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## 3D Steady Model and Simulation for a Proton Exchange Membrane Fuel Cell Performance

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### Abstract

A three-dimensional, steady-state non-isotherm mathematical model for proton exchange membrane fuel cell is developed. The model takes into accounts simultaneously the mass, momentum, energy, species, charge conservation equation and combines electrochemistry reaction inside the cell. The simulation results show that it is easy to improve the fuel cell performance for higher porosity in the diffusion layer, because of the benefit of speeding the gas diffusion, reducing the concentration grads of gas, depressing the ridge board domino effect and falling current density grads.

**Index Terms:** Proton Exchange Membrane Fuel Cell; Porosity; Water Transport; Model; Simulation

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### 1. Introduction

Proton exchange membrane fuel cells (PEMFCs) are promising green power sources for many applications. Simulation research on PEMFC is important for both internal transport phenomena exploration and structural design optimization [1-2].

Water behavior is one of the key factors influence the fuel cell performance. So research on water management issues is very popular in the recent years. The hot topics of these studies were water transportation inside the proton exchange membrane and in the gas diffusion layer [3-8]. At the same time, a few researchers considered the water transport along the gas flow channels [9].

A three-dimensional, steady-state non-isotherm mathematical model for proton exchange membrane fuel cell is developed in the paper. The model takes into accounts simultaneously the mass, momentum, energy, species, charge conservation equation and combines electrochemical reaction inside the cell.

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## 2. Mathematical Model

The basic suppositions of the model: 1. the operation environment of the cell is steady state and non-isotherm. 2. The diffusion layer and the catalyst layer are pore media. 3 There is only laminar flow in the fuel cell flow field. The model is calculated by the FLUENT 6.3 software [10].

### 2.1. Physical model and governing equations

The physical model of proton exchange membrane fuel cell is developed, which include proton exchange membrane, catalyst layer of anode and cathode, gas diffusion layer of anode and cathode, gas channel of anode and cathode, current collector of anode and cathode. This is typical straight channel flow field and used broadly. The computational domain is shown in Fig.1. Governing equations and boundary conditions are the same as the literature of [3].

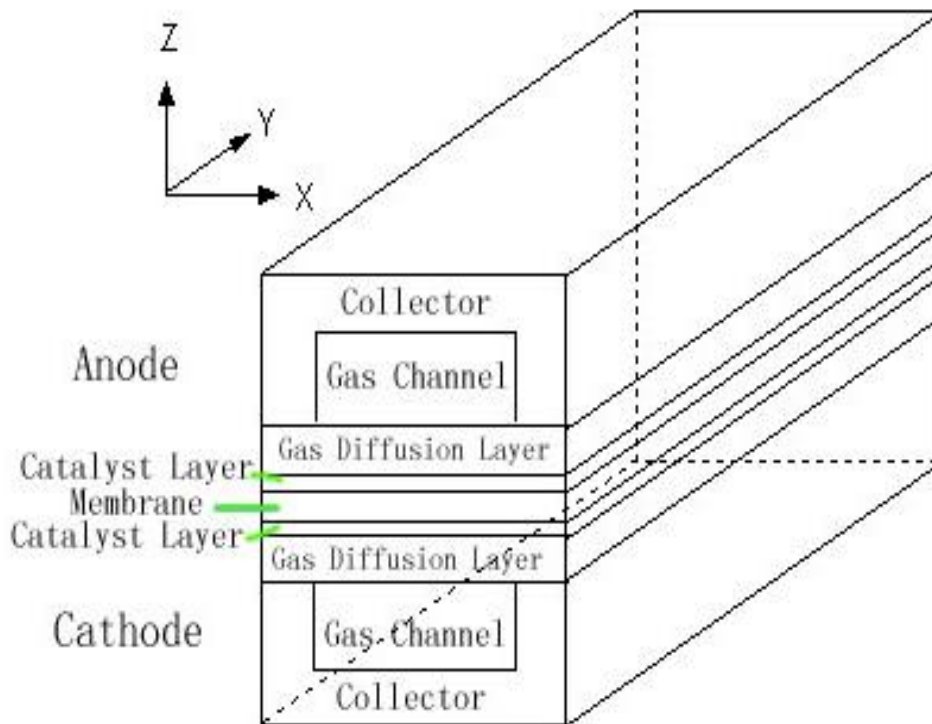


Fig. 1. The physical model of proton exchange membrane fuel cell

### 2.2. Model parameter

The basic parameters referred in the proton exchange membrane fuel cell 3D model are shown in Table 1.

