

Heat and Water Management in a PEM Fuel Cell

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Abstract: - Proton exchange membrane (PEM) fuel cells are promising power-generation sources for mobile and stationary applications. In this paper a non-isothermal, single-domain and two-dimensional computational fluid dynamics model is presented to investigate heat and water transfer in a PEM fuel cell. A set of governing equations, conservation of mass, momentum, species, energy and charge for gas channels, gas diffusion layers, catalyst layers and the membrane regions are considered. These equations are solved numerically in a single domain, using finite-volume-based computational fluid dynamics technique. This model accounts for the major transport phenomena in a PEM fuel cell: convective and diffusive heat and mass transfer, electrode kinetics, and potential fields. The results are shown to be in good agreement with previous work and it is validated with recent experimental data available

Key-Words: - PEM Fuel cell; Heat; Non-isothermal, Single-Domain; CFD

1 Introduction

The high power density and rapid adjustment to power demands make proton exchange membrane fuel cells one of the best candidates for a clean alternative energy sources for the 21st century. The high cost and relatively low reliability of fuel cell are the limiting factors for their widespread use. A better understanding of operating conditions in PEM fuel cell is essential to the development and optimization of fuel cells, the introduction of cheaper materials and fabrication techniques, and the design and development of novel architectures. The difficult experimental environment of fuel cell systems has stimulated efforts to develop model that could simulate and predict multi-dimensional coupled transport of reactants, heat and charged species using computational fluid dynamic methods. At present, much modeling work has been done [1-7]. He et al. [1] developed a two-phase and two-dimensional model of water transport in GDL of a PEM fuel cell. Um et al. [2] proposed a transient, single-phase, single-domain and two-dimensional model for electrochemical and transport processes in a PEM fuel cell. The heat management was neglected by assuming isothermal operation Siegel et al. [3, 4] investigated a Single domain PEM fuel cell model based on agglomerate catalyst geometry. These models are two-dimensional and includes the transport of liquid water within the porous electrodes Liu et al.[5-7] have employed the

mixture model for two-phase behavior in PEM fuel cell, which can describe the liquid water behavior in GDL and gas channel with the advantages of simplicity and low cost of the calculation. Wang et al. [8] also introduced the mixture model to describe two-phase behavior in PEM fuel cell, and they predicted that the liquid water saturation within the cathode will reach 6.3% at $1.4 A cm^{-2}$ for dry inlet air. In the continuation of this work, Wang and co-workers [9] simulated the function of a microporous layer between cathode GDL and catalyst layer with the mixture model. Nguyen et al. [10] presented a computational fluid dynamics model of a PEM fuel cell with serpentine flow field channels. The model accounts for detailed species mass transport, heat transfer, and electrochemical kinetics. In order to set up a tool for the dynamic prediction of cell behaviour and avoid the problems involved in other approaches, a novel approach to the problem presented by Francesco et al. [11]. The Hwang [12] model illustrates the behaviors of the two-phase flow and heat transfer in a porous electrode. This model only investigated the cathode side and the boundary conditions in the interfaces were used in numerical solution. Rowe and Li [13], also Mishra et al. [14] performed study on the water and thermal management on PEM fuel cell using a steady-state, one-dimensional approach. They used the boundary conditions in the interfaces of different regions.

In this model, the computational domain consist two channels, two gas diffusion layers, two catalyst layers, and a polymer electrolyte membrane (PEM). The cell is considered to be two-dimensional and steady state. Then, the governing equations are solved and theoretical performance of a PEM fuel cell is investigated by looking at parameters such as pressure, temperature, current density and species concentration in a single-domain region.

2 Mathematical Model

Figure 1 shows a schematic of a two-dimensional section of the PEM fuel cell corresponding to the geometry of the model considered in this study, which consists of seven different regions: anode and cathode gas channels (aGH, cGH), anode and cathode diffusion layers (aGDL, cGDL), anode and cathode catalyst layers (aCL, cCL), and the membrane (PEM). Inside the fuel cell, hydrogen gas and air are supplied to the cell through the anode and cathode channels, respectively, and the gases diffuse across the respective gas diffusion layers toward the membrane electrode assembly, which includes the two catalyst layers and the membrane. In the anode catalyst layer, hydrogen is consumed to generate protons and electrons, while in the cathode catalyst layer, oxygen reacts with protons and electrons generating water. Based on mass conservation, the mass of hydrogen consumed in the anode side should be equal to the mass of water generated in the cathode side less the mass of oxygen consumed in the cathode side.

