MODELING AND SIMULATION STUDY OF POLYMER ELECTROLYTE MEMBRANE FUEL CELL

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ABSTRACT

Fuel cells are recognized as a promising candidate of power generators for both stationary and automotive applications. A one dimensional unsteady state equation for the reactant gas transport in the gas diffusion layer and in the catalyst layer has been developed to study the unsteady state distribution of oxygen mass fraction in gas diffusion and catalyst layer of the cathode side polymer electrolyte membrane fuel cell. The effect of two parameters namely, diffusivity of oxygen and surface over potential on the mass fraction of oxygen were studied. Also a one dimensional steady state equation for the phase potential has been developed and the distributions of the phase potential in the catalyst layer and in the membrane were studied.

Keywords- Fuel cell, unsteady state equation, Polymer Electrolyte Membrane, Half-cell model, Diffusivity

I. INTRODUCTION

Fuel cell is a device that transforms chemical energy stored in a fuel into electrical energy. The fuel cell will continue to give out product (electricity) as long as raw material (fuel) is supplied. Since fuel cells produce electricity directly from chemical energy, they are more efficient than the combustion engines. The fuel cells are silent, highly reliable and long lasting systems since there are no moving parts. Also there are no undesirable products such as NOx, SOx and particulate emissions. Fuel cells are very useful as power sources in remote locations, such as space craft, remote weather stations, rural locations, and in certain military applications. A new application of fuel cell is micro combined heat and power, which is cogeneration for family homes, office buildings and factories.

A. TYPES OF FUEL CELL

There are five major types of fuel cells classified on the basis of the electrolyte used.

1. Phosphoric acid fuel cell (PAFC).
2. Polymer electrolyte membrane fuel cell (PEMFC).
3. Alkaline fuel cell (AFC).
4. Molten carbonate fuel cell (MCFC).
5. Solid-oxide fuel cell (SOFC).

All the five types of fuel cell work on the same electrochemical principle but they all differ from each other by the operating conditions, incorporating different materials, and fuel tolerance and performance characteristics.

B. PRINCIPLE AND OPERATION OF POLYMER ELECTROLYTE MEMBRANE FUEL CELL

A thin polymer membrane is used as an electrolyte. Protons are the ionic charge carrier in a PEMFC membrane. The schematic diagram of the PEM fuel cell is shown in the figure 1. The oxygen will be supplied in the cathode side and hydrogen is supplied in the anode side, separated by polymer electrolyte membrane. The current which is produced from the fuel cell is collected with the help of the gold plated current collector. The polymer electrolyte membrane fuel cell is the prime candidate for vehicles and other mobile applications of all size down to mobile phones, because of its compactness.

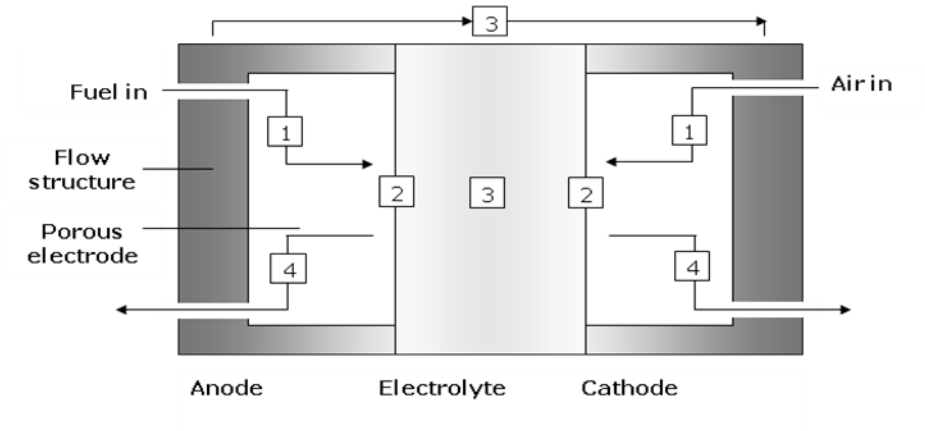

Fig. 1 PEM Fuel Cell

Sequentially, as numbered on the drawing, these steps are as follows:

1. Reactant delivery (transport) into the fuel cell.
2. Electrochemical reaction.
3. Ionic conduction through the electrolyte and electron conduction through the external circuit.
4. Product removal from the fuel cell.

II. MODEL DESCRIPTION

A. HALF CELL MODEL OF A PEM FUEL CELL

A schematic diagram of the cross sectional view of a half- PEM fuel cell is shown in the figure 2. The cathode side of the fuel cell is considered. Oxygen gas transport through a half-PEMFC is simulated. Gas transport from the flow channel to the catalyst layer is by diffusion, which is driven by the concentration gradient.

