Study of the coflow and counterflow distributors geometry in the cathode of a Proton Exchange Membrane Fuel Cell

Li P.F., E.Birgersson
Engineering Science Programme, Faculty of Engineering, National University of Singapore

Abstract

Based on three-dimensional simulation of the cathode of a proton exchange membrane fuel cell, two types of flow-distributors, namely parallel coflow and counterflow channels, are studied through comparison of current densities and current standard deviations at the active layer. A quantitative result shows the coflow channel can sustain a slightly larger current density, and the standard deviation of coflow channel is smaller than counterflow channel as well. Besides study on flow direction, a little study of width of the channel is carried out to show the effect of geometric changes. From the results, larger-width channels have larger current density and better current distribution with smaller current standard deviation.

1. Introduction

Environmental pollution and depletion of conventional fossil fuel call for a cleaner and more abundant energy source. In recent years, fuel cell has attracted more and more people’s attention. The final product of fuel cell is just clean water which has little environmental issues compared to conventional fuels. What’s more, a large resource of hydrogen energy can provide us with a non-exhausted and renewable energy source. Lastly, the wide-range usage of fuel cell, from cell phone and laptop batteries to power source to vehicles, has potential to become one of the most important power supplies of economy development.

One type of fuel cell, on which this paper focuses, is proton exchange membrane fuel cell
(Figure 1). The fuel cell comprises two porous electrodes, namely anode and cathode, with a proton conducting membrane in-between. The basic concept of this type of fuel cell is the oxidation-reduction reaction between hydrogen and oxygen. Oxidation reaction of hydrogen at anode produces electrons and protons. Current flowing through load circuit outside the fuel cell is generated through transfer of electrons from anode to cathode. Simultaneously, protons go through membrane placed in the middle of the fuel cell to undergo reduction reaction with oxygen at the cathode. The specific reactions at the two electrodes are shown below respectively:

\[
\begin{align*}
2H_2 & \rightarrow 4H^+ + 4e^- \quad \text{at the anode;} \\
O_2 + 4H^+ & \rightarrow 2H_2O \quad \text{at the cathode;}
\end{align*}
\]

Therefore, study on mass, momentum and species transfer inside the fuel cell is very crucial to our research on fuel cell. Computer modeling is brought into this field at the time. Some previous work has been done in one or two dimension. M. Vynnychy and E. Birgersson [1] listed some models in their research paper. In order to take more study on the flow-distributor, three-dimensional modeling, based on computational fluid dynamics, is introduced to study the transport phenomena in the fuel cell. Burning et al. [2] and Zhou and Liu [3] used models with parallel flow channels to understand local species behavior and predict current density. Following study of water transport through the membrane on straight channels was implemented by Dutta et al. [4]. The effect of existence of porous backing was studied in his paper as well. Further studies on flow channels on the cathode of fuel cell were continuously carried by many researchers. Dutta et al [5] applied serpentine flow channel onto the cathode to see cell performance. Then porous foam found by Senn and Poulikakos [6] was shown having better performance than straight and serpentine flow channels. Later, interdigitated flow channel developed by Um and Wang [7] can sustain even higher current density than the straight channels. The researches on flow channels have not been resting for a while. More and more researchers make an effort to develop and study new and more complicated flow field distributors.

This paper emphasizes only on the straight flow-distributor geometry in the cathode, parallel coflow and counterflow channels. The model used here simply takes one-phase condition into account instead of two or higher phases. This is only valid in the condition of high temperature and partial pressure of water stays below the saturation partial pressure. With this model, two important parameters, current density and standard deviation, are studied.

2. Model description

2.1 Flow-distributor geometry

(a) Parallel coflow channel:
A series of straight channels passes over the porous backing. Flow runs in one direction. Flow entrances of channels are placed at one side whereas exits are at the other side of the fuel cell. (Figure 2)
Figure 2. Parallel coflow channels

(b) Parallel counterflow channel:
A series of straight channels pass over the porous backing. Flow runs in opposite direction. Half flow entrances and half flow exits of channels exist at one side whereas the other half are at the other side of fuel cell. (Figure 3)

Table 1 List of parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
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</tr>
</tbody>
</table>
2.2 Governing equations

2.2.1 The Navier-Stokes equations

The flow in channels is compressible flow and modeled with the momentum and continuity equations:
\[ \rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla p + \mu \nabla^2 \mathbf{v} + \left( \frac{4\mu}{3} + \mu^v \right) \nabla (\nabla \cdot \mathbf{v}); \quad \frac{\partial p}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \]

Since steady state has been studied in this paper, the partial time derivative vanishes. Hence, continuity equation becomes:
\[ \nabla \cdot (\rho \mathbf{v}) = 0 \]

Where \( \mathbf{v} \) is the velocity, \( \rho \) is the density, \( p \) is the pressure and \( \mu \) is the dynamic viscosity. \( \mu^v \) is second viscosity coefficient.