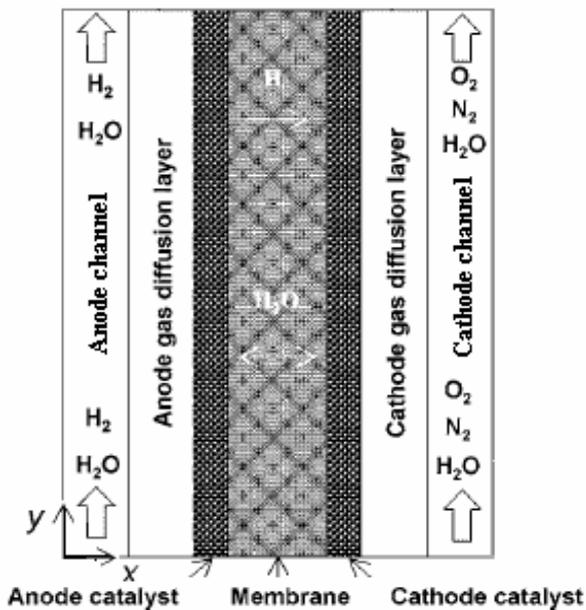


Fig 1. Schematic of a two-dimensional section of the PEM fuel cell

In this study a comprehensive two-dimensional, non-isothermal, one phase, steady state model is adopted. The other assumptions used in this model are as follows: ideal reactant gas mixtures; laminar and incompressible gas flow; impermeable to gases membrane; uniform and fully hydrated cathode catalyst layer; isotropic and homogenous gas diffusion layers, and does not extend into the gas channels; negligible ohmic potential drop in the electronically-conductive solid matrix of porous electrodes and catalyst layers; the single-phase assumption for water transport.

In contrast to usual approach which employs separate differential equations for different regions, we have taken a single-domain approach in which a single set of governing equations valid for all regions. As a result, no interfacial conditions are required to be specified at internal boundaries between these regions. Considering a steady state operation of the cell, the governing equations for the physical phenomena are summarized below.

Conservation of mass across the entire cell is governed by the continuity equation

$$\nabla \cdot (\rho \vec{u}) = 0 \quad (1)$$

Where ρ and \vec{u} are the density of the gas mixture and the velocity vector, respectively. The density of the mixture is calculated using:

$$\rho = \frac{1}{\sum_k y_k / \rho_k} \quad (2)$$

Where y_k is the mass fraction of species k . The density of each species, ρ_k is obtained from the perfect gas law relation:

$$\rho_k = \frac{pM_k}{RT} \quad (3)$$

In which p corresponds to the anode or cathode side pressure, M_k is the molecular weight, T is the temperature and R is the universal gas constant.

The flow field is governed by the steady state Navier–Stokes equations, which express momentum conservation for a Newtonian fluid. A convenient formulation for CFD is:

$$\frac{1}{\varepsilon^2} \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \mu \nabla \cdot \tau + S_{Dar} \quad (4)$$

Where ε , \vec{u} and p are the porosity, velocity and pressure vectors, τ is the viscous stress tensor matrix and S_{Dar} is the Darcy source and that is active only in the GDL and catalyst layers.

$$S_{Dar} = -\frac{\mu}{K} \bar{u} \quad (5)$$

Where μ and K are the dynamic viscosity, and hydraulic permeability.

The steady state species transport equation takes the form:

$$\nabla \cdot (\bar{u} C_k) = \nabla \cdot (D_k^{eff} \nabla C_k) + S_k \quad (6)$$

Where C_k is the molar concentration of species k and D_k^{eff} is the effective species diffusivity. The source terms for hydrogen and oxygen species account for consumption due to reaction in the catalyst layers.

$$S_k = -\frac{s_k j}{nF} \quad (7)$$

Also the source term for water vapor accounts for production of water at the cathode in the catalyst layers.

$$S_k = -\nabla \cdot \left(\frac{n_d}{F} I \right) - \frac{s_k j}{nF} \quad (8)$$

Where n_d is electro-osmotic drag coefficient, s_k is stoichiometry coefficient in electrochemical reaction of species k , n is number of electrons in electrochemical reaction, F is Faraday constant (96487C/mole), j is transfer current density, and I is current density.