Table 1. Basic parameters of a PEMFC model

Parameters	Value
Membrane thickness	$5 \times 10^{-5}$ m
Catalyst layer thickness	$2.5 \times 10^{-5}$ m
Gas diffusion layer height	$2 \times 10^{-4}$ m
Gas channel height	$8 \times 10^{-4}$ m
Current Collector height	$1.2 \times 10^{-3}$ m
Gas channel length	$5 \times 10^{-2}$ m
Gas channel width	$2 \times 10^{-3}$ m
Current Collector width	$4 \times 10^{-3}$ m
Cell Temperature	343K
Anode inlet flux velocity	$1 \times 10^{-7}$ Kg/s
Mass fraction of H <sub>2</sub>	0.8
Cathode inlet flux velocity	$1 \times 10^{-6}$ Kg/s
Mass fraction of O <sub>2</sub>	0.9

### 3. Results and Discussion

#### 3.1. The performance

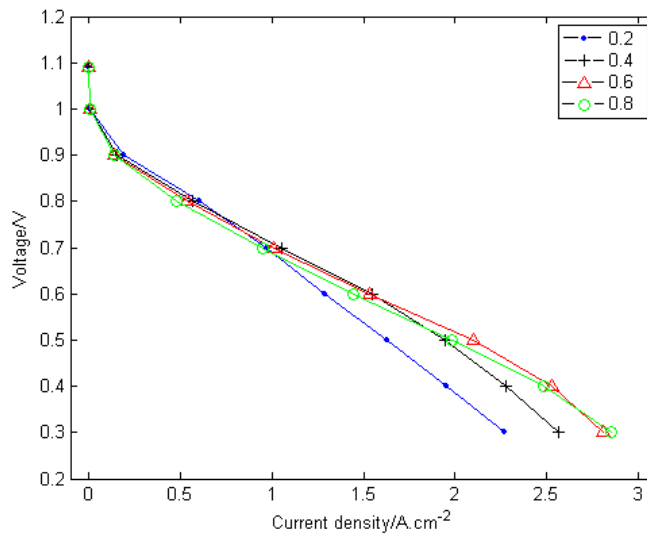


Fig. 2. Polarization curves of proton exchange membrane fuel cell

Fig.2 shows the polarization curves for different porosity at 0.2, 0.4, 0.6 and 0.8. The simulation results displays that the cell's performance at higher porosity is better than at lower porosity when the cell at higher current density. It is opposite when the cell at lower current density. The cell with a porosity of 0.2 has almost

the same current density at the lower current density with the porosity of 0.8 when it is at 0.8V. The fuel cell's polarization curves departs the linearity relation with the voltage attenuates rapidly with the lower porosity when the cell at lower voltage section (e.g. under 0.7V), which put up bigish concentration difference polarization especially when the cell at the porosity of 0.6V. The fuel cell has best performance at the porosity of 0.8 while the worst at 0.2. The reason is that the reactant concentration of the electrode surface begins to change when the fuel is consumed. For example the cell release current at the same time consumes oxygen when oxygen is provided to the cell's cathode, which leads to the oxygen fall across resistance while being transferred. There are two troubles when the mass is been transferred. One is the space resistance, the second is flooding. The space resistance is mainly aroused by the mass transmission and reaction distinction between the flow channel and the ridge part of the flow flied board. The liquid state water bring that the millipore in the diffusion layer occurs to jam which influences the normal gas diffusion. The lower of the porosity, the worse jam will be occurred in the diffusion millipore, and with a more rapid voltage decrease.

