A THEORETICAL SIMULATION OF A PEM FUEL CELL WITH 4-SERPENTINE FLOW CHANNEL

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Abstract

The effects of different operating parameters on the performance of proton exchange membrane (PEM) 4-Serpentine flow channel fuel cell have been studied theoretically by modeling the problem in FLUENT. Pure hydrogen is used on the anode side and oxygen on the cathode side. Computer simulation results are obtained for voltage as a function of current density at different cell temperatures, operating pressures ,different humidities, gas diffusion layer thickness and catalyst layer thickness. The simulation results are compared with the experimental data, and the agreement is found to be good.

Keywords : 4-Serpentine flow channels, Fuel cell, GDL, PEM

Introduction

Polymer electrolyte membrane fuel cell (PEMFC) is the most promising system among several kinds of fuel cells due to their various advantages such as easy start-up, operation at room temperature, no liquid electrolyte and high current density. To achieve high current density, the optimal operating conditions need to be identified for fuel cell systems in addition to design parameters such as membranes and their thickness, catalysts and alloys, particle size, catalyst quantity, catalyst layer thickness, nature of gas diffusion layers and the bi-polar plates.

Parthasarathy et al. (1992) studied temperature dependence of the electrode kinetics of oxygen reduction at the Platinum/Nafion Interface. Vladimir Gurau et al. (1998) studied two dimensional modal for PEM fuel cells. Shimpalee et al.(2000) presented numerical predictions for temperature distribution in PEM fuel cell. Berning et al. (2002) carried out three dimensional computational analysis to describe transport phenomena in a PEM

fuel cell. Ling Wang et al. (2003) studied experimentally the performance of fuel cell at different operating temperatures, cathode and anode humidification temperatures, and pressures.

Berning and Djilali et al. (2003) developed a three-dimensional, non-isothermal model of a PEM fuel cell. Model was solved using commercial software package CFX-4.3. In this effect of various operational parameters such as temperature and pressure, and geometric and material parameters such as GDL thickness, porosity and channel width to land ratio were investigated.

Um and Wang (2004) used a three-dimensional model to study the effects an interdigitated flow field. The model accounted for mass transport, electrochemical kinetics, species profiles and current density distribution within the cell. Interdigitated flow fields result in forced convection of gases, which aids in liquid water removal at the cathode. This would help improve performance at high current densities when transport limitations due to excessive water production are expected.

Hamilton and Pollet (2010) described some recent developments in the area of flow field plates (FFPs) for proton exchange membrane fuel cells. The function, parameters and design of FFPs in PEM fuel cells are outlined and considered in light of their performance.

Wei-Mon Yan et al. (2008) investigated experimentally the cell performance and pressure drop for two commercial size 16 cm×16 cm serpentine flow field proton exchange membrane fuel cells with Core 5621 and Core 57 membrane electrode assemblies at various cell temperatures and humidification temperatures. At cell temperature lower than the humidification temperature, the cell performance improved as the cell temperature increased, while reversely at cell temperature higher than the humidification temperature. At a specified cell temperature, increasing the cathode and/or anode humidification temperature improved the cell performance and their effects weakened as cell temperature decreased. For the constant mass flow rate mode, both cathode and anode pressure drops increased as humidification temperature increased, while anode pressure drops decreased and cathode pressure drops increased as average current density increased. The optimal cell performance occurred at cell temperature of 65° C and humidification temperature of 70° C. The effects of these operating parameters on the cell performance and pressure drop were analyzed based on the catalytic activity, membrane hydration, and cathode flooding.

Xiao-Dong Wang et al. (2008) investigated the effects of the relative humidity (RH) of the reactants on the cell performance and local transport phenomena in proton exchange membrane fuel cells with parallel and interdigitated flow fields. A three-dimensional model was developed taking into account the effect of the liquid water formation on the reactant transport.

B.Sreenivasulu, S.V.Naidu, V.Dharma Rao, G.Vasu / International Journal Of Computational Engineering Research / ISSN: 2250–3005

Antolini, (2004) investigated a significant lowering of the platinum loading of polymer electrolyte fuel cell electrodes from about $4-10 \text{ mg cm}^{-2}$ (platinum black) to about 0.4 mg cm⁻² or even less (carbon supported platinum), by the introduction of ionomer (liquid Nafion) impregnated gas diffusion electrodes, extending the three-dimensional reaction zone. The loss of performance during cell operation due both to the presence of liquid water causing flooding of the catalyst layer and mass transport limitations and to the poisoning of platinum by the use of reformed fuels.

The survey of literature reveals the necessity to understand the effects of various system parameters in a PEM fuel cell in order to improve its performance. Hence an attempt is made to carry out a parametric study by modeling the problem using FLUENT and by obtaining simulation results over wide ranges of parameters such as fuel cell temperature, pressure and relative humidity.

