Numerical Study on Modified Serpentine Flow Fields Effect on Characteristics of PEMFC Water and Gas Transportation

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Abstract. The mass transport properties of fuel cells mainly determined by the flow field structure. Therefore, it is an effective method to improve the running condition and performance of the cell by improving the flow field structure. In this paper, a modified serpentine channel with gradient channel depth and trapezoidal section shape is proposed. The new flow field and the traditional serpentine flow field are solved numerically, the numerical results reveals that compared with the other one the new flow field have a more uniform concentration of reactants, and the water generation in the reflection area is lower due to the high channel pressure. Through the optimizing the flow field the fuel cell have a 23% performance improvement.

Keywords: PEM fuel cell; flow field; transport phenomena; numerical simulation.

1. Introduction
Proton exchange membrane fuel cell (PEMFC) is one of the emerging energy conversion systems which converts the chemical energy stored in fuel and oxidizer into electric energy directly without combustion. PEMFC utilizes polymer electrolyte membranes (PEMs) such as Nafion for proton ion exchange, then converting the Gibbs free energy part of the chemical energy of the fuel into electrical energy by electrochemical reaction.

In the PEM fuel cell system, bipolar plate is one of the prime component. It provides a flow channel for fuel and oxidant distribution to the electrode. In addition, bipolar plate is responsible to carry the electron towards the electric circuit and carry out the exhaust heat and water from the cell. Reasonable flow field structure and parameters can ensure that sufficient reactants are obtained everywhere in the electrode and the product is discharged in time to improve the performance of the battery. A.Kmuar et al. simulated the parallel and serpentine, single-path and multi-path, and the finger flow channels PEMFC models in the form of physical parameters and boundary conditions in the same circumstances [1]. In terms of comprehensive steady-state and dynamic characteristics, the multi-serpentine flow field fuel cell has the best performance. Yan et al. proposed a convergent flow field [2]. It was found that the flow area was reduced due to the flow direction along the flow path, and the flow rate in the channel was increased, which enhanced the mass transfer and drainage performance in the battery, and improved battery performance. Chowdhury M Z et al. numerically solved the different configurations of the improved convergent and divergent serpentine flow fields. Convergent flow field design improves mass transport and effectively removes water[3]. This paper presents a new type of flow channel with gradient channel depth and trapezoidal section shape. The numerical results shows that Compared with the
traditional serpentine flow field, the modified flow field have a more uniform concentration of reactants, and the water concentration in the reaction zone is lower due to the high channel pressure.

2. Model Description
The generalized computational three-dimensional geometrical modeling domain of the modified serpentine flow field (GT) cases is shown in Figure 1 (a), while geometric cross-section shape for inlet and outlet illustrated in Figure 1 (c). The channel depth decreases proportionally along the flow direction in the GT flow field, while in TS the depth stays was consistently. Fig 1(b) shows the structure of a PEMFC with traditional serpentine flow field(TS). Figure (d) shows a constant channel cross section.

![Flow Fields](image)

Figure 1. Schematic of flow fields with GT and TS flow field.

| Parameter                  | Value         |
|----------------------------|---------------|
| Thickness of GDL           | 0.2[mm]       |
| Thickness of CL            | 0.025[mm]     |
| Thickness of membrane      | 0.05[mm]      |
| Inlet Channel Top Width    | 0.5[mm]       |
| Inlet Channel Depth        | 1[mm]         |
| Inlet Channel Bottom Width | 1[mm]         |
| Outlet Channel Bottom Width| 1[mm]         |
| Outlet Channel Top Width   | 0.375[mm]     |
| Outlet Channel Depth       | 0.25[mm]      |
| Channel Width              | 1[mm]         |
| Channel Depth              | 1[mm]         |

3. Electrochemical Equation and Calculation Model
In the electrochemical kinetics of PEMFC, the electrochemical equations are mainly Bulter-Volmer equations and Tafel equations, etc.
The equation in the anode catalytic layer is Bulter-Volmer:
\[ j = j_0^0 \left( \frac{c^* R}{c^* P} e^{anF \eta / (RT)} - \frac{c^* P}{c^* R} e^{-(1-\alpha)nF \eta / (RT)} \right) \]

(1)

Where \( \eta \) is the loss of voltage, \( n \) denotes number of electrons transferred in an electrochemical reaction, \( c^* R \) and \( c^* P \) is the actual indicated concentration of a finite rate material in the reaction; \( j_0^0 \) shows the measured value at the reference point, where the reactants and product concentrations are \( c^* R \) and \( c^* P \).

