates at a relative low temperature (less than 90°C); the PEMFC can start quickly; the PEMFC has a higher current density due to thin membrane electrodes assembly (MEA) compared to other types of fuel cells; and there are no corrosive fluid hazards since there is no liquid electrolyte present in the PEMFC.

Nevertheless, the wide application of a PEMFC is limited due to high capital cost, fuel availability, and durability etc. The difficulty of maintaining suitable thermal management and water management also affects the fuel cell performance significantly. For example, too much water produced on the cathode side will fill the pores of gas diffusion layers (GDLs), and therefore block the diffusion of reactants to reach the catalyst layer. Too little water on the anode side will dry up the membrane so that protons cannot migrate through it. Both cases result in a decrease in the cell output power.

Experimental research and numerical simulation have been used in fuel cell design in order to improve the performance of fuel cells. Experimental data is useful to validate the models. The computational models are efficient in predicting the cell performance under a variety of design parameters. Fuel cell models can be classified into 1D, 2D and 3D according to dimensions. The accuracy of 1D model (Springer et al., 1991), (Gurau et al., 2000) is sacrificed due to some assumptions made in order to simplify the problem to 1D. A 3D model simulates the reactant gas flow in the directions along the flow channel and perpendicular to the flow channel simultaneously, which results in more accurate results but requires longer computational time and larger computing capacity facility (Haralldsson & Wipke et al., 2004) (Berning et al., 2002). A 2D fuel cell model (Siegel et al., 2003) (Biyikoglu, 2005) (Hwang, 2006) combines the benefits of 1D and 3D models and gains its popularity in PEM fuel cell modeling due to its higher computational efficiency compared to 3D models and better simulation accuracy compared to 1D models.

A two-dimensional mathematical model of a PEM fuel cell can be conducted in two different modes: parallel or perpendicular to the gas flow direction in the gas channel

while the other modelling dimension is across the membrane in both cases. Models conducted in the first mode (parallel to the gas flow direction) consider the influence of fluid behavior in the channel; while in the second mode (perpendicular to the gas flow direction), the interdigitated flow pattern can be easily investigated. The goal of the present work is to develop 2-D isothermal PEM fuel cell models in two different modes to investigate the performance of fuel cells such as the mass concentration and velocity distribution of reactants, the polarization curve, the output power density, etc. The results from two modes are then compared to each other. The organization of this paper is as follows: in section 2, the single-phase two-dimensional PEM fuel cell models are developed and the models are solved using the commercial software package COMSOL Multiphysics. The main results obtained from the present work are discussed in section 3. In section 4, the main conclusions derived from the present work are summarized.

2. Model

Fig. 1 schematically shows a 3D single PEMFC and its various components including the membrane, flow channels, gas diffusion layers and catalyst layers on both anode and cathode sides. To conduct a 2 D simulation, there are two options to choose the modeling geometry: one is in x-y plane as shown in Fig. 2(a), and the other is in x-z plane as shown in Fig. 2(b). Both geometries will be studied in this paper.

Figure 1. Three dimensional diagram of a PEMFC and its various components

Figure 2. Two-dimensional PEM fuel cell modelling geometry

2.1 Assumptions

The present model is established based on the following assumptions:

1. Flow is laminar everywhere due to small gas pressure gradient and low Reynolds number.
2. Reactant gases behave as the ideal gas mixture.
3. The electrodes and membrane are made of homogeneous materials.
4. The temperature distribution across the cell is uniform.
5. Water exists only in the gas phase in the fuel cell.
6. The polymer electrolyte membrane is impermeable to reactant gases.
7. Protons can only transport through the electrolyte, and electrons through the solid phase.
8. Three species including oxygen, water and nitrogen are considered on the cathode side while only hydrogen and water are considered on the anode side.
9. The fuel cell is operating at the steady state.

2.2 Governing equations

2.2.1 Flow channels

Based on the model assumptions, the reactant gas flow in the gas channel is governed by the continuity equation to insure the mass conservation and the steady state incompressible Navier-Stokes equation to describe the momentum conservation of Newtonian fluids.