### 3.2. The current density distribution

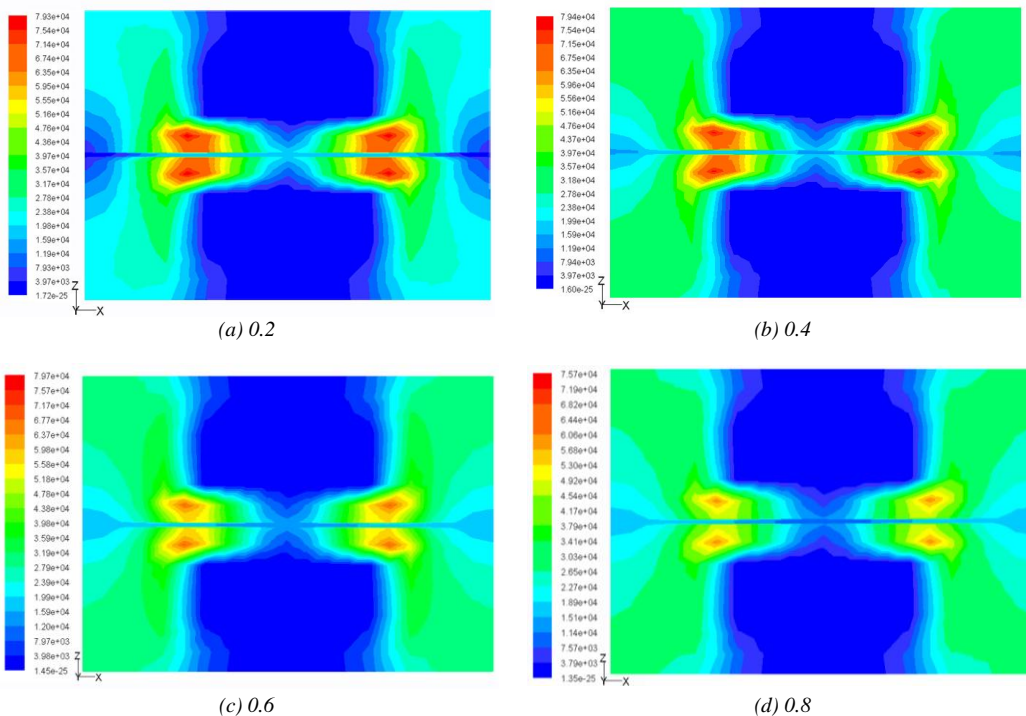


Fig. 3. The current density distributions at  $Y=0m$  slice face with the porosity of 0.2, 0.4, 0.6 and 0.8

The current density distribution at the  $Y=0m$  section of XZ when the cell discharge potential of 0.6V is shown in the Fig.3. The diffusion layer porosity is 0.2, 0.4, 0.6 and 0.8, respectively. The highest current density region is the osculant district of the ridge part of bi-polar board and the diffusion layer, which could be seen the red zone from Fig.3. This is just the area which has the shortest gas transport path and electron transport path. The current density above the flow channel is very small. It is difficult for oxygen to diffuse into the catalyst layer below the ridge portion at lower porosity of 0.2. The current density value reduces along the direction to the center of the ridge portion, the distribution grads of the current density is bigger, falls from the

tiptop of  $7.54 A/cm^2$  to  $0.397 A/cm^2$ . It is contrary when at higher porosity e.g. 0.8. It is easier for oxygen diffusion, the distribution grads is less, falls down from the tiptop of  $6.74 A/cm^2$  to  $1.59 A/cm^2$ .

