NUMERICAL STUDIES ON FLOW FIELD SELECTION OF PROTON EXCHANGE MEMBRANE FUEL CELLS

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Abstract

Proton exchange membrane fuel cell (PEMFC), as one of the ideal source, has attracted attention because of its advantages such as high efficiency, high specific energy and low pollution. Bipolar plate, the essential components of PEMFC, accounts for 60% of the weight of the cell. The design of flow field on bipolar plate has great influence on the performance of PEMFC, operation efficiency and manufacturing cost. In this paper, some common flow field such as multi-passes serpentine flow field, swivel flow field and parallel flow field are selected to analysis the changes of performance of PEMFC, trying to find the reasonable flow field of cathode and anode.

Keywords: PEMFC; Flow field; Cathode and anode; Bipolar plate.

1. INTRODUCTION

Flow field, as one of the key components of PEMFC, plays a role in distributing reactant gas and oxidant evenly, realizing the electrical connection between every cells, supporting stack, collecting and derive current, and isolating the reaction gas [1]. However, how to design a reasonable flow field within an effective area and make it have both excellent mechanical properties and gas flow performance is a difficult problem.

Reasonable different shapes of the flow field, including serpentine flow field, swivel flow field and parallel flow field, can impact the performance of PEMFC [2]. Parallel flow field has a larger number of channels and every channel is parallel with each other [3]. This design will bring a smaller gas flow resistance. It can reduce the pressure loss and improve the efficiency of the PEMFC [4-6]. Serpentine flow field, as one of the important flow field, has been widely used in PEMFC because of its excellent water removal performance [7-8]. Swivel flow field, similar to the serpentine flow field, has the perfect water removal performance [9].

The reasonable flow channel design can not only make the gas distribute in the active region fully and uniformly, but also discharge the liquid water produced by the reaction in time. In this paper, the effects on hydrogen concentration distribution, water distribution, polarization curve and power density curve of different flow field are studied.

2. MATERIAL AND METHODS

In this paper, a three-dimensional model of PEMFC under a steady and constant temperature was applied by COMSOL Multiphysics, the multi-physics direct coupling analysis software.

2.1 Model Hypothesis

The following assumptions are used to simplify the PEMFC model:

- (1) This system operates at steady state;
- (2) All gases involved in the reaction is ideal gas;
- (3) The proton exchange membrane cannot allow any gas to pass through;
- (4) No gravity exists;
- (5) A small amount of liquid water in the flow field is a dispersed water droplet.

2.2 Mathematical Model

The Mathematical model is as follows:

2.2.1 Mass conservation equation

$$\frac{\partial (\varepsilon \rho)}{\partial t} * \nabla \cdot (\varepsilon \rho \overline{u}) = S_m \tag{1}$$

Where ρ is density, ε is porosity, \overline{u} is velocity vector,

 S_m is Mass source term, However, S_m has different values in different areas of PEMFC:

$$S_{mGDL} = S_{mCH} = 0 \tag{2}$$

Formula (2) means that the value of S_m is 0 at the diffusion layer and the flow field at the poles.

For the CL at the two poles, there are:

$$S_{ma} = m_{H_2} = -\frac{M_{H_2}}{2F} i_a,$$

$$S_{mc} = m_{H_2O} + m_{O_2} = \frac{M_{H_2O}}{2F} - \frac{M_{O_2}}{4F} i_c$$
(3)

Where M is molar mass, F is Faraday constant(96487C/mol), i is current density; In subscript, a is anode, c is cathode.

2.2.2 Momentum conservation equation

$$\frac{\partial(\varepsilon\rho\overline{u})}{\partial t} + \nabla\cdot(\varepsilon\rho\overline{u}\overline{u}) = -\varepsilon\nabla p + \nabla\cdot(\varepsilon\mu\nabla\overline{u}) + S_u \quad (4)$$

Where p is pressure, μ is kinetic viscosity, S_u is power source term.

However, in the flow field, $\mathcal{E} = 1$. Therefore, on the premise of this steady state model and neglecting convection and diffusion, the equation can be simplified as follows according to Darcy theorem:

$$\varepsilon u = -\frac{k_p}{\mu} \nabla p \tag{5}$$

2.2.3 Energy conservation equation

$$S_O = (i^s)^2 R_{ohm} + \beta S_{H,O} h_{reaction} + r_w h_{lg} + S_{a,c} \eta$$
 (6)

Where S_Q is energy source term, i^s is surface current density, R_{ohm} is resistivity, β is energy conversion ratio (chemical energy \rightarrow heat energy), S_{H_2O} is formation rate of gaseous water, $h_{reaction}$ is reaction enthalpy, r_w is phase transition rate of water, h_{lg} is phase transition enthalpy of water, $S_{a,c}$ is exchange current density of cathode / anode, η is overpotential.

