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Two Dimensional Modeling of a High Temperature PEM Fuel Cell

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Abstract
A two dimensional model of a high temperature proton exchange membrane fuel cell (HTPEMFC) operating with polybenzimidazole (PBI) based membrane is presented. The model is assumed to be two dimensional, steady-state and isothermal, and it accounts for all transport and polarization phenomena which are used to validate the experimental values. The model predicts electrolyte current density norm, mass transfer ratio in both anode and cathode side. Moreover, the results show that the velocity magnitude of hydrogen and oxygen in gas flow channels, gas diffusion layer (GDL), and catalyst layers.

Keywords: HTPEM fuel cell, polybenzimidazole, two dimensional modeling.

1. Introduction

Fuel cells are electrochemical devices with high energy conversion efficiency, minimized pollutant emission and other advanced features. Proton exchange membrane fuel cell (PEMFC), among the other types, is attractive both for automobile and stationary applications. Several challenges for the PEMFC power technology based on Nafion® membrane are associated with low operating temperature; PEMFC operating at high temperatures has in recent years been recognized as a promising solution to meet these technical challenges [1]. The term *high temperature* used here refers to a temperature range from 100 to 200 □C, relative to the well-developed PEMFC technology typically operating at 80 □C. There are plenty of reasons why there has been growing interest in operating PEMFCs at elevated temperatures, First of all, As a result of not needing the humidifier, compressor and radiator as in the low temperature PEM system (LTPEM), the HTPEM system is very simple and also reducing the balance of plants (BOP) cost to approximately 25% of the fuel cell stack cost [2]. HTPEM is also more resistant against CO poisoning which is a result of using reform liquid fuels. The elevated temperatures in HTPEM, causes carbon monoxide (CO) adsorption onto the platinum (Pt) catalyst particles becomes lower [3]; Hydrogen with a higher CO concentration can be used without the same negative impacts on the performance that observed in LTPEM fuel cells. This makes it possible to directly use hydrogen reformate originating from more economic, and easy to handle energy-carriers such as methanol, ethanol, diesel, etc. Additionally, there is no need for a humidifier due to the composition of the membrane electrode assembly (MEA) which results in a simpler, cheaper and more reliable fuel cell system.

Proton exchange membranes include three general categories:

1. Per-fluorinated ionomer membranes;
2. Partially per-fluorinated membranes;
3. Non-per-fluorinated membranes [4].

Nafion® is an example of a per-fluorinated ionomer membrane, whereas polybenzimidazole (PBI) is an example of a non-per-fluorinated membrane. PBI was first suggested for use in fuel cells by Wainright et al. [5]. PBI has good mechanical strength, high chemical and thermal stability at high temperatures, and it gains its ionic conductivity when doped with a strong acid such as phosphoric or sulfuric acid. PBI is also highly impenetrable to methanol at high temperatures, and has a water drag coefficient of nearly zero, which alleviates cathode flooding and membrane dehydration [6]. It is necessary to have some numerical simulations and mathematical modeling for optimization of this type of fuel cells, since HTPEM fuel cell's technology is relatively newer than other types of fuel cells. Hence, plenty of researches have been conducted about modeling and numerical simulations of HTPEM fuel cells. For instance, Ma et al. studied the conductivities of PBI membranes for the HTPEMFC under controlled temperature and Liu et al [7]. Additionally, E. U. Ubong, Z. Shi, and X. Wang presented a 3 dimensional modeling and experimental study of a high temperature PBI based PEM fuel cell [3].In this study a mathematical model of a HTPEM fuel cell was presented. Also, numerical investigation of steady-state mass transport, and polarization curve was done as well.

2. Mathematical modeling

A 2D single-phase isothermal model is developed here to predict the performance of the HTPEM fuel cell with a PBI membrane.