Formulation of the problem

The dimensions of the fuel cell are 9.6 cm, 0.8948 cm and 9.8 cm in the X, Y and Z directions respectively. The crosssectional area of the membrane electrode assembly is $9.6 \times 9.8 = 94 \text{ cm}^2$. The flow and diffusion of gases and production of electric power in the fuel cell are governed by the coupled transport processes in the membrane, catalyst layer, on gas diffusion electrodes. The reactants hydrogen and oxygen pass through 4-Serpentine flow channels. The schematic diagram of a 4-Serpentine flow channel is shown in Fig.1.



Fig.1 Schematic Diagram of 4-Serpentine flow channel.

A detailed description of the configuration of the PEM fuel cell considered in the theoretical model is presented below. The membrane electrode assembly (MEA) consists of the polymer electrolyte membrane (Nafion 1135, 88 μ m), the anode and cathode catalyst layers and the anode and cathode gas diffusion layer (GDL). The electro-catalyst used is activated carbon supported platinum. The catalyst ink is prepared from platinum-carbon powder with ethyl alcohol. The catalyst ink is a pplied as a layer on the gas diffusion layer (which is a carbon paper).

The catalyst loading on the anode-side is 0.15 mg/cm^2 with a thickness of catalyst layer of $20 \mu m$. A catalyst loading of 0.3 mg/cm^2 is used on the cathode-side with a thickness of catalyst layer of $40 \mu m$. Carbon papers having thickness of 400 μm are used as gas diffusion layers on both sides. The membrane electrode assembly (viz., membrane, GDLs and catalyst layers) is placed between two graphite plates and is pressed between gold-coated copper plates.

The flow of hydrogen and oxygen in a fuel cell takes place in the channel formed by a flow field plate and a carbon paper, which serves as gas diffusion layer. The flow channel contains a number of bends to facilitate diffusion of the gas through the gas diffusion layer (GDL) while the gas passes through the channel.

B.Sreenivasulu, S.V.Naidu, V.Dharma Rao, G.Vasu / International Journal Of Computational Engineering Research / ISSN: 2250–3005

Dimensions of the channel:

Length=98 mm, width=1.5mm, height=0.8mm rib width is 2mm. The various inlet parameters and electrode material properties which are given as inputs to the fluent solver are as follows: cell temperature= 333K, pressure=1atm, humidity = 100%, flow rate of hydrogen= 3.65799×10^{-7} kg/sec, flow rate of oxygen = 5.85278×10^{-6} kg/sec. Permeabilities of membrane, GDL and CL are 1.8×10^{-18} , 1.76×10^{-11} and 1.76×10^{-11} m² respectively. Thermal conductivities of membrane, GDL and CL are 0.5, 1.7 and 0.27 W/m-K respectively. Electrical conductivities of membrane, GDL and CL are 11.6733, 50 and 50 S/m respectively. Porosities of the membrane, GDL and CL are maintained at 0.5. Reference current densities at anode and cathode are 1×10^8 and 650 A/m^3 respectively. Reference concentrations of hydrogen and oxygen maintained at 0.04088 kmol/m³.

The problem of the single fuel cell which contains the membrane electrode assembly with 4-Serpentine flow channel is modeled and solved using FLUENT software. A geometric model is created in GAMBIT module. This model is solved in FLUENT module with appropriate boundary conditions. The three dimensional CFD model of PEM fuel cell in parallel flow arrangement of the gases is shown in Fig.2.



Fig.2 Three-dimensional computational domain (Components are not to scale).

Boundary conditions:

There are several zones which must be specified in the boundary conditions panel are shown in Fig.3. *Anode inlet:* Mass flow rate = 3.65774×10^{-7} kg/s, Temperature =333K, Species (mass fractions): H₂=0.3126, H₂0= 0.6874. *Cathode inlet:* Mass flow rate = 5.85238×10^{-6} Kg/s, Temperature =333K, Species (mass fractions): O₂=0.8792, H₂0= 0.1208. *Anode outlet:* Temperature =333K, Pressure outlet =0 P(gauge pressure).

Cathode outlet: Temperature =333K, Pressure outlet =0 P(gauge pressure). *Anode voltage terminal:* Electric potential=0, Protonic potential=0, Temperature=333K. *Cathode voltage terminal:* Electric potential= Value (say 0.4), Protonic potential=0, Temperature=333K.



Fig. 3 Boundary conditions

Results and Discussion

Results are obtained using FLUENT for the following set of operating conditions: temperature=333K, pressure=1atm, humidity=100%, GDL thickness=400 μ m, catalyst layer thickness at anode is 20 μ m and at cathode 40 μ m. These simulation results are compared with the experimental data of Sreenivasulu (2011), and the comparison is shown in Fig.4. The agreement between the simulation results and experimental data is found to be good.

The validated model is now ready for studying the effects of several operating parameters on fuel cell performance. The performance of the fuel cell based on a certain parameter can be obtained by varying that parameter while keeping all other parameters constant. Results obtained from these parametric studies will allow in identifying the critical parameters on the fuel cell performance. The fuel cell performance at various operating conditions is analyzed using the polarization curves and power curves.