2.2.4 Component conservation equation

$$\frac{\partial(\varepsilon c_k)}{\partial t} + \nabla \cdot (\varepsilon \bar{u} c_k) = \nabla \cdot (D_k^{eff} \nabla c_k) + S_k(7)$$

Where c_k is component concentration, $D_k^{\it eff}$ is effective diffusion coefficient of components, ε is porosity, S_k is component source term, the subscript k is component code, anodic composition include H_2 , H_2O , cathode composition include O_2 , O_2 . It is worth mentioning that the component source term is 0 in the flow field and GDL, and in the CL at the two poles. So, the source term of each component is:

$$S_{H_2} = -\frac{1}{2F} i_a$$

$$S_{O_2} = -\frac{1}{4F} i_c$$

$$S_{H_2O} = \frac{1}{2F} i_c$$
(8)

Where i_a , i_c is the volume current density of anode and cathode, F is Faraday constant(96487C/mol).

2.2.5 Electrochemical equation

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$$S_a = j_{a,ref}^{\nu} \left(\frac{C_{H_2}}{C_{H_{2,ref}}}\right)^{\gamma_a} \left(e^{\frac{\alpha_a F}{RT} \eta_a} - e^{-\frac{\alpha_c F}{RT} \eta_a}\right) \tag{9}$$

$$S_{c} = j_{c,ref}^{v} \left(\frac{C_{O_{2}}}{C_{O_{2,ref}}}\right)^{\gamma_{c}} \left(e^{\frac{\alpha_{c}F}{RT}\eta_{c}} - e^{-\frac{\alpha_{c}F}{RT}\eta_{c}}\right)$$
(10)

Where η is overpotential, j_{ref}^{ν} is reference volume exchange current density, C_i is current molar concentration of component, $C_{i,ref}$ is reference molar concentration of components, γ is concentration index($\gamma_a = 0.5, \gamma_c = 1$), α is transmittance.

2.2.6 Diffusion equation of gas components in porous media

$$D_{i} = \varepsilon^{1.5} (1 - s)^{r_{s}} D_{i}^{0} (\frac{P_{0}}{P})^{\gamma_{p}} (\frac{T}{T_{0}})^{r_{i}} (11)$$

Where \mathcal{E} is porosity, s is saturation of liquid water, D_i^0 is the diffusion coefficient of i at the reference temperature T_0 and reference pressure P_0 , r_s is saturation index, r_p is pressure factor, r_t is temperature exponent. 2.2.7 Transport equation of liquid water

$$\frac{\partial(\varepsilon\rho_l s)}{\partial t} + \nabla \cdot (\rho_l \overline{\nu}_l s) = r_w \tag{12}$$

$$r_w = c_r \max[(1-s)\frac{p_{wv} - p_{sat}}{RT}M_{H_2O} - s\rho_l]$$
 (13)

Where P_{sat} is saturated steam pressure, ρ_l is water density, r_w is water condensation rate.

Table 1 Geometry parameters

T	y parameters
Parameter	Value
GDL length	20mm
GDL width	10mm
GDL thickness	0.38mn
CL thickness	0.05mm
Membrane thickness	0.1mm
GDL porosity	0.4
GDL permeability	1.18e-11[m^2]
GDL electric	222[S/m]
conductivity	
Inlet H ₂ mass fraction	0.743
(anode)	
Inlet H ₂ O mass	0.023
fraction (cathode)	
Inlet oxygen mass	0.228
fraction (cathode)	
Anode inlet flow	0.5[m/s]
velocity	
Cathode inlet flow	0.5[m/s]
velocity	
Anode viscosity	1.19e-5[Pa*s]
Cathode viscosity	2.46e-5[Pa*s]
Hydrogen molar mass	0.002[kg/mol]
Nitrogen molar mass	0.028[kg/mol]
Water molar mass	0.018[kg/mol]
Oxygen molar mass	0.032[kg/mol]
Cell temperature	353.15[K]
Reference pressure	101e3[Pa]
Cell voltage	0.9
Electrolyte phase volume fraction	0.3
Permeability (porous electrode)	kappa_gdl/5
Membrane conductivity	9.825[S/m]

2.3 Main Parameters

The model of PEMFC includes seven parts: anode flow field, anode Gas diffusion layer (GDL), anode Catalyst layer (CL), proton exchange membrane, cathode CL, cathode GDL and cathode flow field. The main parameters are shown in ${\bf Table}\ {\bf 1}.$

3. RESULTS AND DISCUSSION

3.1 Selection of Anode Flow Field

Fig. 1 shows that the concentration difference of hydrogen in the anode. It is obvious that the concentration difference increases gradually with the decrease of the voltage. Specifically, the concentration difference of the multi-passes serpentine flow field, swivel flow field and parallel flow field is abrupt at the voltage of 0.5V, 0.6V and 0.7V. Relatively, the concentration difference of the multi-passes serpentine flow field can maintain a lower level. This shows that the multi-passes serpentine flow field can make the gas distribution more even in the anode GDL. Thus, it can achieve a fuller reaction and more uniform current density.