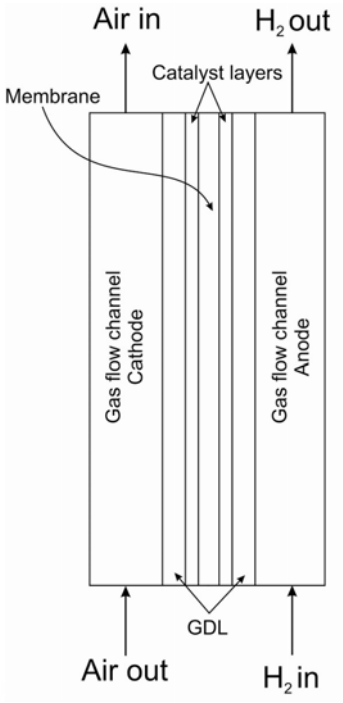

Figure 1: 2D Schematic of HTPEM fuel cells.

Figure 1 indicates a schematic model for a two-dimensional high temperature PEM fuel cell. As it can be seen, this model includes a section of the PBI membrane, both cathode and anode gas flow channels, GDLs, and catalyst layers.

Because HTPEMFC is operating above 100°C at around 2 atm pressure, the water exists only in vapor form. Because of the property of the PBI membranes, the water drag coefficient from the anode to the cathode is assumed to be zero, which is different from the typical low temperature PEMFC with a Nafion® membrane.

2.1. Governing equations

The governing equations in physics of HTPEM fuel cells include conservation of mass, conservation of momentum, conservation of species, and conservation of electric charge. These equations accounts for porous media and it is essential to report them by averaging with volumetric average technique for a specific volume. The results can be observed in below:

1. Conservation of mass and momentum

With the preceding assumptions, the HT-PEMFC operation is governed by the following conservation equations.

$$\nabla.\vec{u} = Q/\rho \tag{1}$$

$$\rho\vec{u}.\nabla\vec{u} = \nabla\{-pI + \mu[\nabla\vec{u} + (\nabla\vec{u})^{\mathrm{T}}]\} \tag{2}$$

where $\vec{u}$ is the gas mixture velocity vector, ρ is the gas mixture density, Q is the source term, p is the pressure, and μ is the dynamic viscosity of the mixture. The above equations change into Darcy's equation which accounts for porous media.

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla.(\rho\vec{u}) = Q_m \tag{3}$$

In the above equation, ρ is the density of the fluid, ε is the porosity, and Q_m is a mass source term. Porosity is defined as the fraction of the control volume that is occupied by pores. Thus, porosity can vary from zero for pure solid regions to unity for domains of free flow.

2. Conservation of species

The multispecies mass transports in the whole computational domain including the gas channels and GDL are described by the Maxwell–Stefan equation. It solves for the fluxes of each species in terms of mass fraction. The general form of the Maxwell–Stefan equation is shown below

$$\nabla\{-\rho w_i\sum_{j=1}^{N} D_{ij}[\frac{M}{M_j}(\nabla w_j + w_j\frac{\nabla M}{M}) + (x_j - w_j\frac{\nabla P}{P})] + w_i\rho\vec{u}\} \tag{4}$$

where D_{ij} is the binary diffusion coefficient, x is the molar fraction, w is the mass fraction, M is the molecular mass, R is the universal gas constant and T is the cell operating temperature.

3. Conservation of electric charge

In a PEMFC, the current can be split into two parts: ionic current and electronic current. Protons travel through the ionic conductor membrane to form an ionic current, while electrons transfer only through the solid matrix of electrodes, which results in an electronic current. The current continuity equations are obtained by using Ohm's law

$$\begin{aligned}\nabla.(-\sigma_s\nabla.\phi_s) &= S_s\\ \nabla.(-\sigma_m\nabla.\phi_m) &= S_m\end{aligned} \tag{5}$$

2.2. Boundary conditions

The species fraction at the inlet is calculated based on the humidified air and corresponding temperature. At the outlet of the flow channel, back-pressure is set to the atmospheric pressure. The flow is assumed to be fully developed. The no-slip boundary condition is applied to the impermeable walls and surfaces. The anode current collector is set to 0 V and the cathode current collector is equal to the fuel cell operating voltage. The rest of the boundaries are set to be insulated.

