Three Dimensional Computational Study on Proton Exchange Membrane Fuel Cell by Operation Conditions*

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Abstract
A single-phase, fully three-dimensional simulation model for a proton exchange membrane(PEM) fuel cell was used to examine the interdigitated flow field with electrochemical reaction and ion, electron, and water transport(electro-osmotic drag flux and back diffusion flux) through the polymer membrane. The numerical results showed that the fuel cell with an interdigitated flow field resulted in better performance than a fuel cell with a conventional flow field due to its strong convective transport across gas diffusion layer(GDL). However, the pressure drop in an interdigitated flow field is much greater than in conventional flow field. To investigate the effect of relative humidity on the performance of a PEM fuel cell, the humidification condition was set to 100% at the anode flow field and was changed by 0-100% at the cathode flow field. Maximum power density was obtained for a 70% humidified condition at the cathode where the oxygen concentration is moderately high while maintaining high ion conductivity at the polymer membrane.

Key words: Proton Exchange Membrane Fuel Cell, Conventional Flow Field, Interdigitated Flow Field, Relative Humidity

1. Introduction
A proton exchange membrane(PEM) fuel cell is an electrochemical device that directly converts the chemical energy to electric and heat energy. A PEM fuel cell using a very thin membrane has been considered for a promising candidate of future power sources for transportation and in portable power systems. Its features, including high power density, simple construction, and fast startup, make it suitable for applications in automotive and domestic appliances. (1-3)

The PEM fuel cell is a sandwich of two graphite bipolar plates with small flow fields separated by a membrane electrode assembly(MEA). The MEA consists of a membrane and two electrodes with a dispersed Pt catalyst. The gas diffusion layer(GDL) is porous to supply reactants to the electrodes in unexposed areas of the flow channel. It is well known that flow field design, including GDL, is very important to supply the reactant and expel the product effectively, and hence directly affects the performance of the fuel cell. (4)

Simulation and modeling of the mass transport and management of water and heat in flow fields are being used extensively in researches and industrial applications to gain better understanding of the fundamental processes of PEM fuel cell and to optimize PEM fuel cell flow field designs before building a prototype for engineering application. (5)

Therefore, many researches have examined optimal flow fielded configurations. Most
flow field studies have focused on conventional and serpentine flow fields. Recent demand for higher power density PEM fuel cell requires a decrease of concentration over voltage at high current density, and an increase of current density at the mid-cell voltage range. An interdigitated flow field was recently proposed wherein the mass transfer rate by convection inside a GDL is greater than diffusion transfer rate by the diffusion mechanism through a GDL gas diffusion layer. In PEM fuel cells with a conventional flow field, the fuel gas is transported to the diffuser layer mainly by means of the diffusion effect. In the cells with an interdigitated flow field, baffles are added at the end of each flow channel to force the fuel gas transported into the diffuser layer by convection; thus the limiting current density can be extended. (6-9)

Weng et al (10) presented that the reactant RH and the flow field design all significantly affect cell performance. For the same operating conditions and reactant RH, the interdigitated design has better cell performance than the conventional design. With a constant anode RH=100%, for lower operating voltages, a lower cathode RH reduces cathode flooding and improves cell performance, while for higher operating voltages, a higher cathode RH maintains the membrane hydration to give better cell performance. And Zhang et al (11) presented that fuel cell performance could be depressed significantly by decreasing RH from 100 to 25%. AC impedance and cyclic voltammetry techniques were employed to diagnose the RH effect on fuel cell reaction kinetics. Reducing RH can result in slower electrode kinetics, including electrode reaction and mass diffusion rates, and higher membrane resistance.

However, most papers showed that bypass flow in the interdigitated flow channel improved the performance of fuel cell and also resulted in the increase of the pressure loss along the channel. But our work focused on the effect of operating condition such as relative humidity on the performance of PEM fuel cell along with the comparison of flow fields of fuel cell with conventional flow channel and interdigitated flow channel.

It is very important to find out optimum relative humidity condition of fuel cells with different flow configurations for optimum control of the fuel cell system.

In this paper, we developed a 3-D computational fluid dynamics (CFD) model for a PEM fuel cell which can deal with both anode and cathode conventional and interdigitated flow fields. A commercial program, FLUENT (Version 6.3), was modified with UDF (User-Defined Functions) to simulate the 3-D PEM fuel cell model (12-17). With this simulation, we investigated the effect of the flow fields structure and the relative humidity of the reactant on the performance of PEM fuel cell along with the comparison of flow fields of fuel cell with conventional flow channel and interdigitated flow channel.

