

Modeling High Pressurized Three Dimensional Polymer Electrolyte Membrane Fuel Cell

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ABSTRACT

A fuel cell is an energy conversion device that converts the chemical energy of fuel into electrical energy. Fuel cells operate continuously if they are provided with the reactant gases, not like batteries. Fuel cells can provide power in wide range. Fuel cells are environmentally friendly; the by-product of hydrogen/oxygen fuel cell is water and heat.

This paper will show a numerical modeling of high pressurized Polymer Electrolyte Membrane fuel cell. Numerical modeling requires understanding the physical principles of fuel cells, fluid flow, heat transfer, mass transfer in porous media, electrochemical reactions, multiphase flow with phase change, transport of current and potential field in porous media and solid conducting regions, and water transport across the polymer membrane; and this will result in optimal design process.

This paper will show fuel cell models that are used in this analysis. Such as; electrochemical model: predicts local current density, voltage distributions. Potential field model: predicts current and voltage in porous and solid conducting regions. Multiphase mixture model: predicts liquid water and gas flow in the porous diffusion layers. Thin film multiphase model: tracks liquid water flow in gas flow passages. The numerical results of the theoretical modelling of high pressurized fuel cells and transport effects of the PEM fuel cells are shown in this paper. Results including contour plot of mass and mole fraction of H₂, O₂, and H₂O across the catalyst layers and the membrane are shown in this paper. As shown in this paper the concentration of the H₂, O₂, and H₂O are clear.

INTRODUCTION

A fuel cell is an energy conversion device that converts the chemical energy of fuel into electrical energy. Fuel cells operate continuously if they are provided with the reactant gases, not like batteries. Fuel cells can provide power in wide range. Fuel cells are environmentally friendly; the by-product of hydrogen/oxygen fuel cell is water and heat.

This paper will show a numerical modeling for high pressurized of Polymer Electrolyte Membrane fuel cell. Numerical modeling requires understanding the physical principles of fuel cells, fluid flow, heat transfer, mass transfer in porous media, electrochemical reactions, multiphase flow

with phase change, transport of current and potential field in porous media and solid conducting regions, and water transport across the polymer membrane; and this will result in optimal design process.

This paper will show fuel cell models that are used in this analysis. Such as electrochemical model which predicts the local current density, voltage distributions. Potential field model which predicts current and voltage in porous and solid conducting regions. Multiphase mixture model which predicts liquid water and gas flow in the porous diffusion layers. Thin film multiphase model which tracks liquid water flow in gas flow passages.

DISCUSSION

A fuel cell is an electrochemical energy conversion device that combines hydrogen and oxygen to produce electricity, with water and heat as its by-product. In principle, fuel cells operate like batteries. Unlike batteries, fuel cells do not run down or require recharging. It will produce energy in the form of electricity and heat as long as there is a flow of chemicals into the cell. A Polymer Electrolyte Membrane (PEM) fuel cell, also called Proton Exchange Membrane, is one of the most promising technologies. A PEM fuel cell uses a simple chemical reaction to combine hydrogen and oxygen into water, producing electric current in the process. The PEM fuel cell uses one of the simplest reactions of any fuel cell.

Polymer electrolyte membrane (PEM) fuel cells deliver high power density and offer the advantages of low weight and volume, compared to other fuel cells. PEM fuel cells use a solid polymer as an electrolyte and porous carbon electrodes containing a platinum catalyst. They need only hydrogen, oxygen from the air, and water to operate and do not require corrosive fluids like some fuel cells. They are typically fueled with pure hydrogen supplied from storage tanks or onboard reformers.

Polymer electrolyte membrane fuel cells operate at relatively low temperatures, around 100°C. PEM fuel cells are used primarily for transportation applications and some stationary applications. Due to their fast startup time, low sensitivity to orientation, and favorable power-to-weight ratio, PEM fuel cells are particularly suitable for use in passenger vehicles. However, it requires that a platinum catalyst be used

to separate the hydrogen's electrons and protons. The platinum catalyst is extremely sensitive to CO poisoning, making it necessary to employ an additional reactor to reduce CO in the fuel gas if the hydrogen is derived from an alcohol or hydrocarbon fuel.

Pressurized hydrogen gas is fed to the anode. This gas is forced through the catalyst by the pressure. When hydrogen atoms come in contact with the catalyst, it splits into two H^+ ions and two electrons e^- . The electrons are forced to travel in an external circuit because the membrane is electrically insulating. The protons migrate through the electrolyte to the cathode, where they reunite with oxygen and the electrons to produce water and heat. On the cathode catalyst of the fuel cell, oxygen molecules are fed to the cathode and react with the electrons and protons, where it forms two oxygen atoms. Each of these atoms has a strong negative charge. This negative charge attracts the two H^+ ions through the membrane, where they combine with an oxygen atom and two of the electrons from the external circuit to form a water molecule (H_2O) [1-5].