3. Results and Discussion

The aforementioned fuel cell model is solved using finite element-based commercial software COMSOL Multiphysics®. Table 1 shows the physical and base model parameters.

Table 1: Base model Parameters

Parameters	Value	Unit
L	0.02	m
H_{ch}	0.001	m
H_{GDL}	380e-6	m
$H_{electrode}$	50e-6	m
$H_{membrane}$	100e-6	m
ε_{GDL}	0.4	-
ε_{cl}	0.4	-
κ_{GDL}	1.18e-11	-
κ_{cl}	2.36e-12	-
σ_{GDL}	222	S m^{-1}
$\sigma_{membrane}$	9.825	S m^{-1}
$\omega_{Hydrogen,in}$	0.743	-
$\omega_{Oxygen,in}$	0.228	-
$\omega_{Water,in}$	0.023	-
$U_{in,a}$	0.2	m s^{-1}
$U_{in,c}$	0.5	m s^{-1}
μ_a	1.19e-5	Pa s
μ_c	2.46e-5	Pa s
$M_{Hydrogen}$	0.002	kg mol^{-1}
M_{Oxygen}	0.032	kg mol^{-1}
M_{water}	0.018	kg mol^{-1}
$M_{nitrogen}$	0.028	kg mol^{-1}
$D_{Hydrogen,water}$	1.808e-4	m^2 s
$D_{Nitrogen,water}$	5.056e-5	m^2 s
$D_{Oxygen,Nitrogen}$	4.713e-5	m^2 s
$D_{Oxygen,water}$	5.539e-5	m^2 s

Figure 2 shows the computational domain. As it can be seen, a non-uniform mesh grid is generated to minimize the computational cost while maintaining the accuracy.

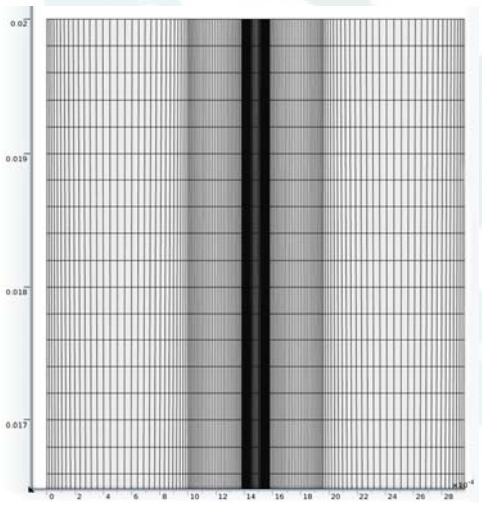

Figure 2: Mesh grid for 2D model of HTPEM fuel cell.

As we can see in figure 3, the velocity magnitude in air channel is greater than that of in fuel (hydrogen) channel. Since porosity magnitude is low in GDL and catalyst layers diffusivity is the dominant force for mass transport in these regions.