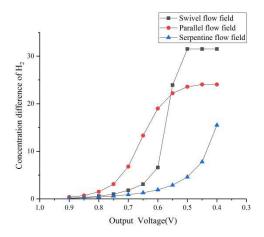


Fig.1 Concentration difference of anode

As is shown in **Fig. 2**, when the voltage is 0.55V, the distribution of hydrogen concentration in the three flow field is appreciable different.

Specifically, there are three obvious fault in the gas

concentration distribution of swivel flow field: inlet-first roundabout, the first roundabout-the second roundabout, the second rotation-outlet. =The concentration gradients are 32-34 mol/m^3 , 29-31 mol/m^3 , 25-28 mol/m^3 , respectively. The decrease of the inlet gas concentration is due to the obvious gas resistance at the roundabout of the swivel flow field. It will lead to the decrease of the inlet pressure at the back end of the flow field. Eventually, the uneven distribution of the gas will be caused.

The gas distribution centralized in the inlet at the anode of the parallel flow field, the gas concentrations of flow field are below 25 except for the inlet. The uneven distribution of the concentration is due to the slow gas flow rate in the parallel flow field.

The hydrogen distribution of mult-passes serpentine flow field is evener. The concentration difference less than $10 \text{ } mol/m^3$ at the 0.55V of voltage and the concentration only drop at the outlet. This is because of

the lack of gas supply in the rear section of the flow field. To sum up, multi-passes Serpentine flow field is the best choice for the anode flow field.

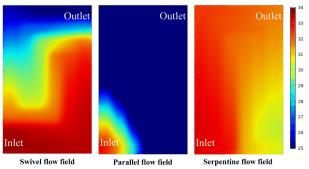
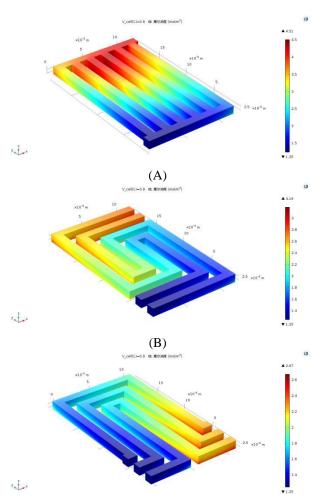


Fig. 2 Hydrogen distribution in different flow field under the voltage of 0.55V

3.2 Selection of Cathode Flow Field

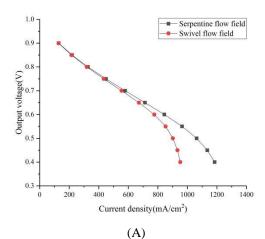
Fig. 3 reveals that the liquid water distribution of cathode. The distribution of the parallel flow field increases obviously in the second half of the flow field. It indicates that the distribution characteristics of the parallel flow field lead to the liquid water produced by the reaction cannot be fully discharged from the flow field. However, multi-passes serpentine flow field and swivel flow field can remove liquid water easily due to enough pressure drop. The contrast in **Fig. 3** is not enough to determine the optimal flow field for the cathode, but the parallel channel is excluded.



(C)

Fig. 3 Liquid water distribution of cathode: (A)parallel flow field; (B)swivel flow field; (C) multi-passes serpentine flow field.

A further comparative study on multi-passes serpentine flow field and swivel flow field is displayed in **Fig. 4**. At the same potential, the current density of multi-passes serpentine flow field is greater than that of swivel flow field and the maximum power density of multi-passes serpentine flow field is higher than that of swivel flow field. This shows that multi-passes serpentine flow field is more suitable for the cathode of PEMFC than swivel flow field.



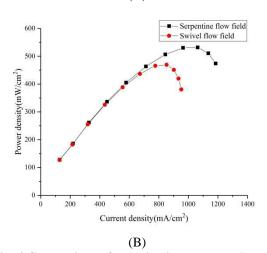


Fig. 4 Comparison of polarization curve and power density curve: (A)Comparison of polarization curve; (B)Comparison of power density curve.

4. CONCLUSION

In this paper, the effects of three different flow field on the hydrogen concentration distribution, water distribution of cathode, polarization curve and power density curve in the same area of GDL were studied. The conclusions are as follows:

(1) In anode, the multi-passes serpentine flow field can make the distribution of hydrogen more uniform and guarantee a small concentration difference even under the condition of lower voltage.

- (2) In cathode, multi-passes serpentine flow field and swivel flow field are easy to remove liquid water and the water removal effectiveness of parallel channel is worse because of the lower pressure drop.
- (3) Compared with swivel flow field, the current density and the power density of the multi-passes serpentine flow field are both dominant under the same condition. It indicates the optimum channel is multi-passes serpentine flow field at cathode.

5. ACKNOWLEDGEMENTS

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