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Nomenclature

- $A_{sv}$: specific surface area of the control volume, $m^{-1}$
- $D_{w}$: diffusion coefficient of water, $m^2 s^{-1}$
- $F$: Faraday constant, $96,487 Cmol^{-1}$
- $I$: local current density, $Am^{-2}$
- $k$: thermal conductivity, $W(mk^{-1})$
- $M$: molecular weight, $kgmol^{-1}$
- $M_{e, dry}$: equivalent weight of a dry membrane, $kgmol^{-1}$
- $n$: number of electrons in electrochemical reaction
- $n_d$: electro-osmotic drag coefficient
- $P$: Pressure, $pa$
- $T$: Temperature, $K$
- $u$: velocity vector, $ms^{-1}$
- $x, y, z$: Cell coordinates
2. Numerical Models

Governing equations for calculating the fully three dimensional flow field are expressed under following assumptions

1) The gas mixture is incompressible, ideal fluid
2) The flow in the flow channel is laminar
3) Isothermal condition
4) Butler-Volmer kinetics for electrochemical reaction rate

2.1.1 Mass conservation equation

\[ \nabla \cdot (\varepsilon \mu u) = S_m \]  

Where \( \varepsilon \) is the porosity of porous materials. \( S_m \) denotes source terms corresponding the consumption of hydrogen and oxygen in the anode and cathode, and the production of water in the cathode

\[ S_m = S_{H_2} + S_{aw} : \text{Anode Side} \]  
\[ S_m = S_{O_2} + S_{ew} : \text{Cathode Side} \]

2.1.2 Momentum conservation equation

The fluid flow in fuel cell is described as following equation based on Darcy’s law.

\[ \nabla (\varepsilon \rho u u) = -\varepsilon \nabla p + \nabla (\varepsilon \mu \nabla u) + S_u \]  

Where \( S_u \) is expressed as

\[ S_u = -\frac{\mu u}{\beta_x} \]  
\[ S_u = -\frac{\mu v}{\beta_y} \]  
\[ S_u = -\frac{\mu w}{\beta_z} \]

2.1.3 Species conservation equation

\[ \nabla (\varepsilon \rho u C_k) = \nabla (D_k \nabla C_k) + S_k \]  

Where source term \( S_k \) denotes,
\[ S_t = \left\{ \begin{array}{c} \frac{I(x,y)}{2F} M_H A_y : S_{ht} \\ \frac{\alpha(x,y)}{F} I(x,y) M_H A_y : S_{aw} \\ \frac{I(x,y)}{4F} M_O A_y : S_{lt} \\ 1+2\alpha(x,y) \frac{I(x,y) M_H A_y}{2F} : S_{cw} \end{array} \right. \]

Current density \( I(x,y) \) is described as

\[
I(x,y) = \frac{\sigma}{l_m} [E - V_c - \eta(x,y)]
\]

Where \( \alpha(x,y) \) is expressed as

\[
\alpha(x,y) = n_j - \frac{F}{R(x,y)} D_j(x,y) \frac{C_c - C_o}{T_a}
\]

Expressions for water transport and other variables are listed in Table 1.

<table>
<thead>
<tr>
<th>Table.1 Equation for modeling electrochemical and water transport effects</th>
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<tr>
<td>Water activity</td>
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<td>Nernst equation</td>
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<td>Water content in the membrane</td>
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<td>Electro-osmotic drag coefficient</td>
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<td>Water content in the membrane</td>
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<tr>
<td>Membrane conductivity</td>
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<tr>
<td>Water content in the membrane</td>
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<td>Over potential</td>
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<td>Back diffusion</td>
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2.2 Numerical analysis

<table>
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<tr>
<th>Table.2 Physical Parameters</th>
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<tbody>
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<td>Channel Length(cm)</td>
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<td>Channel Width(cm)</td>
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<tr>
<td>Channel Height(cm)</td>
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<tr>
<td>GDL thickness(cm)</td>
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<tr>
<td>Catalyst layer thickness(cm)</td>
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<td>Inlet temperature(K)</td>
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<td>Anode side pressure(atm)</td>
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Figure 1 shows the comparison of conventional and interdigitated flow field structure respectively. The dimensions of flow field is set to $0.762 \times 0.762 \times 4.0 \text{ cm}$. The flow fields of anode and cathode is divided into $40 \times 50 \times 24$. At the inlets, the fluid is supposed to flow into the channel at known velocity and the atmospheric pressure is applied at the outlets. Other specifications necessary for calculation is shown in Table 2.