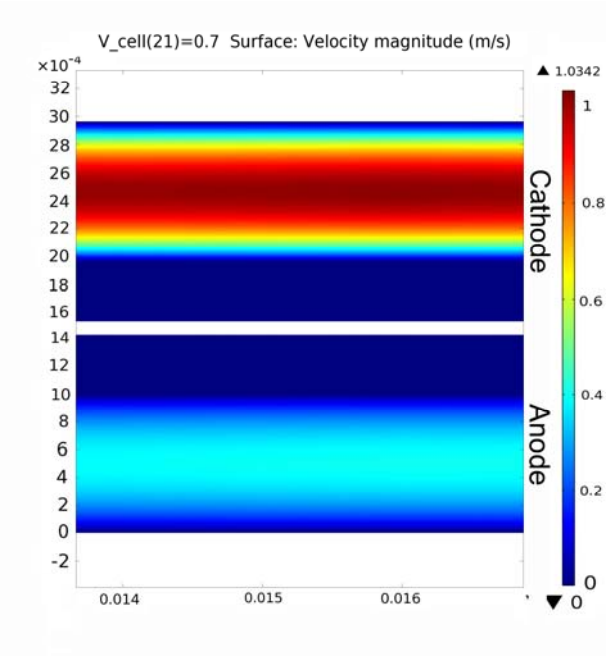

Figure 3: Velocity magnitude in different layers of HTPEM.

According to the Ohm's law:

$$i = -\sigma \nabla \phi \qquad (6)$$

the conductivity is the proportional factor for current-potential. Therefore, the slope of current curve indicates the effective conductivity accounted for the porosity at the media.

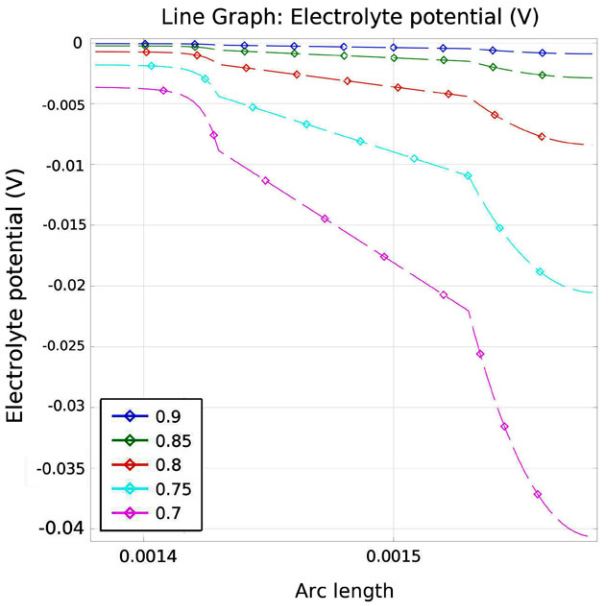

Figure 4: Electrolyte potential curve in different layers.

Figure 5 shows the polarization plot for aforementioned HTPEM fuel cell. It can be observed that the cell average current increases as the cell voltage decreases.

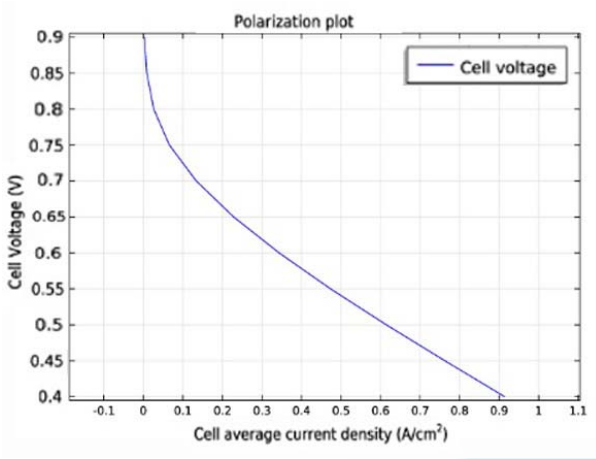

Figure 5: Polarization plot for HTPEM fuel cell.

Electrolyte current density at the center of polymer membrane for 0.5 voltage can be found in figure 6.