The transfer current densities and Surface overpotential are expressed as follows:

$$j_a = (ai_0)_a^{ref} \left(\frac{C_{H_2}}{C_{H_2}^{ref}} \right)^{1/2} \left(\frac{\alpha_a + \alpha_c}{RT} \cdot F \cdot \eta \right) \quad (9a)$$

$$j_c = -(ai_0)_c^{ref} \left(\frac{C_{O_2}}{C_{O_2}^{ref}} \right) \exp\left(-\frac{\alpha_c}{RT} \cdot F \cdot \eta\right) \quad (9b)$$

Where

$$\eta_a = -\phi_m \quad (10a)$$

$$\eta_c = V_{cell} - \phi_m - U_0 \quad (10b)$$

$$U_0 = 1.23 - 0.9 \times 10^{-3} (T - 298.1) \quad (11c)$$

Where C is molar concentration, α is transfer coefficient, η is overpotential, ϕ is phase potential, V_{cell} is cell potential and U_0 is thermodynamic equilibrium potential. The superscript "ref" indicates a reference state and Subscripts "a, c, 0, m, H_2 , O_2 " indicate anode, cathode, standard

condition, membrane, hydrogen and oxygen, respectively.

Electrochemical reactions in the PEM fuel cell are:

$$\sum_k s_k M_k^z = ne^-, \begin{cases} M_k \equiv \text{chemical formula} \\ s_k \equiv \text{stoichiometry coefficient} \\ n = \text{number of electrons} \end{cases} \quad (11)$$

Hydrogen oxidation reaction in anode side is:



Oxygen reduction reaction in cathode side is:



The potential distribution can be calculated by applying the generic transport equation without the convective terms.

$$\nabla \cdot (\sigma_m \nabla \phi_m) + S_m = 0 \quad (13)$$

Where σ_m is the proton conductivity on the membrane, and the source term, S_m represents the production/consumption of protons due to electrochemical reactions in the catalyst layers. The rate of the electrochemical reaction is described by the Butler–Volmer relation, where the electrical potential is assumed to be constant in each electrode. It is set to zero on the anode side, and in the cathode side is the difference between the cell voltage and open circuit voltage.

$$S_m = j \quad (14)$$

The energy equation is presented in Eq. (14) and contains sources for ohmic heating due to ionic resistance, reversible heat, heat produced due to activation losses.

$$\nabla \cdot (\rho C_p \bar{u} T) = \nabla \cdot (k^{eff} \nabla T) + S_T \quad (15)$$

Where C_p is heat capacitance and k^{eff} is effected thermal conductivity.

The source terms S_T in catalyst layers and membrane are given by respectively.

$$S_T = j(\eta + T \frac{dU_0}{dT}) + \frac{I^2}{\sigma^{eff}} \quad (16)$$

$$S_T = \frac{I^2}{\sigma^{eff}} \quad (17)$$

The mass diffusion coefficient of species k , D_k , in the anode and cathode gas channels is

calculated as a function of temperature and pressure. For the porous regions, the expression is modified into the effective species diffusivity, D_k^{eff} using Bruggeman correlation [2].

$$D_k^{eff} = \varepsilon_i^{1.5} D_k = \varepsilon_i^{1.5} D_0 \left(\frac{T}{T_0}\right)^{1.5} \left(\frac{P}{P_0}\right) \quad (18)$$

The proton conductivity, σ_m , and the electro-osmotic drag coefficient, n_d , for water in the membrane are correlated with the water content of the membrane, λ , which is in turn a function of the water activity, a .

$$a = \frac{C_w^g RT}{P^{sat}} \quad (18)$$

$$\lambda = \begin{cases} 0.043 + 17.81a - 39.85a^2 + 36.0a^3 & \text{for } 0 < a \leq 1 \\ 14 + 1.4(a-1) & \text{for } 1 < a \leq 3 \end{cases} \quad (19)$$

$$n_d = \frac{2.5\lambda}{22} \quad (20)$$

$$\sigma_m^{eff} = \frac{1}{2} \sigma_m = \frac{1}{2} (0.0005139\lambda - 0.000326) \times \exp(1268.0(\frac{1}{303} - \frac{1}{T})) \quad (21)$$

3 Numerical Procedures

The governing equations were discretized using a finite volume based finite difference method and solved using a computational fluid dynamic code. In this code the pressure and velocity fields are treated with the SIMPLER pressure correction algorithm, where a single-domain model is used. It should be mentioned that by using this model although some species do not exist practically in certain regions of fuel cell, the species transport equation can still be applied throughout the entire computational domain by using the large source term technique [2]. For instance, no hydrogen or oxygen virtually exist in the membrane and in this region a sufficiently large source term is assigned to the hydrogen or oxygen transport equation, which freezes the hydrogen or oxygen mole fraction at zero. Stringent numerical tests were performed to ensure that the solutions were independent of the grid size. The coupled set of equations was solved iteratively, and the solution was considered to be convergent when the relative error in each field between two consecutive iterations was less than 10^{-6} . The CPU

time ranged from 10 to 20 minute on a Pentium IV PC (3. GHz, 1GB RAM).