Most fuel cells designed for use in vehicles produce less than 0.9 volts of electricity—far from enough to power a vehicle. Therefore, multiple cells must be assembled into a fuel cell stack. The potential power generated by a fuel cell stack depends on the number and size of the individual fuel cells that comprise the stack and the surface area of the PEM.

Fuel cells are more energy-efficient than internal combustion engines in terms of the amount of energy used per weight of fuel and the amount of fuel used vs. the amount wasted. However, hydrogen gas is very diffuse, and only a small amount in terms of weight can be stored in onboard fuel tanks of a reasonable size. This can be overcome by increasing the pressure under which the hydrogen is stored or through the development of chemical or metal hydride storage options. Researchers are developing high-pressure tanks and hydride systems that will store hydrogen more effectively and safely.

Fluent is used to model the flow in PEM fuel cells [6]. Two electric potential fields are solved. One potential is solved in the membrane and catalyst layer. The other is solved in the catalyst layers, the diffusion layers, and the current collectors. Surface reactions on the porous catalyst region are solved and the reaction diffusion balance is applied to compute the rates. Based on the cell prescribed voltage, the current density value is computed. Alternatively, a cell voltage can be computed based on a prescribed average current density. The electrochemical processes of the rate of the hydrogen oxidation and the rate of oxygen reduction are treated as heterogeneous reactions that take place on the catalyst surfaces inside the two catalyst layers on both sides of the membrane. The driving force behind these reactions is the surface over-potential: the difference between the phase potential of the solid and the phase potential of the electrolyte/membrane. Therefore, two potential equations are solved for in the PEM model: one potential equation accounts for the electron transport through the solid conductive materials the other potential equation represents the ionic transport of H^+ .

There are two types of external boundaries. Those through which there passes an electrical current and those through which there passes no current. As no protonic currents leave the fuel cell through any external boundary, there is a zero flux boundary condition for the membrane phase potential on all outside boundaries. For the solid phase potential there are external boundaries on the anode and the cathode sides that are in contact with the external electric circuit and only through these boundaries pass the electrical current generated in the fuel cell. On all other external boundaries there is a zero flux boundary condition. The Butler-Volmer function is used to model the transfer currents inside the catalyst layers. The driving force for the kinetics is the local surface over-potential also known as the activation loss. It is generally the difference between the solid and membrane potentials. The gain in electrical potential from crossing from the anode to the cathode side can then be taken into account by subtracting the open-circuit voltage on the cathode side [6].

Many challenges must be overcome before fuel cell vehicles will be a successful competitive alternative for users. Since the conversion of the fuel to energy takes place via an electrochemical process, not combustion, the process is clean, quiet and highly efficient about two to three times more efficient than combustion.

THEORETICAL MODELING OF PEM FUEL CELL

The electrochemistry modeling concerns with calculation of the rate of the hydrogen oxidation and the reduction rate of oxygen. Heterogeneous reactions are assumed for these electrochemical processes that take place on the catalyst surfaces on both sides of the membrane [6-9]. The driving force behind these reactions is the surface over-potential: the difference between the phase potential of the solid and the phase potential of the electrolyte/membrane. Therefore, two potential equations are solved. The first potential equation accounts for the electron transport e^- through the solid conductive materials, as shown in equation 1. The other potential equation is shown in equation 2 represents the ionic transport of H^+ [6].

$$\nabla \cdot (\sigma_{sol} \nabla \Phi_{sol}) + R_{sol} = 0 \quad (1)$$

$$\nabla \cdot (\sigma_{mem} \nabla \Phi_{mem}) + R_{mem} = 0 \quad (2)$$

Where: σ = electrical conductivity (1/ohm-m), Φ = electric potential (volts), and R = volumetric transfer current ($A=m^3$).

There are two types of external boundaries; first type through which there passes an electrical current and second type those through which there passes no current. Note that there is no protonic currents leave the fuel cell through any external boundary; there is a zero flux boundary condition for the membrane phase potential, Φ_{mem} , on all outside boundaries. Also note that for the solid phase potential, Φ_{sol} , there are external boundaries on the anode and the cathode sides that are in contact with the external electric circuit and only through

these boundaries pass the electrical current generated in the fuel cell. On all other external boundaries there is a zero flux boundary condition for Φ_{sol} .