Fig. 4 Comparison of simulation results with the experimental data.

FLUENT results are obtained for voltage as a function of current density at four different cell temperatures (40, 50, 60 and 70°C), five operating pressures (1, 2, 3, 4 and 5 atm), four different humidities (10, 25, 50, and 65%), three different GDL thicknesses (200, 300 and 400 μ m), and three different cathode catalyst layer thicknesses (20, 30 and 40 μ m). These results are presented and discussed below.

Effect of Temperature

The pressure and electrode porosity are kept constant at 1atm. and 0.5 respectively, while the temperatures are varied from 40 to 70°C. The polarization curves of the cell at different operating temperatures are shown in Fig. 5. It is observed that the voltage across the fuel cell increases with an increase in temperature. The performance is better in all regions along the polarization curve. This is because the gas diffusivity, exchange current density and membrane conductivity are high at higher temperatures. The P-I curves are also shown in Fig. 6 for the same conditions as mentioned above.



Fig.5 Effect of temperature on cell performance (V-I curve).



Effect of Pressure

Pressure is another operating parameter that has a large effect on fuel cell performance. The polarization curves at different cell operating pressures are shown in Fig. 7. The cell temperature and electrode porosity are maintained at 343 K and 0.5 respectively. It is observed from Fig.7 that as the operating pressure is increased from 1 to 5 atm. the fuel cell performance increases. This is due to an increase in gas diffusivity with an increase in pressure. However additional energy is required to compress the gases to raise the pressure, which may outweigh the gain in efficiency. For the same conditions the P-I curve also shown in Fig. 8.



Fig.7 Effect of pressure on cell performance (V-I curve).



Fig.8 Effect of pressure on cell performance (P-I curve).

Effect of Gas Humidity

The effect of gas humidity on cell performance is shown in Figs.9 and 10. It is observed that the performance of fuel cell increases with humidity up to 65%, and there is no further improvement in the performance with an increase in humidity above 65%. Below 65% of reactant stream humidity the voltage drop occurs due to insufficient amount of water at the electrolyte membranes of the fuel cell. These membranes must maintain a minimum level of moisture in order to properly conduct ions.



Fig.9 Effect of humidity on cell performance (V-I curve).



Fig.10 Effect of humidity on cell performance (P-I curve).

Effect of GDL Thickness.

The effect of GDL thickness is shown in Figs. 11 and 12. When the GDL thickness is 200 μ m, the average potential is higher than the case of 300 μ m and 400 μ m. A thinner GDL results in a larger oxygen transfer from the gas channel to the catalyst layer, and thus a larger potential is generated. The effect of the GDL thickness on the fuel cell performance is again mostly on the mass transport, as the Ohmic losses of the electrons inside the GDL can be neglected due to the high conductivity of the carbon fiber paper.



Fig.12 Effect of GDL thickness on cell performance (P-I curve).

Effect of cathode catalyst layer thickness

Figure 13 and 14 shows the effect of cathode catalyst layer thickness on performance of the fuel cell. The theoretical results for different catalyst layer thickness (20, 30 and 40 μ m) and at a 20 μ m constant anode catalyst layer are shown in Figs.13 and 14. It is observed from Figs. 13 and 14 the performance is increases by an increase with catalyst layer thickness. It is also observed that the performance is superior for 40 μ m compared to the 20 μ m and 30 μ m. This is due to the fact that the reactant gases do not have as many reaction sites in the later case as in the former case. However the performance is decreases beyond certain thickness due to in catalyst layer's electric and ionic resistance and to the increase in mass transport limitation. Due to increased mass transport resistance in higher catalyst thickness, at higher current densities, the reactant gases are unable to reach all the reaction sites and the catalyst at the inner half of the catalyst layer (i.e., adjacent to the membrane) largely remain underutilized.



Fig.13 Effect of catalyst layer thickness on cell performance (V-I curve).



Fig.14 Effect of catalyst layer thickness on cell performance (P-I curve).

CONCLUSIONS:

The following conclusions can be drawn from the results.

- 1. The theoretical model developed for single PEM fuel cell simulates effectively the various conditions that exist in a real fuel cell, which is evident from the comparison of the theoretical results with experimental data.
- 2. The fuel cell performance is improved with an increase in temperature from 40°C to 70°C. This is due to increase of gas diffusivity, exchange current density and membrane conductivity at higher temperature.
- 3. As the operating pressure is increased from 1 to 5 atm, the fuel cell performance also increases due to increase in inlet concentration of oxygen.
- 4. A thinner GDL results in a larger oxygen transfer from the gas channel to the catalyst layer, and thus a larger potential is generated.
- 5. As the catalyst layer thickness increases there is an improvement in the performance was observed. However the performance is decreases beyond certain thickness due to in catalyst layer's electric and ionic resistance and to the increase in mass transport limitation.

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