4 Results and Discussion

Model validation is checked using numerical and experimental results in literature. The experimental setup input data shown in table 1, were used in this model from Ref 13. In Fig. 2, the calculated results for polarization curve are compared and validated with the experimental results. The accuracy of this model is so that there is no adjustment required for reactive surface area or the exchange current density and porosity is required to readjust the present model prediction with the experimental results.

Table 1 Physical properties

Description	Unit	Value
T_{cell}	K	353.0
P_a	atm	3
P_c	atm	3
t_{GDL}	m	2×10^{-4}
t_{CL}	m	7×10^{-6}
t_{PEM}	m	1.8×10^{-4}
ξ_a	-	1.5
ξ_c	-	3
ε_{GDL}^{eff}	-	0.6
ε_{CL}^{eff}	-	0.6
ε_{MC}^{eff}	-	0.26
K	m^2	2×10^{-12}
$c_{H_2}^{ref}$	mol/m^3	40.88
$c_{O_2}^{ref}$	mol/m^3	40.88
R	$J/mol \cdot K$	8.34
k_{GDL}^{eff}	$W/m \cdot K$	1.6
k_{CL}^{eff}	$W/m \cdot K$	1.5
k_{PEM}^{eff}	$W/m \cdot K$	0.34
F	C/mol	96487
μ_a	$pa \cdot s$	2×10^{-5}
μ_c	$pa \cdot s$	1×10^{-5}
$D_{0,H_2,a}$	m^2/s	1.1028×10^{-4}
$D_{0,H_2,o,a}$	m^2/s	1.1028×10^{-4}
$D_{0,O_2,c}$	m^2/s	3.2348×10^{-5}
$D_{0,H_2,o,c}$	m^2/s	7.35×10^{-5}

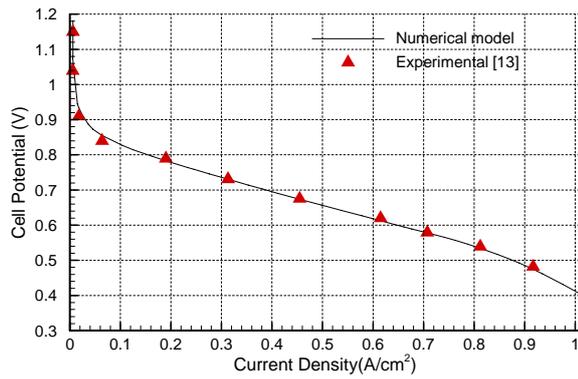


Fig. 2 Comparison between the numerical model and experimental results Ref 13.

Fig. 3 shows the flow-velocity vectors for $I = 0.7 A.cm^{-2}$. Two marks on each plot represent the local maximum and minimum velocities in the module. It is seen that the maximum velocities occur at the outlet channel. The velocity in the GDLs and membranes is almost zero; therefore gas reactants enter these regions only by diffusion.

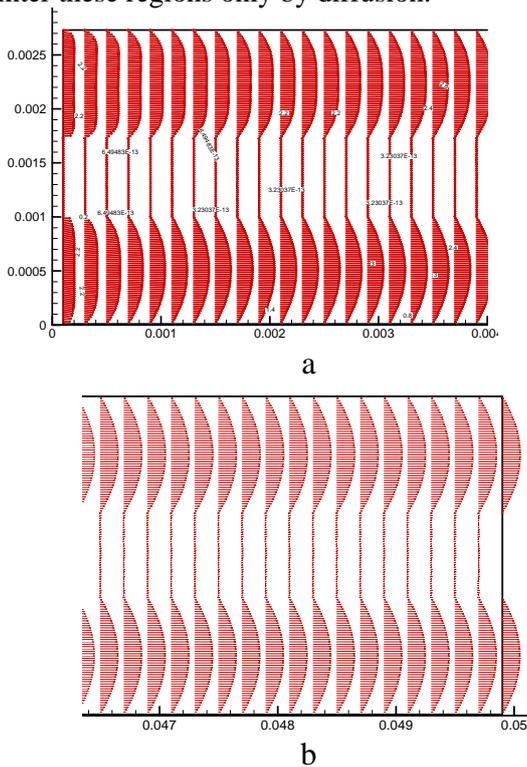


Fig. 3 the flow-velocity vectors, (a) inlet cross-section, (b) outlet cross-section

