A Simulation Study on the Optimization of Flow Channel Pattern in High Temperature Proton Exchange Membrane Fuel Cell

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Abstract. High temperature proton exchange membrane fuel cell (HT-PEMFC) has been one of the most promising candidates for the power source of vehicles. Correspondingly, as a factor significantly influencing the performance of the HT-PEMFC, the structure of the flow channel has been extensively discussed. In this study, the multi-channel flow patterns of fuel cell was proposed, and the effect of the channel number on the fuel cell performance was investigated by numerical simulations. The results showed that the HT-PEMFC with multi flow channels performed a power density of 0.392 W cm⁻², better than that of single-channel fuel cell. Furthermore, after a comprehensive consideration of performance and production cost, the bipolar plates with three flow channels is recommended. It is noted that the as-designed flow pattern contributes to the improvement of the HT-PEMFC power density.

1. Introduction
Nowadays, the high temperature proton exchange membrane fuel cell (HT-PEMFC) has been one of the most expected power sources [1, 2]. Comparing with the conventional PEMFC which works under room temperature to 100°C, HT-PEMFC has a higher operation temperature from 120 °C to 180 °C. Higher temperature means faster electrochemical reaction and higher poison-tolerant. These advantages allow HT-PEMFC to exhibit high efficiency without high-purity hydrogen [3-5]. The high operation temperature also helps to simplify the water management system and air intake system. However, HT-PEMFC is severely hindered by the short service life, the non-uniform distribution of reactants, the abuse of membrane electrode, the improper design of bipolar plates and so on. All these hurdles should be leaped before the commercialization of this kind of fuel cell. For instance, the optimization of the flow channel pattern in bipolar plates has been approved to be an effective method. [6-8]. Taccani et al. [3] explored the effect of the flow field geometry on the overall performance of the PBI-based high temperature PEMFC. In his study, two serpentine flow fields and parallel channels flow field were investigated, and the former has better cell performance but higher pressure drop. Liu et al. [9] designed and fabricated various flow patterns on graphite plates, and proposed a novel symmetric serpentine flow field to meet the requirement of the relatively large size fuel cell application. And the results showed that the serpentine flow channel was still favourable and the as-designed symmetric serpentine flow channel was satisfied.

Despite of the breakthrough outcomes and achievements, it is unrealistic and costly to go deep to detail and mechanism in a flow field only by experimental methods. Therefore, numerical simulation were introduced into this field. Mostafa et al. [10] designed bipolar plates with a bio-inspired flow...
pattern, and optimized their lung-shaped flow channel by means of numerical simulation, in order to obtain the appropriate design to enhance the power and energy density. Arbabi and Roshandel[11] conducted a series of simulations focusing on optimizing the dimensions and configuration of a leaf venation patterns. It was found that the leaf-like flow pattern achieved less pressure drop, more uniform pressure and velocity distributions.

Herein, the authors investigated the flow channel patterns with different channel numbers from 1 to 4, in order to reveal the effect of the channel number on the performance of HT-PEMFC, as well as on the pressure drop and on the concentration distribution of the gas. Results of this study would serve as a guide for flow channel pattern design.

2. Simulation

Fig. 1 schematically illustrates the representative PEMFC module with a single flow channel. As shown in Fig. 1, the cell has two bipolar plates, gas diffusion layers (GDL), catalyst layer and membrane. A three-dimensional, single phase is numerically simulated. The dimensional parameters are listed in Table 1. The governing equations were established and were coupled to solve the multi-physical problems.

![Figure 1. The schematic illustration of the model.](image)

2.1. Continuity equation

As for the convection and diffusion of the fluids in flow channels and GDL, they can be described by continuity equation shown as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

where $\rho$ and $\mathbf{v}$ are density and velocity vector of the fluids, respectively. The first term on the left side of the equation described the mass accumulating as a function of time. The second term expresses the variation of mass flow. Momentum equation

The momentum conservation in the solving domain can be described by the following equation:

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{v}) + S_m$$

where $p$ and $\mu$ represent pressure and viscosity in the solving domains. $S_m$ is the source term resulted from momentum and differs in various domains.