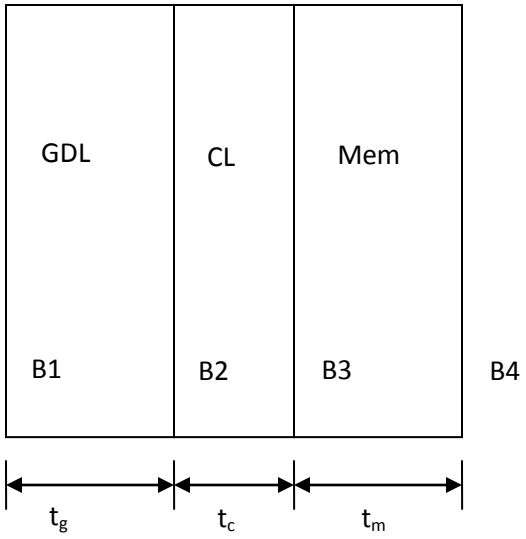

Fig. 2 Half cell model of PEM Fuel cell

B. GOVERNING EQUATIONS

A steady state one dimensional transport equation for the oxygen mass fraction, w, in the diffusion layer can be expressed by

$$\rho\varepsilon_2 \frac{\partial e}{\partial t} = \frac{\partial}{\partial x}(\varepsilon_1^{\tau_1} \rho D \frac{\partial w}{\partial x})$$

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$$\rho\varepsilon_2 \frac{\partial w}{\partial t} = \frac{\partial}{\partial x}(\varepsilon_2^{\tau_2} \rho D \frac{\partial w}{\partial x}) - \frac{kM_{o_2}}{2} w \exp(\frac{\alpha nF}{RT}\eta)$$

The expression for the phase potential in the catalyst layer is

$$\rho\varepsilon_2 \frac{\partial \phi}{\partial t} = \frac{\partial}{\partial x}(\varepsilon_2^{\tau_2} \sigma \frac{\partial \phi}{\partial x}) - nFkw \exp(\frac{\alpha nF}{RT}\eta)$$

The expression for the phase potential in the catalyst layer is

$$\rho\varepsilon_3 \frac{\partial \phi}{\partial t} = \frac{\partial}{\partial x}(\sigma \frac{\partial \phi}{\partial x})$$

The membrane ionic conductivity is evaluated by

$$\sigma = (0.005193\lambda_w - 0.00326)\exp[1268(\frac{1}{303} - \frac{1}{T})]$$

III. RESULTS AND DISCUSSION

The mathematical model described in the previous section is solved using the software MATLAB. The spatial profile of oxygen mass fraction in the gas diffusion layer and the catalyst layer of PEM fuel cell is simulated using MATLAB under steady state and unsteady state conditions. The result show good agreement with the results found in the literature. In this chapter the effect of effective diffusivity and surface over potential on the spatial profile of mass fraction of oxygen is discussed.

A. SIMULATION METHODOLOGY

The split boundary value problem for oxygen mass fraction in the gas diffusion layer and in the catalyst layer under steady state conditions were solved in MATLAB by using the finite difference method with 100 grid points in the gas diffusion layer and 50 grid points catalyst layer in the x direction. The unsteady state equation for oxygen mass fraction in the gas diffusion layer and in the catalyst layer were solved using forward difference in time and central difference in space method.

B. EFFECT OF EFFECTIVE DIFFUSIVITY ON THE MASS FRACTION OF OXYGEN

The effect of effective diffusivity on the mass fraction of oxygen in the gas diffusion layer and in the catalyst layer is shown in the figure 3. The simulation is done for three diffusivity values (D1=2.837*10-5 m2/s, D2= 2.837*10-8 m2/s, D3=2.837*10-10 m2/s). From the figure it is observed that when the diffusivity of the oxygen is high, oxygen diffuses more easily and hence there is almost no concentration gradient across the gas diffusion layer and catalyst layer. For lower diffusivity of oxygen, the concentration of oxygen falls rapidly along the length of the two layers, making available less oxygen at the membrane layer.