2.2.2 Maxwell-Stefan diffusion and convection equation

\[ \nabla [(\rho \mathbf{v}) wO_2] = \nabla \cdot [(\rho \mathbf{D}) \nabla wO_2] \]
\[ \nabla [(\rho \mathbf{v}) wH_2O] = \nabla \cdot [(\rho \mathbf{D}) \nabla wH_2O] \]

Where \( \mathbf{D} \) is the diffusion tensor, \( wO_2 \) and \( wH_2O \) are mass fractions of oxygen and water vapor.

2.3 Boundary conditions

2.3.2 Inlet

Pressure gradient across channel is \( dp \), therefore pressure at flow entrance and no viscous stress is involved.

For parallel coflow channel:
\[ \eta(\nabla \mathbf{v} + (\nabla \mathbf{v})^T) \mathbf{n} = 0; \quad p = p_0 + dp; \quad \mathbf{v} \cdot \mathbf{i} = v_x; \quad y- \text{ and } z- \text{ components of velocity are both } 0; \quad wO_2 = w_{O_20}; \quad wH_2O = w_{H_2O0}; \]

Where \( \eta \) is the overpotential, \( v_x \) is the x-component of velocity and \( \mathbf{n} \) is the unit normal

For parallel counterflow channel:
\[ \eta(\nabla \mathbf{v} + (\nabla \mathbf{v})^T) \mathbf{n} = 0; \quad p = p_0 + dp; \quad \mathbf{v} \cdot \mathbf{i} = -v_x; \quad y- \text{ and } z- \text{ components of velocity are both } 0; \quad wO_2 = w_{O_20}; \quad wH_2O = w_{H_2O0}; \]
2.3.3 Outlet

\[ \eta \left( \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right) \mathbf{n} = 0; \quad p = p_0; \quad \mathbf{n}_i \cdot \mathbf{n} = (\rho \omega_i \mathbf{u}) \cdot \mathbf{n} \]

Where \( \mathbf{n}_i \) and \( \omega_i \) represent the mass flux and mass fraction of species \( i \) and \( \rho \) is the density.

2.3.4 Active layer / porous backing interface

\[ \mathbf{n}_{O_2} \cdot \mathbf{n} = M_{O_2} \frac{i_c}{4F}; \quad \mathbf{n}_{H_2O} \cdot \mathbf{n} = -M_{H_2O} \frac{i_c}{F} \left( \frac{1}{2} + t_{H2O} \right) \]

where \( \mathbf{n}_{O_2} \) and \( \mathbf{n}_{H_2O} \) represent the mass flux of \( O_2 \) and \( H_2O \). \( F \) denotes Faraday’s constant (C/mol), \( t_{H2O} \) is the water transport number or drag number (the number of water molecules dragged across the PEMFC membrane for each electron transferred), and \( i_c \) is the current density (A/m\(^2\)) given by the expression

\[ i_c = (-S_a \delta i_0) \frac{\omega_{O2}}{\omega_{O2,0}} \exp \left( \frac{F \eta}{2RT} \right) \]

Here \( S_a \) denotes the specific surface area (m\(^2\)/m\(^3\)), \( \delta \) is the thickness of the active layer (m), \( R \) represents the gas constant (J/(mol·K)), \( T \) equals the temperature (K), \( i_0 \) gives the exchange current density (A/m\(^2\)), and \( \eta \) is the overpotential (V). The mass fraction of oxygen, \( \omega_{O2} \), normalized with a reference fraction, is also included.

The mass and heat flux in the model is based on the Maxwell-Stefan diffusion and convection equations. This equation is applied on both flow channels and active layer (porous backing):

\[ \mathbf{v} \cdot \left[ -\rho \omega_{\mathbf{j}} \sum_{j=1}^{N} \frac{M_j}{M} \left( \nabla \omega_j + \frac{\omega_j M_j}{M} \right) + \rho \omega_{\mathbf{j}} \mathbf{u} \right] = 0 \]