Figure 1 Schematic of the flow channel structure (a) conventional and (b) interdigitated flow field

3. Results and Discussions

To validate the numerical simulation model used in this study, the i-V polarization curves were compared with the experimental results from a PEM Fuel Cell with a conventional flow field obtained under the same operating condition as shown in Figure 2. (18)

Figure 2 Comparison of i-V polarization at present study and experimental study at anode side humidity 100% and cathode side humidity 0%.

There is only a small difference between the numerical simulation and the experimental data. However, at high current density, the discrepancy between the numerical simulation and the experimental results is somewhat large, and the model always over-predicts the current density. The low current density in the high current density region shown by the experimental results may be caused by the presence of liquid water in the catalyst layers and the GDL. The presence of liquid water tends to decrease the effective porosity of the GDL and Pt catalyst layers, and increase the mass transfer resistance. However comparison of the relative performance of PEM fuel cell with different flow configurations using a single phase model may give the data necessary to design of the flow field.
Figure 3 two-dimensional velocity vectors in the flow field (a) conventional flow field (b) interdigitated flow field at anode side humidity 100% and cathode side humidity 0%.

Using this numerical simulation model and the operating conditions listed in Table 2, numerical simulations were carried out for examining interdigitated and conventional flow fields. The performance of the two types of flow fields under same operating conditions was simulated numerically.

To compare the mass transport inside the gas diffusion layer (GDL) of the two flow fields, the velocity vector distribution at the 1/4, 1/2 and 3/4 section along the flow direction...
of each flow fields was presented Figure 3. The velocity vector in the conventional flow field in Figure 3-(a) is going toward the GDL and has a symmetric shape, which indicates that most reactants are transported by a diffusion process. On the other hand, for the interdigitated flow field in Figure 3-(b), velocity vectors in both the anode and cathode sides point from the inlet to the outlet of gas channel due to the forced convection mechanism of mass transport in the GDL. This convective transport makes the mass transport of hydrogen and air into the catalyst layer more effective. And that the strong convection by bypass flow in GDL in the interdigitated flow channel is more effective to remove the water rather than diffusion flow in the diffusion flow channel as shown in Fig.3. Color distribution in Fig. 3 represents the mean square root of magnitude of velocities($V_x, V_y, V_z$). So, color of magnitude is in red color at the central region where velocity is high and in the blue color at the wall and near GDL where velocity is low.

Figure 4 shows the velocity vector distribution at the x-z cross section on the GDL at anode side. The velocity vector in the GDL of conventional flow field in Figure 4-(a) represents the mass transport by the diffusion mechanism, because velocity vectors are directed along the flow channel. The velocity field in the GDL of the interdigitated flow field in Figure 4-(b) shows the mass transport by the convection between the flow fields.

![Figure 4](image)

(a)Conventional flow field  (b)Interdigitated flow field

Figure 4 Comparison of distribution of velocity vector on the gas diffusion layer at anode side humidity 100% and cathode side humidity 0%.

And it is important to know the pressure loss in each flow field since a higher pressure loss requires a higher pumping power. The pressure loss is caused by diffusion and convection flow in conventional and interdigitated flow fields. Pressure drop for interdigitated flow field is higher due to strong convective flow across the GDL than that for conventional flow channel. While a higher fuel supply in interdigitated flow field improves performance due to the higher mass transfer by convection flow, it also accompanies a higher pressure drop in the flow field.

Figure 5 shows the local current density distribution on the membrane at the different cell voltage at conventional and interdigitated flow field at co-flow condition. Figure 5-(a) and 5-(b) shows the contour of current density on the polymer membrane at 0.5V. The current density at inlet was the highest and decreased along the flow field. Maximum hydrogen and oxygen are supplied at the entrance region under co-flow condition because the fuel and oxygen are consumed along the flow channel.

The contour of current density pattern was symmetric pattern to center line of the Z axis in conventional flow fields. But contour of current density pattern was asymmetric to center line of the Z axis in interdigitated flow fields. This is because the concentration of hydrogen and oxygen is the highest at the inlet flow field and getting decreasing as it moves to the outlet.