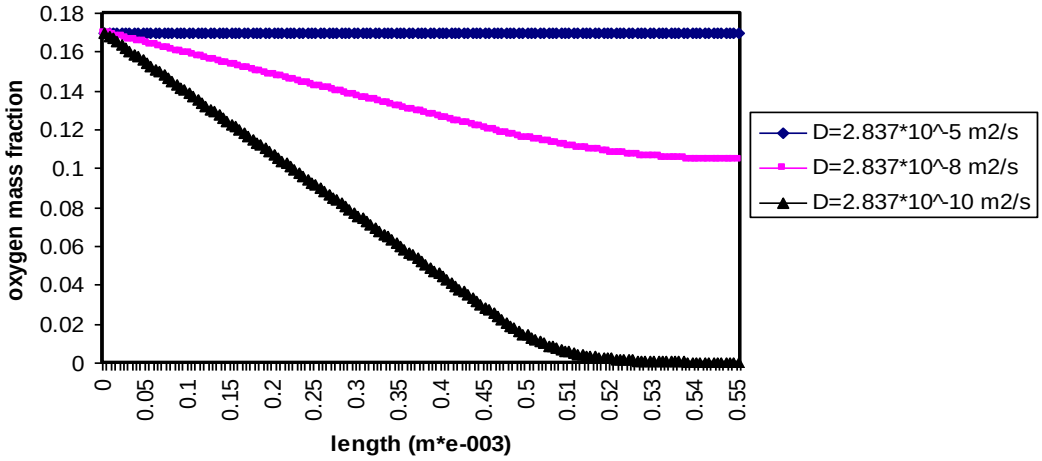

Fig 3. Effect of effective diffusivity on the mass fraction

C. EFFECT OF SURFACE OVER POTENTIAL ON THE MASS FRACTION OF OXYGEN

The effects of surface over potential on the mass fraction of oxygen in the gas diffusion layer and in the catalyst layer were shown in the figure 4. The simulation is done for three values of surface over potential (η1=0.15V, η2=0.25V, η3=0.4V). From the figure it is observed that as the surface over potential value (η3=0.4) increases the mass fraction of oxygen decreases. The significance of the surface over potential is that, as the surface over potential is increased, the activation barrier for the reaction is decreased by an amount –αnFη. Hence more reaction will occur and the mass fraction of oxygen will be reduced.

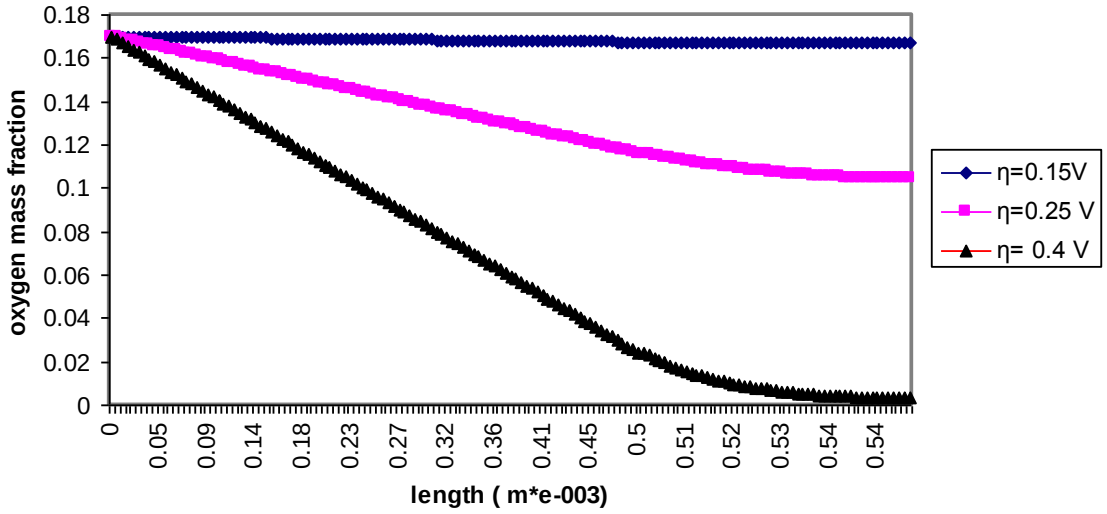

Fig 4. Effect of effective diffusivity on the mass fraction

D. UNSTEADY STATE DIFFUSION OF OXYGEN IN THE GAS DIFFUSION LAYER AND IN THE CATALYST LAYER

The unsteady state diffusion of oxygen in the gas diffusion layer and in the catalyst layer for a time step of 0.0001 was shown in the figure 5. From the figure it is clear that at time t=0 the oxygen mass fraction in the gas diffusion layer and in the catalyst layer is zero. At time t=1, the oxygen enters the gas diffusion layer and the mass fraction of oxygen is 0.17 at the inlet. As the time elapses the oxygen diffuses into the gas diffusion layer and catalyst layer and reaches the final profile. The diffusion of oxygen in the gas diffusion layer and in the catalyst layer attains the steady state within 1 second.