N-S Equation:

$$\rho(u \cdot \nabla)u = \nabla \cdot [-PI + \mu(\nabla u + (\nabla u)^T)] \quad (1)$$

Continuity Equation:

$$\nabla \cdot u = 0 \quad (2)$$

where u is velocity vector, m/s; P , pressure, Pa; ρ , mixture density, kg/m³; μ , dynamic viscosity, kg/(m s).

The multi-component diffusion and convection in flow channels are described by the Maxwell-Stefan equation. It solves for the fluxes in terms of mass fraction. The general form of the Maxwell-Stefan equation is shown below:

Maxwell-Stefan Equation:

$$\frac{\partial}{\partial t} \rho \omega_j + \nabla \cdot [-\rho \omega_j \sum_{j=1}^N D_{ij} \{ \frac{M}{M_j} (\nabla \omega_j + \omega_j \frac{\nabla M}{M}) + (x_j - \omega_j) \frac{\nabla P}{P} \} + \omega_j \rho u] = R_i \quad (3)$$

where D_{ij} is the diffusion coefficient, m²/s; R_i , the reaction rate and is zero in the flow channel, kg/(m³.s); x , the mole fraction; ω , the mass fraction; M , the molecular mass, kg/mol. The density of mixture gas ρ is a function of mixture components and is described by the following equation:

$$\rho = \left(\sum_i x_i M_i \right) P / (RT) \quad (4)$$

where x_i is the mole fraction; R , the universal gas constant, 8.314 J/(mol.K); T , the cell temperature, K. The subscript i (or j) represents each species of hydrogen and water on the anode side, and oxygen, water, nitrogen on the cathode side.

On the cathode side, the transport equations are solved for two species since the third species can always be obtained from the mass balance equation given as following:

$$w_{N_2} = 1 - w_{O_2} - w_{H_2O} \quad (5)$$

On the anode side, the hydrogen transport equation is solved first, and then the mass fraction of water can be obtained by:

$$w_{H_2O} = 1 - w_{H_2} \quad (6)$$

2.2.2 Gas diffusion layers and catalyst layers

Since gas diffusion layers (GDL) and catalyst layers are porous media, the velocity distribution is therefore formulated by Darcy's law and mass conservation equation.

Darcy's Law:

$$u = -\frac{\kappa}{\mu} \nabla p \quad (7)$$

where κ is the permeability, m²; and μ the dynamic viscosity, Pa.s;

Continuity equation:

$$\nabla \cdot (\rho u) = S \quad (8)$$

where S is the source term, $\text{kg}/(\text{m}^3\cdot\text{s})$. The continuity equation for the gas flow mixture describes the sum of all the involved gas species at each side. The source term, S , accounts for the total consumption and production during the electrochemical reactions.

In the catalyst layer, the reaction rate R_i corresponding to each species is given as:

$$R_{H_2} = -\frac{j_a}{2F} M_{H_2} \quad (9)$$

$$R_{O_2} = -\frac{|j_c|}{4F} M_{O_2} \quad (10)$$

$$R_{H_2O} = \frac{|j_c|}{2F} M_{H_2O} \quad (11)$$

2.2.3 Current transport

The continuity of current in a conducting material is described by

$$\nabla \cdot i = 0 \quad (12)$$

In a PEM fuel cell, the conducting materials are porous electrodes and membrane. The current is therefore split into two parts: the ionic current and the electronic current. Protons travel through the ionic conductor (the membrane) to form an ionic current denoted by i_e , while electrons can only be transferred through the solid matrix of electrodes which results in an electronic current denoted by i_s . The continuity equation of current then becomes:

$$\nabla \cdot i = \nabla \cdot i_s + \nabla \cdot i_e = 0 \quad (13)$$

In the catalyst layer, where a chemical reaction occurs on a three-phase boundary, electrons are either transferred from the solid matrix to electrolyte or vice versa. This two-way transfer of electrons between solid matrix and electrolyte makes the transfer current density, denoted by j , a source term in one phase, and a sink term in the other phase. The potential equations for both solid and electrolyte phases are obtained by applying Ohmic's law to Eq. (13).