3.3. Distribution of gas concentration

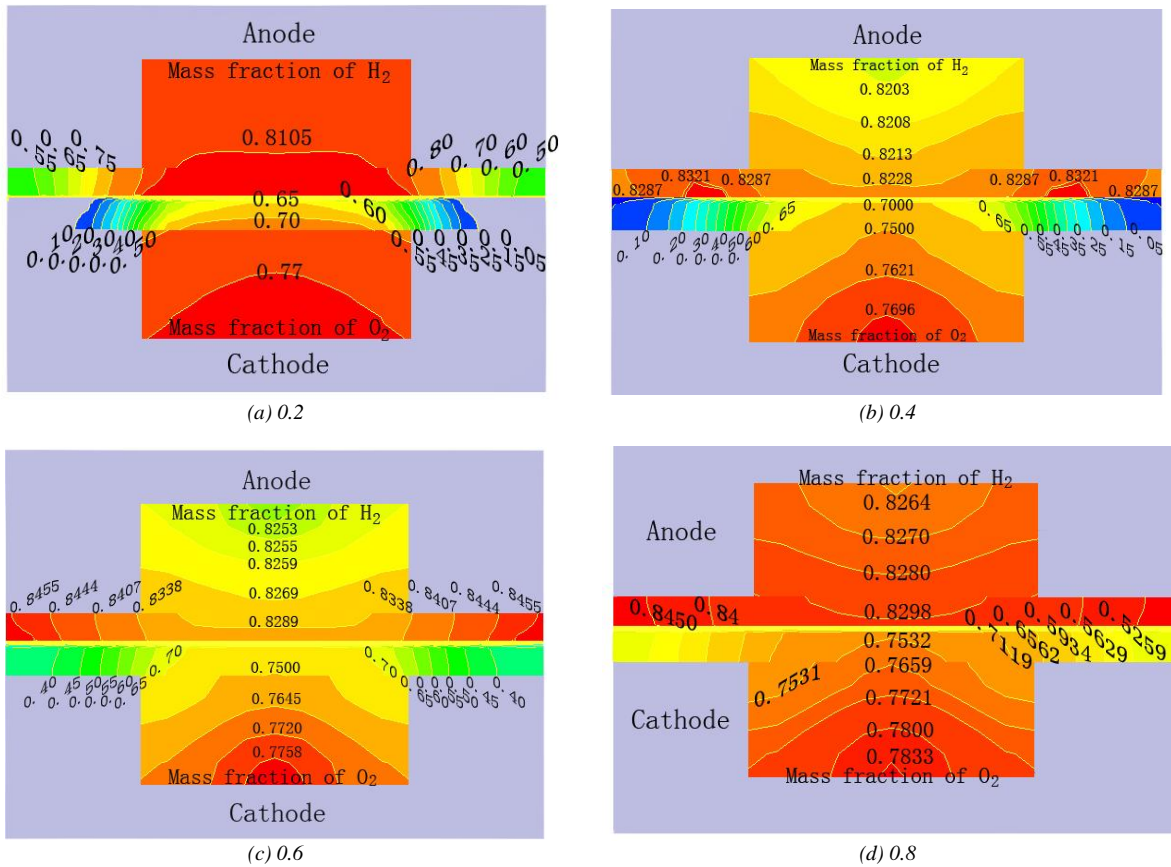
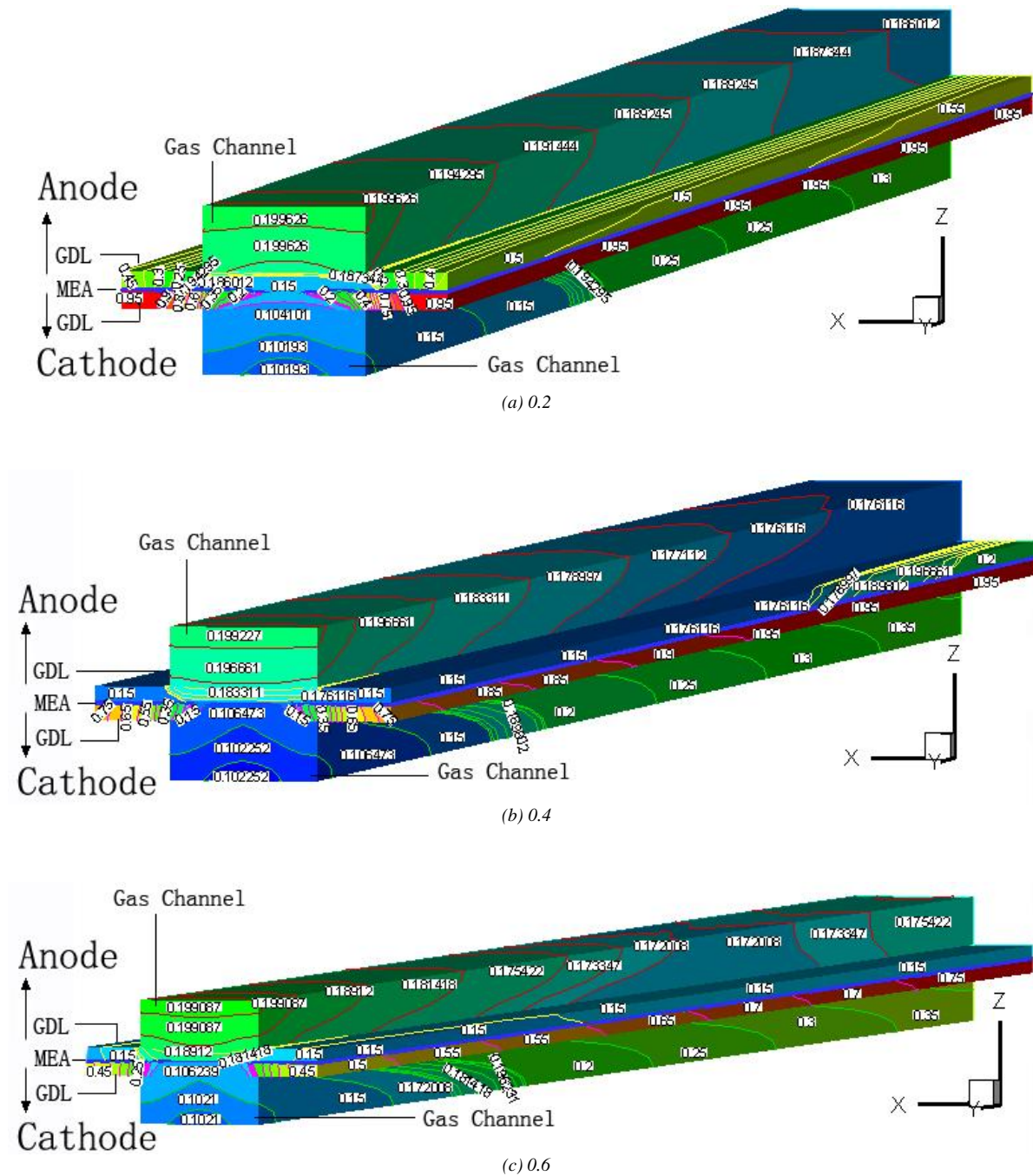