Here \( \rho \) denotes the density of the mixture (kg/m\(^3\)), \( M \) equals the total molar mass of the mixture (kg), \( M_j \) represents the molar mass of species \( j \) (kg), \( \omega_j \) gives the mass fraction of species \( j \), and \( \mathbf{u} \) is the velocity (m/s). The multicomponent Fick diffusivities, \( D_{ij} \), is calculated as follows:

\[ D_{ui} = \frac{(\omega_2 + \omega_3)^2}{x_1 D_{13} + x_2 D_{12} + \frac{x_1 x_2}{D_{12} D_{13}}} \quad D_{12} = \frac{\omega_1 (\omega_2 + \omega_3) + \omega_2 (\omega_1 + \omega_3)}{x_1 D_{13} + x_2 D_{12} + \frac{x_1 x_2}{D_{12} D_{13}}} \]

Where \( x_j \) denotes the molar fraction of species \( j \) and \( D_{ij} \) are the Maxwell-Stefan diffusivities (m\(^2\)/s). The Maxwell-Stefan diffusivities can be described with the equation:

\[ D_{ij} = k \frac{\eta^{1.75}}{\rho [v_i^{1/3} + v_j^{1/3}]^2 \left[ \frac{1}{M_i} + \frac{1}{M_j} \right]^{1/2}} \]

Here \( k \) is a constant equal to 3.16·10\(^{-8}\) Pa·m\(^2\)/s, \( T \) represents the temperature expressed in kelvin, \( \rho \) equals pressure (Pa), \( v_i \) is the molar diffusion volume of species \( i \) expressed in m\(^3\)/mol, and \( M_i \) is the molar mass of species \( i \) expressed in kg/mol.

2.3.5 Symmetry boundary
Because of the symmetry of flow channels (Figure 4), computational domain can be reduced to a unit cell, which is the smallest characteristic domain.

For the channels:
\[
\mathbf{n} \cdot \mathbf{v} = 0; \quad \mathbf{t} \cdot \left[-p \mathbf{I} + \eta (\nabla \mathbf{v} + (\nabla \mathbf{v})^T)\right] \mathbf{n} = 0;
\]
\[
\mathbf{n} \cdot \nabla \mathbf{w}_{O_2} = \mathbf{n} \cdot \nabla \mathbf{w}_{H_2} = 0
\]

For the porous backing:
\[
\mathbf{n} \cdot \mathbf{v}_{\text{avg}} = 0; \quad \mathbf{t} \cdot \left[-p \mathbf{I} + \eta \left(\nabla \mathbf{v}_{\text{avg}} + (\nabla \mathbf{v}_{\text{avg}})^T\right)\right] \mathbf{n} = 0
\]
\[
\mathbf{n} \cdot \nabla \mathbf{w}_{O_2}^{\text{int}} = \mathbf{n} \cdot \nabla \mathbf{w}_{H_2}^{\text{int}} = 0
\]

Where \( \mathbf{v}_{\text{avg}} \) is the superficial average and \( \mathbf{t} \) is the unit tangent the boundary. \( \mathbf{w}_{O_2}^{\text{int}} \) and \( \mathbf{w}_{H_2}^{\text{int}} \) are the intrinsic average.

2.3.5 Walls
Walls are assumed to be no slip.

For the channels:
\[
\mathbf{v} = 0; \quad \mathbf{n} \cdot \nabla \mathbf{w}_{O_2} = \mathbf{n} \cdot \nabla \mathbf{w}_{H_2} = 0
\]

For the porous backing:
\[
\mathbf{n} \cdot \mathbf{v}_{\text{avg}} = 0; \quad \mathbf{t} \cdot \left[-p \mathbf{I} + \eta \left(\nabla \mathbf{v}_{\text{avg}} + (\nabla \mathbf{v}_{\text{avg}})^T\right)\right] \mathbf{n} = 0
\]
\[
\mathbf{n} \cdot \nabla \mathbf{w}_{O_2}^{\text{int}} = \mathbf{n} \cdot \nabla \mathbf{w}_{H_2}^{\text{int}} = 0
\]

3 Numerics

3.1 Dimension of models:

The unit cell that has been studied consists of two of half parallel channels and the corresponding porous backing under the channels (Figure 4). Since the channel is symmetric, only half of the channel is involved in computation by using symmetry boundary.
3.2 Mesh

Mesh type has been selected to be quad, whose mesh unit is rectangle. The mesh points on the width, length and height of a channel is 1, 30, 2 respectively (Figure 4). This mesh selection gives totally 186 mesh units for one channel. Each mesh unit has volume of approximately $2.258 \times 10^4 \text{ cm}^3$. Mesh of porous backing is classified into two types: porous backing in contact with channels and not in contact with channels (Figure 4). The part in contact with channels has the same mesh as the channels; however, the mesh unit volume is $4.516 \times 10^5 \text{ cm}^3$. The other part has 4, 30, 2 points on the width, length and height respectively. 465 mesh units are obtained through this mesh, and the volume of each mesh unit is about $7.226 \times 10^5 \text{ cm}^3$. The computational process has two steps: 1. Fluid dynamics and 2. Diffusion and convection (involving electrokinetics). The number of degree of freedom of step one is 13554, and for step two, the number of degree of freedom is 23546. The computation runs in a note-book computer with a 2GHz Core Two CPU and 1 GB RAM. The whole process takes about 80 seconds for low current density and roughly 130 seconds for high current density.