The source terms in equations 1 and 2 are non-zero only inside the catalyst layers. For the membrane phase: on the anode side $R_{mem} = +R_{an} (> 0)$ and on the cathode side $R_{mem} = -R_{cat} (< 0)$. For the solid phase: on the anode side $R_{sol} = -R_{an} (< 0)$ and on the cathode side $R_{sol} = +R_{cat} (> 0)$. The source terms in equations 1 and 2 are also known as the exchange current density (A/m^3), and are shown in equations 3 and 4 [6].

$$R_{an} = J_{an}^{ref} \left(\frac{(H_2)}{(H_2)_{ref}} \right)^{\gamma_{an}} \left(e^{\alpha_{an} F \eta_{an} / RT} - e^{-\alpha_{an} F \eta_{an} / RT} \right) \quad (3)$$

$$R_{cat} = J_{cat}^{ref} \left(\frac{(O_2)}{(O_2)_{ref}} \right)^{\gamma_{cat}} \left(e^{\alpha_{cat} F \eta_{cat} / RT} - e^{-\alpha_{cat} F \eta_{cat} / RT} \right) \quad (4)$$

Where: J^{ref} is the volumetric reference exchange current density (A/m^3), $ref.$ is the local species concentration, reference value ($kgmol/m^3$), γ is the dimensionless concentration dependence, α is dimensionless transfer coefficient, and F is Faraday constant (9.65×10^7 C/kgmol). Equations 3 and 4 are the general formulation of the Butler-Volmer function. Equations 5 and 6 are the simplified form of the Butler-Volmer function which is known as the Tafel formulation [6].

$$R_{an} = J_{an}^{ref} \left(\frac{(H_2)}{(H_2)_{ref}} \right)^{\gamma_{an}} \left(e^{\alpha_{an} F \eta_{an} / RT} \right) \quad (5)$$

$$R_{cat} = J_{cat}^{ref} \left(\frac{(O_2)}{(O_2)_{ref}} \right)^{\gamma_{cat}} \left(e^{\alpha_{cat} F \eta_{cat} / RT} \right) \quad (6)$$

The driving force for the kinetics is the local surface overpotential, η . It is the difference between the solid and membrane potentials, Φ_{sol} and Φ_{mem} . The gain in electrical potential from crossing from the anode to the cathode side can be taken into account by subtracting the open-circuit voltage V_{oc} on the cathode side as shown in equations 7 and 8 [6-9].

$$\eta_{an} = \Phi_{sol} - \Phi_{mem} \quad (7)$$

$$\eta_{cat} = \Phi_{sol} - \Phi_{mem} - V_{oc} \quad (8)$$

When hydrogen atoms come in contact with the catalyst, it splits into two H^+ ions and two electrons e^- . The electrons are forced to travel in an external circuit because the membrane is electrically insulating. The protons migrate through the electrolyte to the cathode, where they reunite with oxygen and the electrons to produce water and heat. On the cathode catalyst

of the fuel cell, oxygen molecules are fed to the cathode and react with the electrons and protons, where it forms two oxygen atoms. Each of these atoms has a strong negative charge. This negative charge attracts the two H^+ ions through the membrane, where they combine with an oxygen atom and two of the electrons from the external circuit to form a water molecule (H_2O). The following reactions occur, respectively, at the anode and the cathode, as shown in equations 10 and 11:



The volumetric source terms for the species equations and energy equation include ohmic heating, heat of formation of water, electric work and latent heat of water are given in equations 11 to 14 [6].

$$S_{H_2} = -\frac{M_{\omega, H_2}}{2F} R_{an} \quad (11)$$

$$S_{O_2} = -\frac{M_{\omega, O_2}}{4F} R_{cat} \quad (12)$$

$$S_{H_2O} = \frac{M_{\omega, H_2O}}{2F} R_{cat} \quad (13)$$

$$S_h = I^2 R_{ohm} + h_{reaction} + \eta R_{an,cat} + h_{phase} \quad (14)$$

Heterogeneous reactions that take place on the catalyst surfaces in the porous media for the electrochemical reaction of the catalyst layers are assumed. Therefore, the species concentrations of hydrogen and oxygen in the rate calculation, equations 3 and 6 are the surface values. The reactions are treated as surface reactions in the two catalyst layers, and it is assumed that the diffusive flux of any reacting species is balanced by its rate of production [6].

$$\frac{\rho D_i}{\delta} (y_{i,surf} - y_{i,cent}) \eta = \frac{M_{\omega,i}}{nF} R_{an,cat} \quad (15)$$

Where: D_i is the mass diffusivity of species i (m^2/s), η is the specific reacting surface area of the catalyst layer, or surface-to-volume ratio ($1/m$), $y_{i,surf}$ is the mass fraction of species i at the reacting surface, $y_{i,cent}$ is the mass fraction of species i at the cell center, and δ is the average distance between the reaction surfaces and the cell center (m). The left hand side of equation 15 represents the diffusive flux at the reacting surface and the right hand side represents the rate of mass generation. The average distance from the center of the cell to the reacting surface is assumed as $\delta = 1/s$. Equation 15 is used to obtain the surface values of H_2 and O_2 concentrations, applying a Newtonian solution procedure. These surface values are then used to compute the rates in equations 3 to 6 [6-13].