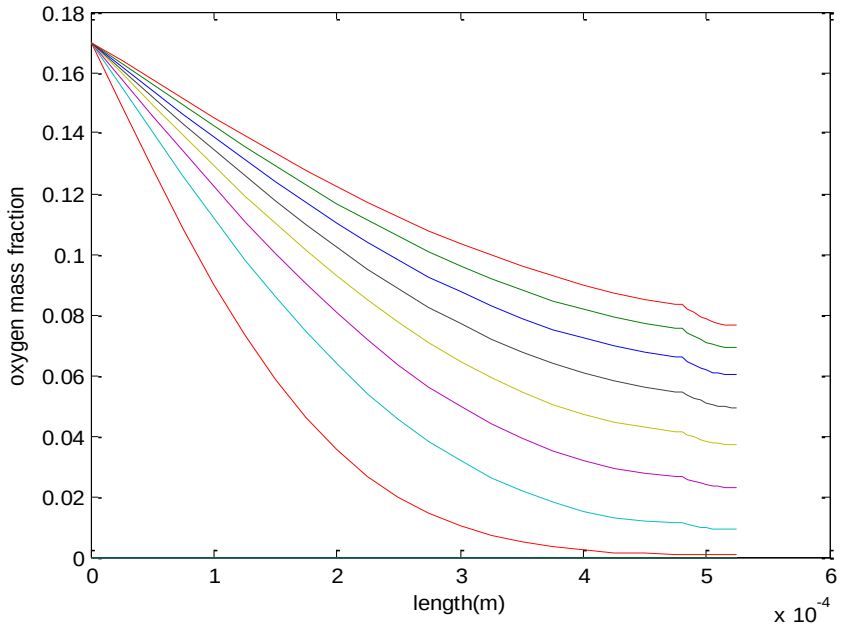

Fig 5. Unsteady state diffusion of oxygen in the gas diffusion layer and in the catalyst layer

E. THE PHASE POTENTIAL DISTRIBUTIONS IN THE CATALYST LAYER AND IN THE MEMBRANE

The steady state one dimensional equation for phase potential in the catalyst layer and in the membrane were solved in MATLAB by using the finite difference method with 50 grid points in the catalyst layer and 100 grid points in the membrane in the x direction. The phase potential distributions in the catalyst layer and in the membrane were shown in the figure 6.

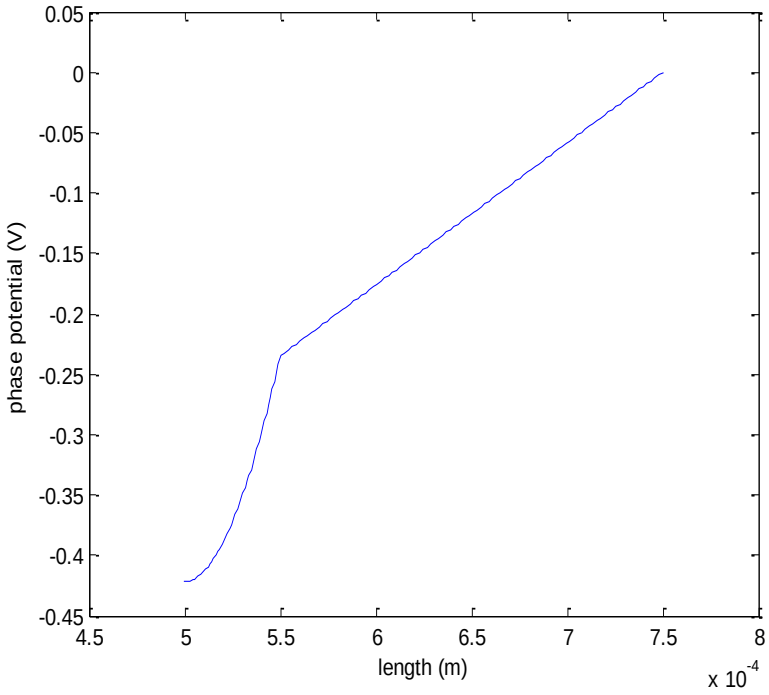

Fig 6. Steady state distribution of phase potential

IV. CONCLUSION

In the present work a one dimensional unsteady state equation for the reactant gas transport in the gas diffusion layer and in the catalyst layer has been developed to study the unsteady state distribution of oxygen mass fraction in the gas diffusion layer and in the catalyst layer of the cathode side of a polymer electrolyte membrane fuel cell. The effect of two parameters namely, diffusivity of oxygen and surface over potential on the mass fraction of oxygen were studied. Also a one dimensional steady state equation for the phase potential has been developed and the distributions of the phase potential in the catalyst layer and in the membrane were studied. The split boundary value problem for the oxygen mass fraction and phase potential were solved in MATLAB by using the finite difference method with 100 grid points in the gas diffusion layer and in membrane and 50 grid points in the catalyst layer in the x direction. The result shows good agreement with the results found in the literature.

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