Electron transport

$$\nabla \cdot (-\sigma_s \nabla \phi_s) = S_s \quad (14)$$

Proton transport

$$\nabla \cdot (-\sigma_e \nabla \phi_e) = S_e \quad (15)$$

Where ϕ is the phase potential, V; σ , the effective electric conductivity, s/m ; S the current source term, A/m^3 ; the subscript s denotes the property of a solid phase and e denotes that of an electrolyte phase. The source terms in the electron and proton transport equations, i.e., Eq. (14-15), result from the electrochemical reaction occurring in the catalyst layers of anode and cathode sides.

Anode Catalyst layer:

$$S_e = j_a \quad ; \quad S_s = -j_a \quad (16)$$

Cathode Catalyst layer:

$$S_e = j_c \quad ; \quad S_s = -j_c \quad (17)$$

where j_a and j_c are the transfer current density corresponding to the electrochemical reaction at the anode and cathode catalyst layers, which is formulated by the agglomerate model. In the catalyst layers, the agglomerate is formed by the dispersed catalyst, and this zone is filled with electrolyte. Oxygen is dissolved into the electrolyte and reaches the catalyst site. The agglomerate model describes the transfer current density as following (Broka, 1995):

Anode:

$$j_a = -\frac{6(1-\varepsilon)FD_H^{agg}}{(R^{agg})^2} (c_H^{agg} - c_H^{ref} \exp(-\frac{2F}{RT}\eta)) \cdot (1 - \sqrt{\frac{j_{o,a}s}{aFc_H^{ref}D_H^{agg}}R^{agg}} \coth \sqrt{\frac{j_{o,a}s}{aFc_H^{ref}D_H^{agg}}R^{agg}}) \quad (18)$$

Cathode:

$$j_c = R \frac{12(1-\varepsilon)FD_O^{agg}}{(R^{agg})^2} c_O^{agg} \cdot (1 - \sqrt{\frac{j_{o,c}s(R^{agg})^2}{4Fc_O^{ref}D_O^{agg}} \exp(-\frac{0.5F}{RT}\eta)}) \cdot \coth \sqrt{\frac{j_{o,c}s(R^{agg})^2}{4Fc_O^{ref}D_O^{agg}} \exp(-\frac{0.5F}{RT}\eta)} \quad (19)$$

where c^{agg} is the gas concentration at the surface of the agglomerates, mol/m³; c^{ref} the dissolved gas concentration at a reference state, mol/m³; F, the Faraday constant, coulomb/mol; D^{agg} the diffusion coefficient, m²/s of the dissolved gas inside the agglomerate; R^{agg} the agglomerate radius, m; j_0 the exchange current density, A/m²; s the specific surface area, m²/m³; η the electrochemical overpotential, V, which is expressed by the potential difference between solid matrix and electrolyte and is defined as:

Anode side:

$$\eta = \phi_s - \phi_e \quad (20)$$

Cathode side:

$$\eta = \phi_s - \phi_e - U_{oc} \quad (21)$$

where the open-circuit potential U_{oc} is given by

$$U_{oc} = 1.23 - 0.9 \times 10^{-3} (T - 298) \quad (22)$$

The dissolved gas concentration at the surface of the agglomerates is corresponding to the molar fraction in the gas phase through Henry's Law:

$$c^{agg} = \frac{c_{gas} P}{H} \quad (23)$$

where H is the Henry's constant, $\text{Pa}\cdot\text{m}^3/\text{mol}$.