In the flow channel and GDL, $S_m$ is equal to 0. In the porous electrodes, the source term can be given by the pressure drop described by Darcy Law:

$$S_m = -\frac{\mu}{K} \mathbf{v}$$

where $\varepsilon$ and $K$ are the porosity and permeability of the porous electrodes, respectively.
Table 1. The important dimensional parameters of the model

| Dimension                              | Value | Unit |
|----------------------------------------|-------|------|
| Channel length                         | 20    | mm   |
| Total channel width                    | 1     | mm   |
| Channel height                         | 1     | mm   |
| Rib width                              | 0.8   | mm   |
| Total (Total channel width + Rib width)| 1.8   | mm   |
| Gas diffusion layer thickness          | 0.35  | mm   |
| Porous electrode thickness             | 0.05  | mm   |
| Membrane thickness                     | 0.1   | mm   |
| Total height                           | 3     | mm   |

2.2. Specimens equation

The specimen conservation can be described as follows:

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\varepsilon \mathbf{p} x_i) = \nabla \cdot \left( \rho D_i^{\text{eff}} \nabla x_i \right) + S_{i,i}$$ (4)

where $x_i$, $D_i^{\text{eff}}$ and $S_{i,i}$ are on behalf of mass fraction, effective diffusion coefficient and specimen source term of various substances. In the porous medium, the effective diffusion coefficient can be derived from the following equation:

$$D_i^{\text{eff}} = D_i \varepsilon$$ (5)

Especially in high working temperature, the Eq. 5 can be simplified as:

$$D_i^{\text{eff}} = D_i \frac{\varepsilon}{\tau}$$ (6)

In particular, the specimen of the gas can be described by Stefan-Maxwell equation:

$$\nabla y_i = RT \sum_i y_i N_j - y_j N_i \frac{\varepsilon^{1/5}}{p D_i^{\text{eff}}}$$ (7)

where $y_i$ and $N_i$ are the mole fraction and the flux of the gas. When $D_i^{\text{eff}}$ is used to describe binary specimen of the gas, it can be expressed as:

$$D_i^{\text{eff}} = \frac{a}{p} \left(T_j \right)^b \left(p,p_j\right)^{1/3} \left(\sqrt{T_i T_j} \right)^{5/12} \left(M_j \right)^{0.5} \varepsilon^{1.5}$$ (8)

where $T_i$ and $p_i$ represent the temperature and pressure of the gas specimen. $T_j = \sqrt{T_i T_j}$. $M$ is the mole fraction of the gas. $M_j = \frac{1}{M_i} + \frac{1}{M_j}$. For Hydrogen, oxygen and nitrogen, a and b are usually considered as 0.0002745 and 1.832. As for vapor, a is equal to 0.000364 and b is equal to 2.334 [12].

2.3. Charge conservation and electrode reaction kinetics

The charge conservation in solid phase of the cell follows the equation:

$$\nabla \cdot (\sigma_i \nabla \varphi_i) = S_i$$ (9)

where $\sigma_i, i = 1,2$ is on behalf of the conductivity of the liquid and solid phase. $\sigma_i, i = 1,2 \Phi_{i,i=1,2}$ is the potential in the liquid and solid phase. For source term $S_{i,j=1,2}$ in cathode and anode, they are equal to $j_c$ and $j_a$, which are denoted as the exchange current density of electrodes. Further, $j_c$ and $j_a$ can be obtained from Butler-Volmer equation:
\[ j_a = i_0 \left( e^{\frac{a_0 n F \eta_a}{RT}} - e^{\frac{(1-a_0 n F \eta_a)}{RT}} \right) \]  
\[ j_c = i_0 \left( e^{\frac{a_0 n F \eta_c}{RT}} - e^{\frac{(1-a_0 n F \eta_c)}{RT}} \right) \]