The temperature rises within a PEM fuel cell is due to heat generation caused by exothermic nature of reactions and Joule heating. The temperature changes across the entire cell for $I = 0.7 A.cm^{-2}$ are shown in Fig. 4. The cathode side temperature is higher than the anode side. This is due to heat generation by the reaction in the cathodic catalyst

layer, which is much larger than heat generation in the anode side. On other hand, exchange current density of the anodic reaction is several orders of magnitude higher than the cathodic reaction. The heat generation in the catalyst layers is transferred by both convection and conduction in all regions within the PEM fuel cell and causes to increase the cell temperature. The maximum temperature occurs in the cathode catalyst layer since major heat generation takes place in this region. The temperature distribution within the membrane is not linear due to significant heat generation of Joule heating. The non-uniform temperature distribution may become even worse for fuel cell stacks and thus, thermal management is very critical in PEM fuel cell performance.

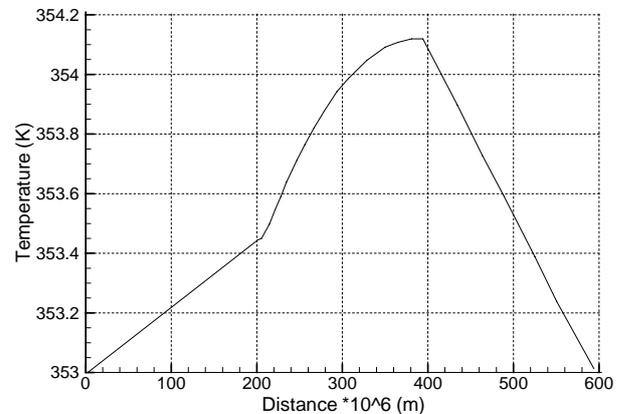


Fig. 4 Temperature distribution across the entire cell, correspond to the parameter combination given in table 1.

Fig.5 shows the water flux across the membrane as a function of the local current density where relative humidity is 100% in the anode gas stream. At low current densities, the water flux is negative. Because water is transported from the cathode to the anode due to back diffusion arising from the water concentration gradient, but at high current densities it becomes positive, signifying the dominant effect of electro-osmotic drag of water transport. Also by considering the same curve in the cathode catalyst layer, the influence of electro-osmotic drag is readily apparent. At low current density, there is very little change in water content across the membrane electrode assembly. This is due to a relatively low amount of drag and the fact that vapor activity at anode and cathode is almost identical. At high current density, the water content curve becomes steeper as the anode dehydrates and the cathode water content increases. Also, the total amount of water contained in the MEA decreases. This occurs because the vapor activity of the anode stream has dropped due to water removal upstream

leaving less water available to hydrate the anode.

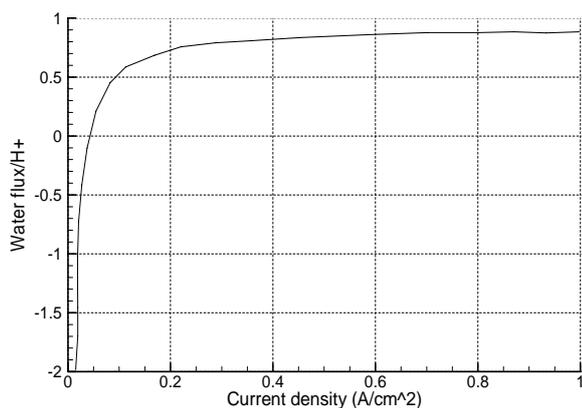


Fig 5. Net water flux across the membrane

4- Conclusion

A Two-dimensional, single-domain and non-isothermal model of a PEM fuel cell has been developed to investigate thermal and water transport and effects on cell performance. Thermal response and water transport have been investigated. The thermal management and water management is coupled. A study was performed for four critical parameters: current density, operating temperature, relative humidity and thermal conductivity of gas diffusion layer. The results show that, the gas reactants enter the GDLs and membranes only by diffusion. Also, the maximum velocities occur at the outlet channel and maximum temperature occurs in the cathode catalyst layer since major heat generation takes place in this region. At low current densities, the water flux is negative but at high current densities it becomes positive, signifying the dominant effect of electro-osmotic drag of water transport

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