2.3 Numerical procedure

COMSOL Multiphysics, a commercial solver based on the finite element technique, is used to solve the governing equations. The stationary nonlinear solver is used since the source terms of the current conservation equation make the problem non-linear. Furthermore, the convergence behavior of this non-linear solver is highly sensitive to the initial estimation of the solution. To accelerate the convergence, the following procedures are adopted: the Conductive Media DC module is firstly solved based on the initial setting; secondly, Darcy's Law and Incompressible Navier-Stokes modules are solved together using the results from the previous calculation as initial conditions. After the previous two modules converge, all the coupled equations including Maxwell-Stefan Diffusion and Convection module are solved simultaneously until the convergence is obtained as shown in Fig. 3.

Figure 3. Solving procedure in COMSOL Multiphysics

3. Results and discussion

Using the aforementioned procedures, the X-Z geometry as described in Fig. 2a and the X-Y geometry in Fig. 2b are simulated separately. The X-Z mode represents the PEM fuel cell with straight or serpentine channels on the bipolar plates while the X-Y mode represents those with interdigitated channels. The material properties used in the model are selected

from Meng and Wang, 2005. The parameters describing the electrochemical reaction are based on the agglomerate model from (Broka, 1995).

Figure 4 shows the polarization curve obtained from the X-Z model. Figure 5 shows the profile of oxygen mass fraction on the cathode side for the cell operating voltages of 0.8 volt and 0.3 volt. The reactant gas concentration decreases along the flow direction and across the membrane direction due to the consumption of fuel in the electrochemical reaction at the catalyst layer. A higher fuel concentration gradient is found at 0.3 volt (the left figure in Fig.5), which is due to the faster consumption of fuel when the cell is working at low output voltage but high current density.

Figure 4. Polarization curves: the X-Z model

Figure 6 shows the polarization curve of X-Y model. Figure 7 shows the concentration profile of oxygen of X-Y model. The flow channel is not included in this model; however, this model can provide more detailed descriptions of fuel cell performance across the membrane direction. The oxygen mass fraction decreases from the inlet to outlet, and it decreases faster at the low voltage and high current density conditions, which is again due to the faster fuel consumption in chemical reactions since that the consumption rate is proportional to the cell operating current density.

Fig. 8 and Fig. 9 show the distribution of solid phase and electrolyte phase potentials across the membrane obtained from the X-Z and X-Y models, respectively. The potential distribution displays a similar behaviour for two different models. An obvious potential drop is found within the membrane due to the low proton conductivity of membrane. The ohmic losses, however, are very small on both anode and cathode electrodes. A high overpotential is found on the cathode side due to the slow kinetic reaction of oxygen reduction.

Figure 5. Oxygen mass fraction distribution in the X-Z mode (Left: Vcell=0.8 V, Right: Vcell=0.3V)

Figure 6. Polarization curves: the X-Y mode

Figure 7. Oxygen mass fraction distribution in the X-Y mode (Left: $V_{cell}=0.8\text{ V}$, Right: $V_{cell}=0.3\text{ V}$)

Figure 8. Electrical potential distribution in the electrodes and membrane profiles: the X-Z model (Solid line: solid phase potential, Dashed line: electrolyte phase potential)

Figure 9. Electrical potential distribution in the electrodes and membrane profiles: the X-Y model (Solid line: solid phase potential, Dashed line: electrolyte phase potential)

4. Conclusions

Two-dimensional, single-phase and isothermal models of PEM fuel cells were developed in two different modes. These models are solved using commercial software package, COMSOL Multiphysics, based on finite element techniques. The models are able to investigate the transport phenomena and electrical potential distribution in the various PEM fuel cell components including the gas channels, gas diffusion layers, catalyst layers and membrane.

The polarization curves were presented. The X-Z model was used to study the fuel cell with straight channels or serpentine channels design. The X-Y model is suitable for the fuel cell with interdigitated flow patterns. Both X-Z and X-Y model show the fuel mass fraction decrease faster when the cell is working at low voltage and high current density region. In both X-Y and X-Z models, the potential distribution indicated a major potential drop occurring across the membrane, and a higher overpotential was found on the cathode catalyst layer. These two modes of models can be combined together to describe the overall behavior of PEM fuel cells in all directions.

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