where the \( \eta_a \) is the active potential. \( i_0 \) under different temperature and pressure can be obtained from the corrected equation:

\[ i_0 = i_0^{ref} \left( \frac{p_r^{ref}}{p_r} \right)^{\gamma} \left( \frac{E}{E_{ref}} \right) \]

where \( p_r \) is the partial pressure of the specimen. \( p_r^{ref} \) is the reference pressure. \( \gamma \) is the concentration coefficient, which respectively represents 0.5 and 1 in the anode and cathode. \( E_c \) called the active energy is equal to 66 kJ mol\(^{-1}\). Particularly, the potential can be derived from the \( \eta_{act} \), the over reactive potential:

\[ \eta_{act} = \phi_1 - \phi_2 - E_{eq} \]

where \( E_{eq} \) is the equilibrium potential and can be expressed by the formula:

\[ E_{eq} = -\left( \frac{\nabla H - T \nabla S}{nF} \right) + \frac{RT}{nF} \ln \left( \frac{P_{O_2} P_{H_2}}{P_0^2} \right)^{\frac{1}{12}} \]

Comprehensively considering Eq. 13 and Eq. 14, the \( V_{cell} \) can be given by:

\[ V_{cell} = \phi_{Vc} - \phi_{Vc} \]

where \( V_{cell} \) is the voltage of the fuel cell, indicating the performance of HT-PEMFC.

| Table 2. Some important technical parameters used in modeling |
|---------------------------------|---------|---------|
| Dimension                      | Value   | Unit    |
| Porosity of GDL                | 0.4     | 1       |
| Conductivity of GDL            | 222 [13]| S m\(^{-1}\) |
| Conductivity of membrane       | 9.825 [13]| S m\(^{-1}\) |
| H2-H2O binary diffusion coefficient | 1.8076*10\(^{-4}\) [13]| m\(^2\) s\(^{-1}\) |
| N2-H2O binary diffusion coefficient | 5.0559*10\(^{-4}\) [13]| m\(^2\) s\(^{-1}\) |
| O2-H2O binary diffusion coefficient | 5.5394*10\(^{-5}\) [13]| m\(^2\) s\(^{-1}\) |
| O2-N2 binary diffusion coefficient | 4.7131*10\(^{-5}\) [13]| m\(^2\) s\(^{-1}\) |
| Working temperature            | 453.15  | K       |

2.4. Boundary conditions and hypothesis

Boundary conditions exerts a critical role in the modeling process. In this case, the working temperature of HT-PEMFC is configured as 180 °C (453.15 K) much higher than that of conventional PEMFC which usually ranges from 50 to 100 °C. For the flow channels, the inlet velocities of the anode and cathode are set as 0.2 m s\(^{-1}\) and 0.5 m s\(^{-1}\), respectively. The pressure of outlet is equal to pressure. The potential of anode is considered as 0, while that of cathode is equal to the voltage of the fuel cell. The no slip boundary condition is utilized in the inner wall of the flow filed. The important technical parameters are listed in Table 2.

In the present paper, some hypotheses are made not only to simplify the calculation but also to guarantee the convergence of the numerical simulation:

1. The reactive gas is incompressible and considered as ideal gas.
2. The fluid is considered as laminar flow in the flow fields.
3. The electrochemical reaction only occurs at the catalyst surface.
4. The porous medium is homogeneous and exhibits isotropy for physical parameters.
(5) There is no water of liquid state existing in the physical fields due to the high working temperature.

(6) The contact resistance between each layer is ignored during the modeling process.