Figure 6 shows i-V and power density polarization curves for conventional and interdigitated flow field. In the low cell voltage region, the power density for fuel cell with
the interdigitated flow field was higher than that with the conventional flow field. It is obvious that the interdigitated flow field outperforms the conventional flow field, especially at high current densities. The limit current density in a fuel cell with the interdigitated flow field is improved compared to that of the fuel cell with the conventional flow field. This is because high oxygen and hydrogen transfer rate in fuel cell with interdigitated flow field can be provided by strong forced convection at high current density, which cannot be satisfied by the conventional flow field due to the diffusion limitations. Voltage of 0.5V for the maximum power density was found to be the optimal operating condition for PEM fuel cell. These results indicate that the trade off between performance and pressure loss should be considered for the efficient design of the flow field.

Figure 5 Distributions of current density on the membrane at different cell voltage at anode side humidity 100% and cathode side humidity 0%.

Figure 7 show the average current density curves for conventional and interdigitated flow fields for various anode relative humidity with constant 100%.

Figure7 shows that maximum current density existed at the relative humidity of 60% in the cathode side in conventional flow field. On the other hand, maximum current density was obtained at relative humidity of 70% in the cathode side in the interdigitated flow field.

To investigate the effects of relative humidity in the cathode side on performance of the fuel cell, moral concentration of water and oxygen with different relative humidity were presented in Figure 8.

Figure 8-(a) shows that moral concentration of water increased linearly along the flow
direction conventional flow field. In the interdigitated flow field, moral concentration of water increased along the flow direction but there were spikes at the inlet and outlet region due to strong bypass flow shown in Figure 6. Generally the moral concentration of water in the conventional flow field and interdigitated flow field increased with increasing relative humidity in the cathode side. Figure 8-(b) shows that moral concentration of oxygen was decreased with increasing relative humidity in the cathode side in the conventional flow field and interdigitated flow field except existence of spikes in the inlet and outlet region. It is known that ion conductivity of membrane affects performance of fuel cell greatly. Figure 9 shows the ion conductivity of membrane along the flow direction in the conventional and interdigitated flow field. As shown in Fig.8-(a), water vapor concentration along the flow channel at the cathode side increases as electrochemical reaction forming water takes place. But the ion conductivity of membrane is determined by the balance of the electro-osmotic drag from anode side and back diffusion from cathode side. Normally, the electro-osmotic drag from anode side is more dominant to determine the ion conductivity of membrane and the electro-osmotic drag tends to be higher at the inlet region than at the exit region of flow channel.

As expected, the ion conductivity of membrane increased with increasing relative humidity in the cathode side in both flow fields. It is thought that the maximum current density can be obtained by trade off of increasing ion conductivity of membrane and decreasing moral concentration of oxygen with increasing relative humidity in the cathode side.

![Figure 6](image6.png)

**Figure 6** Comparison of polarization curve at conventional and Interdigitated flow field at anode side humidity 100% and cathode side humidity 0%.

![Figure 7](image7.png)

**Figure 7** Comparison of current density curve at different relative cathode side humidity
Figure 8 Comparison of moral concentration of water and oxygen at different relative cathode side humidity

Figure 9 Comparison of membrane ion conductivity at different relative cathode side humidity

4. Conclusions

By using a fully 3-D simulation model for PEM fuel cell that can deal with anode and cathode flow together, following conclusions for PEM fuel cell with conventional and interdigitated flow field could be obtained.

1) The same operating conditions, the performance of PEM fuel cell with interdigitated
flow field design has better fuel cell performance than the conventional flow field design due to strong mass transport by convection mechanism across GDL.

2) The contour of current density pattern was symmetric pattern to center line of the $Z$ axis in conventional flow fields. But contour of current density pattern was asymmetric to center line of the $Z$ axis in interdigitated flow fields. This is because the concentration of hydrogen and oxygen is the highest at the inlet flow field and getting decreasing as it moves to the outlet.

3) It is thought that the maximum current density can be obtained by trade off of increasing ion conductivity of membrane and decreasing moral concentration of oxygen with increasing relative humidity in the cathode side

4) Maximum current density existed at the relative humidity of 60% in the cathode side in conventional flow field. On the other hand, maximum current density was obtained at relative humidity of 70% in the cathode side in the interdigitated flow field.

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