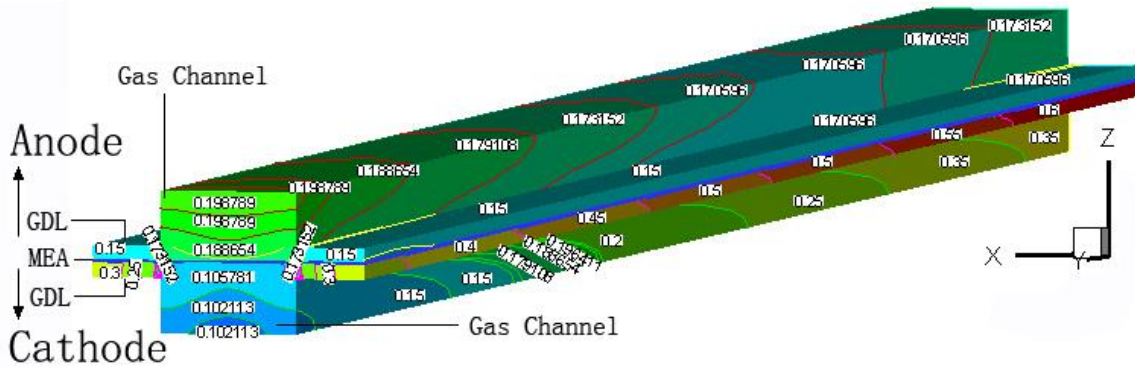
Fig. 4. The gas species distributions at Y=0m slice face with the porosity of 0.2, 0.4, 0.6 and 0.8