4 Results and discussion

The simulation has been carried out for different values of some parameters. The following table (Table 3) shows the range of values of these parameters.

<table>
<thead>
<tr>
<th>$\eta$ (V)</th>
<th>$v_{O_2}$ (m/s)</th>
<th>$v_{H_2O}$ (m/s)</th>
<th>$v_{N_2}$ (m/s)</th>
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</thead>
<tbody>
<tr>
<td>7.66E-4</td>
<td>7.27E-4</td>
<td>7.79E-4</td>
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<td>7.27E-9</td>
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</tr>
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<td>4.66E-9</td>
<td>4.27E-9</td>
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<td>1.66E-9</td>
<td>1.27E-9</td>
<td>1.79E-9</td>
<td></td>
</tr>
</tbody>
</table>

In the following context, average current density and standard deviation over the active layer are expressed as $i_{cavg}$ and $i_{cstd}$ respectively. $i_{cavg}$ and $i_{cstd}$ are defined as follows:

$$i_{cavg} = \frac{1}{A} \int_A i_c \, dA$$

$$i_{cstd} = \sqrt{\frac{1}{A} \int_A \left( i_c^2 - i_{cavg}^2 \right) \, dA}$$

Where $A$ is the area of the active layer at the bottom of porous backing. These two quantities are the criteria to judge the performance of fuel cell. High current density is not enough to
predict good performance of a fuel cell. Uniformity is desired as well since catalyst utilization and degradation relates to the distribution of current at the active layer. The uniform distribution of current at the active layer can also lead to better performance of a fuel cell.

4.1 Effect of $\eta$ on $i_{\text{avg}}$ and $i_{\text{std}}$.

Inlet velocities of oxygen, water vapor and nitrogen is fixed in this process as well as pressure difference.

<table>
<thead>
<tr>
<th>$v_{\text{O}_2}$ (m/s)</th>
<th>$v_{\text{H}_2\text{O}}$ (m/s)</th>
<th>$v_{\text{N}_2}$ (m/s)</th>
<th>$dP$ (pa)</th>
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</thead>
<tbody>
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<td>1.27E-9</td>
<td>1.79E-9</td>
<td>25.325</td>
</tr>
</tbody>
</table>

Plots of $i_{\text{avg}}$ and $i_{\text{std}}$ against $\eta$ are generated under different values of $\eta$ from 0.2 to 0.35. Computation runs in the case of coflow channel.

From figure 5, an exponential increase of $i_{\text{avg}}$ takes place when the value of $\eta$ gains; however, $i_{\text{std}}$ undergoes an exponential increase as well. Therefore, increase of overpotential can give a higher current density but with rather non-uniform distribution at the active layer.

4.2 Effect of inlet velocity of gases on $i_{\text{avg}}$ and $i_{\text{std}}$.

By fixing other parameters, $\eta$ and $dP$, this time inlet velocity of oxygen, water vapor and nitrogen has been varied (Table 3) to see the effect on $i_{\text{avg}}$ and $i_{\text{std}}$.

<table>
<thead>
<tr>
<th>$\eta$ (V)</th>
<th>$dP$ (pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>25.325</td>
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</tbody>
</table>
The computation is carried out with four different sets of values of inlet velocities (Table 3). Again, this process runs in coflow channel as well.

The figure 6 shows that current density decreases and standard deviation gains as inlet velocity increases. However, higher inlet velocities of gases into the channels can facilitate the reaction in the cathode since increase of concentration of reactants can push the chemical equilibrium to the direction of products. Therefore, an optimal value of the inlet velocity is desired to achieve the best performance of fuel cell. Nevertheless, from figure 6, little change of \( i_{\text{avg}} \) and \( i_{\text{std}} \) occurs in the low-velocity region. Table 4 gives the specific values at low-velocity region. Hence, the optimal inlet velocity is at power -6.