For large activation overpotentials (greater than 50~100 mV at room temperature), ignoring the second exponential term in the Butler-Volmer equation, it can be simplified to:

\[ \eta_{act} = \frac{RT}{anF} \ln j_0 + \frac{RT}{anF} \ln j \]

(2)

\( \eta_{act} \) of \( \ln j \) curve should be a straight line, By fitting \( \ln j \) or \( \ln \eta_{act} \), \( j_0 \) and \( \alpha \) can be obtained. If the equation is generalized as follows[4]:

\[ \eta_{act} = a + b \ln j \]

(3)

The above equation is Tafel equation, \( b \) is called Tafel slope.

The assumptions of the established mathematical model in this paper can be referred to[5,6].

| Parameter                              | Value          |
|----------------------------------------|----------------|
| Open-circuit voltage                   | 0.95[V]        |
| Anode exchange current density         | 2e+09[A m^-3]  |
| Anode concentration exponent          | 0.5            |
| Anode reference concentration          | 0.0564[A m^-3] |
| Cathode exchange current density       | 10000[A m^-3]  |
| Cathode concentration exponent        | 1              |
| Cathode reference concentration       | 0.00339[A m^-3]|
| Hydrogen reference diffusivity         | 1.1e-04[m^2s^-1]|
| Oxygen reference diffusivity           | 3.2e-05[m^2s^-1]|
| Water reference diffusivity            | 7.35e-05[m^2s^-1]|
| GDL porosity                           | 0.5            |
| Catalyst layer porosity                | 0.5            |
| Stoichiometry of H2 and air            | 1.5/2          |

4. Results and Discussion

The internal phenomena of Oxygen concentration distribution and water mass transport are analyzed at catalyst layer and gas diffusion layer. From the analysis results, it can be seen that these internal phenomena are closely related to each other and affect the performance of the cell. Water transport is one of the most complicated problems in cathode flow field of proton exchange membrane fuel cell. Water is produced by electrochemical reactions in the catalyst layer. Another source of water is due to the humidification of the air to facilitate transport of proton membrane hydrate to improve performance. However, excessive water can cause the cathode to flooding and reduce the transport of the active material, leading to performance degradation. As the concentration of reactants in the reaction zone decreases, it is the result of the continuous diffusion process, and the pressure loss increases with the accumulation of water. According to the Figure 3(c), the water concentration along the channel increases slowly from the inlet to the outlet, mainly on the surface of the catalyst layer, especially at the outlet channel. Due to the gradual decrease of channel height, GT channel has a higher pressure than ST channel shows in Figure 3(d). It can effectively remove the excess water on the catalyst layer. The oxygen mass fraction at the interface between the catalyst layer and the gas diffusion layer for GT was
shown in the Figure3 (a). The reactants not only flow through the channel, but are forced to flow through the diffusion layer under the rib plane between the two adjacent channels. Due to the high pressure in the small area of channel bending, oxygen is highly concentrated in the channel bending area. This is due to the turbulence characteristics of the flow at the bend of the channel leading to a higher pressure drop, which leads to an increase in the oxygen mass fraction. According to the figure 3 (d), a maximum reduction of 27% in the oxygen mass fraction of an outlet area compared to that of an inlet area. Figure 2 shows that compared with TS, GT has a better cell performance, it benefit from an average 2.7% better oxygen concentration, 6.8% reduction water concentration at the catalyst layer.

Figure 2. Cell performance with GT and TS flow fields.

Figure 3. The concentration distribution of oxygen and water in GT(a)(c) and TS(b)(d);at0.6V.

5. Conclusions
The internal transport of proton exchange membrane fuel cell was explained by analyzing the electrochemical, mass transport and properties of the flow field in the flow channel, catalyst layer and
cathode. Through numerical study, the transport characteristics of modified serpentine flow field (GT) and traditional serpentine flow field (TS) fuel cell are explored substantially. The modified serpentine flow field has good expression in performance, oxygen transport and water concentration distribution benefit from the rectangular cross section and the decreasing channel height. On the other hand, non-uniform reaction gas distribution and excessive water concentration are being predicted in the traditional serpentine flow field. The traditional flow field has uneven oxygen mass distribution along the direction of the flow field, and water flooding occurs in the outlet channel and its adjacent reaction zone. All of these, cause to an adverse effect on the cell performance are resulted from the lack of an effective structure to facilitate water removal. The modified serpentine flow field have a 23% performance improvement, average 2.7% better oxygen concentration and 6.8% reduction water concentration at the catalyst layer.

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