3. Results and Discussions

A CFD model is built to explore the effects of flow patterns on the performance of HT-PEMFC. Four types of flow channel were proposed and respectively denoted as FN1, FN2, FN3 and FN4 according to the configuration of channel number. Fig. 2(a) and (b) demonstrated the voltage and power density curves as a function of current density. Observed from the above pictures, on one hand, the profiles of voltage vs. current density showed a negative correlation while the that of power density vs. current density exhibited a positive correlation. On the other hand, when the output voltage of the cell reached 0.4 V, the current and power densities of the FN1 to FN4 were 0.904 V and 0.361 W cm-2, 0.935 V and 0.374 W cm-2, 0.980V and 0.392 W cm-2, 1.006 V and 0.397 W cm-2, respectively. It was noted that the performance of HT-PEMFC had a positive correlation with the number of flow channel. It was also found that compared with FN1 the cell performance of FN3 had nearly 8.3% incensement in terms of the power density, indicating that the cell performance could be apparently influenced by the number of flow channel. Interestingly, it was also obtained that compared with FN1, the cell performance of FN4 only increased about 10.0%, meaning that the cell performance became slightly sensitive to channel number from now on.

![Fig. 2. The plots of (a) voltage and (b) power density vs. current density.](image)

Fig. 3 showed the pressure drop of the reactant gas along length of the flow channel. For FN1 to FN4, the inlet pressures were 1.343, 2.744, 5.424 and 10.669 KPa, then finally decreased to the reference pressure of 0 Pa at the outlet. It was obtained that the pressure decreased as the number of flow channel increased, showing a contrary varying tendency with the cell performance. The above phenomena are largely determined by the width of channel. The more flow channels, the less width of the cross section there is. Since the flow rate in this paper is controlled as a constant, the fluids can reach a higher velocity. According to the Darcy law derived from Eq. 3:

$$\Delta p = -\frac{\mu}{K}v$$

where $\Delta p$ is the pressure drop. The Eq. 16 clearly reveals that the pressure drop increases with the velocity increasing. In this case, the higher velocity of the fluids facilitates the gas exchange between each layer, correspondingly bringing about higher pressure drop in the flow field but better performance in the electrochemical filed. Generally, a larger pressure drop means a higher requirement for the air intake system, to some extent resulting in higher cost for the whole fuel cell. Therefore, the FN4 flow pattern with the largest pressure drop of 10.669 was not considered an appropriate option. It was noted that the pressure drop of HT-PEMFC was much lower than that of conventional PEMFC [6]. The temperature plays a critical role in this regard. Since the working temperature was specified as...
180 ° which exceeds the boiling point a lot, the water was excluded from the flow channel as the form of vapor, leading to a great lower pressure drop and simultaneously simplifying the water management system.

![Figure 3. The curves of pressure varying with the central axis of the flow channel.](image)

To directly exhibit the concentration distribution of the hydrogen along with flow direction, the contour images with isolines were used. Fig. 4 illustrated the isoline distribution of H2 concentration. It was clear that the more flow channels were used, the flatter isolines could be obtained, implying a more uniform distribution of the gas concentration. The number of the flow channel exerts a critical role in this result. For the bipolar plates with a single channel, the maximum velocity is always found in the central axis of the channel due to the properties of the Newtonian fluids. As number of the channel increases, the maximum velocity can now be found in all the central axis of the channels, subsequently balancing the velocity distribution. Once the velocity distributes more evenly, the gas correspondingly achieves a uniform exchanging, leading to a homogeneous concentration of hydrogen.

From the mentioned above, it seemed that the flow pattern with 3 channels was a suitable option for the practical application of HT-PEMFC by considering both the cell performance, the flow characteristics and production cost.

![Figure 4. The concentration distribution represented by contour with isoline.](image)
4. Conclusion
In this study, the authors proposed the multi-channel flow pattern in the high temperature PEMFC, and investigated the effect of the channel number on the fuel cell performance by numerical simulations. Results showed that more flow channels lead to higher power density, which is 0.392 W·cm⁻² for 3-channel and 0.397 W·cm⁻² for 4-channel. Comparing with the original single channel design, they are 8.3% and 10% increasing, respectively. However, when the channel number exceeds three, the power density would grow slowly as the channel number increase. Therefore, considering of the production cost, the 3-channel flow pattern would be the most economical and practical. Furthermore, the simulation study would serve as a guide for flow channel pattern design, and would ultimately be helpful to the commercialization of the HT-PEMFC.

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6. References
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