### Table 4 Values of \( i_{\text{avg}} \) and \( i_{\text{std}} \) at low-velocity region.

<table>
<thead>
<tr>
<th>( \nu_{O2} ) (m/s)</th>
<th>( \nu_{H2O} ) (m/s)</th>
<th>( \nu_{N2} ) (m/s)</th>
<th>( i_{\text{avg}} ) (A cm(^{-2}))</th>
<th>( i_{\text{std}} ) (A cm(^{-2}))</th>
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<td>11.82</td>
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</table>

\( \nu_{O2} \quad \nu_{H2O} \quad \nu_{N2} \)

**Figure 6.** (a) Negative logarithms of inlet velocities of oxygen, water vapor and nitrogen versus \( i_{\text{avg}} \); (b) Negative logarithms of inlet velocities of oxygen, water vapor and nitrogen versus \( i_{\text{std}} \)

### 4.3 Comparison of coflow channel and counterflow channel

The main difference between these two types of channels is the direction of flow, which gives very different distribution of current at the active layer. Figure 7 shows the distribution of current at the active layer for coflow and counterflow channels at different values of \( \eta \) from 0.2 to 0.35.
In order to compare the current density and standard deviation at the active layer, a combined plot of $i_{c_{avg}}$ and $i_{c_{std}}$ of the two types of channels with respect to eta is shown as follows (Figure 8):
The coflow channel can be capable of generating slightly larger current density than counterflow channel, and has better current distribution (smaller deviation). Nevertheless, Vynnychy and E. Birgersson [8] in their paper predicted a just opposite conclusion. They got higher local current density in counterflow channels, and pointed out that the reason why counterflow behaves better is the alternating inlets and outlets providing for an increasing mass transfer in the spanwise direction. They gave a clear proof to show this prediction is reasonable. According to this contradiction, further study is required as there might be some conditions that the coflow channels can have a better performance.

4.4 Effect of changes of width of channels on $i_{c_{avg}}$ and $i_{c_{std}}$.

Effects of different widths of channels are highlighted here. Table 5 shows four different widths that have been studied. Again coflow channel model is used. Graph of current distribution at $eta = 0.2$ and plots of $i_{c_{avg}}$ and $i_{c_{std}}$ of different widths of channels are shown in following figure (Figure 9).

**Figure 8.** (a) $i_{c_{avg}}$ versus $i_{c_{avg}}$ of coflow and counterflow channels; (b) $i_{c_{avg}}$ versus $eta$ of coflow and counterflow channels; (c) $i_{c_{avg}}$ versus $eta$ of coflow and counterflow channels;
Table 5: Widths and fixed parameters

<table>
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<th>Width 1</th>
<th>Width 2</th>
<th>Original Width</th>
<th>Width 3</th>
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</table>

<table>
<thead>
<tr>
<th>$v_{O2}$ (m/s)</th>
<th>$v_{H2O}$ (m/s)</th>
<th>$v_{N2}$ (m/s)</th>
<th>$dp$ (pa)</th>
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<tbody>
<tr>
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<td>1.27E-9</td>
<td>1.79E-9</td>
<td>25.325</td>
</tr>
</tbody>
</table>

(a) (b) (c) (d)

(e) (f)

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- $v_{O2}$: Velocity of Oxygen
- $v_{H2O}$: Velocity of Water Vapour
- $v_{N2}$: Velocity of Nitrogen
- $dp$: Pressure Drop
The results are quite clear that the wider the channels the better fuel cell performs. This conclusion leaves a very good point to think about. If the channel is wide enough that the channel manages to cover the whole porous backing. This point leads to another type channel which is foam. Vynnychy and E. Birgersson [8] give the description and prediction of foam in their paper. Their research results show that the foam behaves much better than coflow and counter flow channels. Foam can sustain much larger current density and has very small standard deviation compared to conventional parallel channels.

5 Conclusion

Based on a three-dimensional gas-phase model, two types of flow-distributors, namely coflow and counterflow channels, has been studied. Effects of different widths of channels have been considered. The local current density and standard deviation at the active layer has been computed and treated as the criteria to predict the performance of fuel cell during the simulation. Several parameters, such as overpotential, inlet velocities of oxygen, water vapor and nitrogen, have been discussed.

The results show coflow channels sustain higher local current density with comparably smaller standard deviation, and large width of channels is preferred as it gives higher local current density and better current distribution.

The simulation is constrained in one-phase flow. In real case, liquids and gases are mixed in the cathode of fuel cell. Hence, one-phase is not enough. Furthermore, the model is set at the isothermal environment, which is not practical as well. The further study is required to incorporate two phases of flow and other thermal effects.

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7 References