The numerical results of the theoretical modeling of pressurized PEM fuel cells are shown in figures 1 to 2. Figure 1 shows contour plot of mass fraction of H_2 , O_2 , and H_2O across the catalyst layers and the membrane. As shown in this figure the species concentrations of the H_2 , O_2 , and H_2O are clear. Figure 3 shows the contour plots of the relative humidity across the catalyst layers and the membrane.

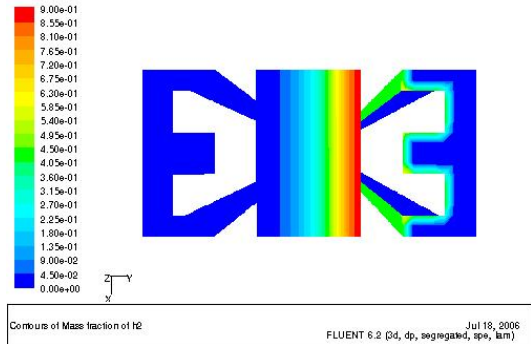


Fig. 1(a) Contour plots of mass fraction of H_2

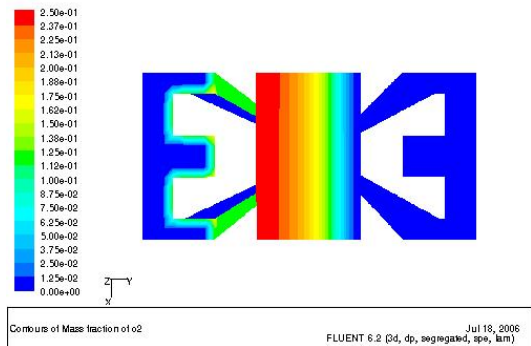


Fig. 1(b) Contour plot of mass fraction of O_2

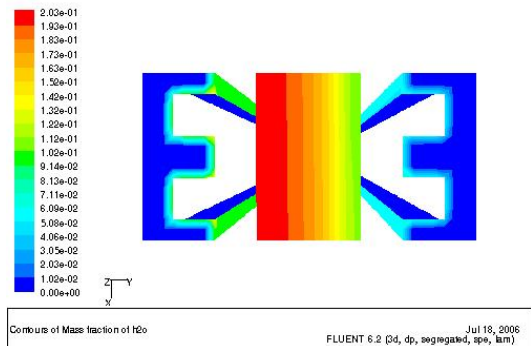


Fig. 1(c) Contour plots of mass fraction of H_2O

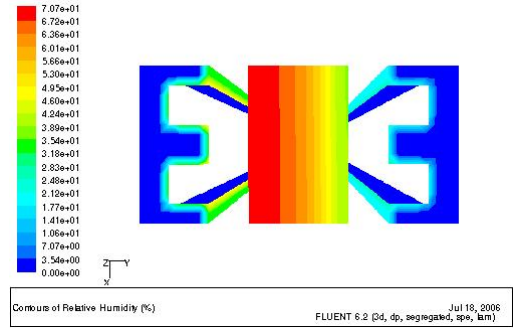


Fig. 2 Contour plots of Relative Humidity

CONCLUSION

Two electric potential fields are solved. One potential is solved in the membrane and catalyst layer. The other is solved in the catalyst layers, the diffusion layers, and the current collectors. Surface reactions on the porous catalyst region are solved and the reaction diffusion balance is applied to compute the rates. Based on the cell prescribed voltage, the current density value is computed. Alternatively, a cell voltage can be computed based on a prescribed average current density. The electrochemical processes of the rate of the hydrogen oxidation and the rate of oxygen reduction are treated as heterogeneous reactions that take place on the catalyst surfaces inside the two catalyst layers on both sides of the membrane. The driving force behind these reactions is the surface over-potential: the difference between the phase potential of the solid and the phase potential of the electrolyte/membrane. Therefore, two potential equations are solved for in the PEM model: one potential equation accounts for the electron transport through the solid conductive materials the other potential equation represents the ionic transport of H^+ .

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