Fig.4 displays the hydrogen and oxygen gas mass concentration distribution at the Y=0m section of XZ when the cell discharge potential of 0.6V with the diffusion layer porosity is 0.2, 0.4, 0.6 and 0.8. It can be seen that the hydrogen gas in the gas channel of the anode distributing uniformly with the mass fraction value of 0.8105 when the porosity is 0.2. Differently, the oxygen gas distribution grads are larger than this, decline from 0.77 to 0.65. The hydrogen gas distribution in the diffusion layer of the anode falls down from 0.8105 to 0.50. On the contrary, oxygen gas distribution in the diffusion layer of the cathode drops sharply from 0.60 to 0. This situation will be relaxed when the porosity is 0.8, all the gas distribution grads is smaller than that at 0.2. Another result is that the hydrogen gas distribution grads are smaller than the oxygen gas distribution grads. There is some relationship with the molecule volume. Therefore, the higher the diffusion layer porosity is, the smaller the gas concentration grads of the diffusion will be. It is benefit for gas transport with high porosity, reducing the oxygen gas concentration grads and ridge part effect, especially when the oxygen gas diffuses

from flow channel down to the ridge portion of the bi-polar board. The cell performance could be increased accordingly.

### 3.4. Water distribution





(d) 0.8

Fig. 5. The water mass fraction distribution in fuel cell with the porosity of 0.2, 0.4, 0.6 and 0.8

The water mass fraction distribution of the fuel cell with the cell discharge potential of 0.6V is shown in Fig.5. The oxygen gas is humidified before entering flow channel in the cathode of the cell, thus water of the gas channel and the gas diffusion layer root in building from reaction and transferring through the proton exchange membrane from anode side to cathode side. The water mass fraction of the gas diffusion layer is always 0.95 when the porosity of the diffusion layer is 0.2. There are two grads when the porosity is 0.4. One is along the XZ slice face, the water mass fraction from the center of the diffusion layer to the boundary in the inlet slice face are 0.1065, 0.15, 0.35, 0.65, 0.75. The second grad along the YZ slice face, e.g. the water mass fraction distribution from the inlet to outlet of the slice face at  $X=2 \times 10^{-3}$  m are 0.75, 0.85, 0.90 and 0.95. There are also two grads when the porosity is 0.6 or 0.8. The water mass fraction distribution is from 0.1068 to 0.3 at the inlet slice face, and from 0.3 to 0.6 along the gas channel direction in the slice face at  $X=2 \times 10^{-3}$  m, respectively. In conclusion, the water mass fraction distribution minish from the gas diffusion layer to the gas channel in any XZ slice face, and increases along the gas channel direction. The higher the porosity is, the smaller the water mass fraction distribution grads will be, which explains that higher porosity is propitious to water transfer in the diffusion layer.

The different in the anode is that the water mass fraction distribution grads in the diffusion layer along the gas channel direction are not as great as that in the cathode. The main distinctness is that water mass fraction increases in the gas channel along the channel direction in the cathode side, while depressed in the anode side, although the depress extent is small. This is mostly because the net flux of water in the proton exchange membrane falls down from cathode to anode side, which means that the water concentration increasing in the diffusion layer of the anode side and then diffuse to the gas channel. Yet the gas concentration falls down near the outlet, which leads to the water building from reaction decrease. The water of the gas channel transfer to the diffusion layer in order to avoid the membrane drying at the anode side.

#### 4. Conclusions

- (1) The liquid water bring that the millipore in the diffusion layer occurs to jam which influences the normal gas diffusion. The lower of the porosity, the worse jam will be occurred of the diffusion millipore, and with more rapidness of the voltage.
- (2) The highest current density region is the osculant district of the ridge part of bi-polar plate and the diffusion layer. This happens to be the area which has the relatively shortest of gas transport path and electron transport path. The current density above the flow channel is very small. It is difficult for oxygen to diffusion into the catalyst layer below the ridge portion when at lower porosity.

- (3) The higher the porosity of the diffusion layer is, the smaller the gas concentration grads of the diffusion will be. It is benefit for gas transport with high porosity, reducing the oxygen gas concentration grads and ridge part effect, especially when the oxygen gas diffuses from flow channel down to the ridge portion of the bi-polar board. The cell performance could be increased accordingly.
- (4) The water mass fraction distribution monishes from the gas diffusion layer to the gas channel in any XZ slice face, and increases along the gas channel direction. The higher the porosity is, the smaller the water mass fraction distribution grads will be, which explains that higher porosity is propitious to water transfer in the diffusion layer.

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