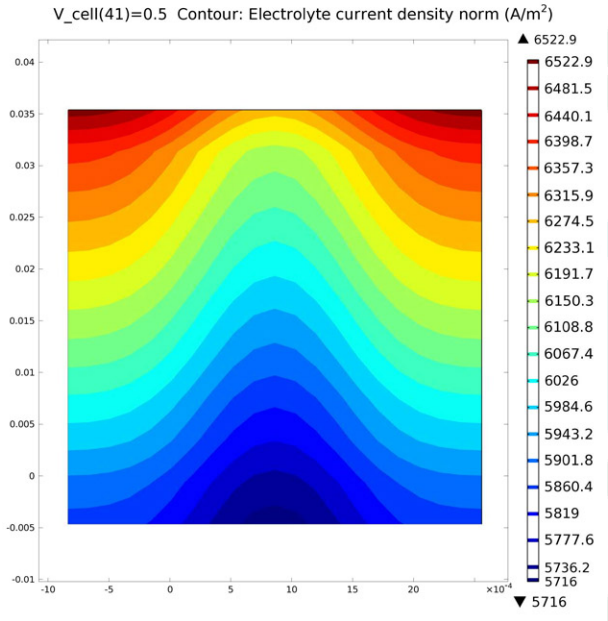

Figure 6: Electrolyte current density norm.

Figure 7 illustrates mass fraction magnitude of hydrogen and oxygen. The oxygen mass fraction at the inlet is 0.21 similarly to the molar fraction of oxygen in the air. Numerical computations show that the oxygen mass fraction decrease through the air channel flow since it is consumed in reactions. The crucial point is that mass fraction distribution of oxygen is constant at the reaction layer and it causes chemical reaction's rate to be constant as well and it is necessary since the efficiency of fuel cell is highly related to it. As it can be seen in figure 7, hydrogen mass fraction at the inlet is 0.74, and then it decreases through the fuel channel flow.

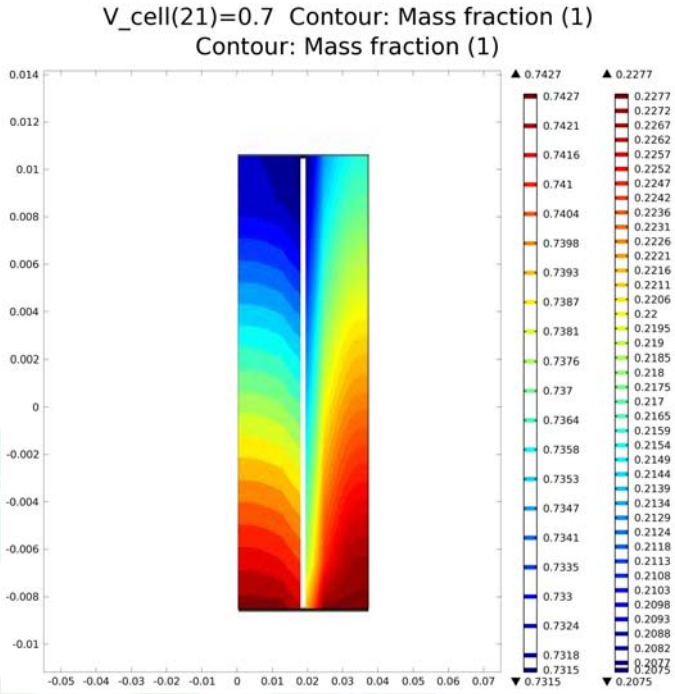

Figure 7: Mass fraction contour both for anode and cathode.

Conclusions

Numerical simulation was conducted to study an HT-PEMFC with PBI membrane by developing a 2D isothermal model. The model has clear physical and mathematical basis and it can be used to estimate properties of an HTPEM fuel cell from its current-voltage curve. Furthermore, it can be concluded that significant transport limitations exist at both electrodes, due to the low diffusivity and solubility of phosphoric acid systems. Aforementioned model did not take into account heat transfer phenomenon since it was assumed to be isothermal; hence this can be the subject of future studies.

List of symbols

C	concentration
D	Diffusion coefficient
i	Local current density
l	thickness
M	Molar
P	pressure
T	temperature
$\vec{u}$	Velocity vector
I	Index matrix
w	Mass fraction
x	Molar fraction

Greek symbols

σ	electrical conductivity
μ	viscosity
κ	permeability
ε	porosity
ρ	density
φ	electrical potential

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