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Simulation effect of operating temperature on performance of PEMFC based on serpentine flow field design

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Abstract

Polymer electrolyte membrane fuel cells (PEMFCs) transform directly chemical energy into electricity based on the reaction between hydrogen and oxygen. This research evaluated the effect of temperature on fuel cell operation relying to a 3-D fuel cell model simulation. The results of this research showed that the operating temperature relates to the water formation inside fuel cell; as a result, it affects directly to fuel cell performance. If the operating temperature is too low, the formed water exists at liquid phase, then it blocks gas channels. This phenomenon can degrade the fuel cell performance. In case of high operating temperature, the dryness of the membrane will decrease the electrical conductivity and lead to increase resistive loss. Therefore, maintaining suitable membrane humidity is very important to ensure optimal operation of a PEMFC system.

Keywords: Polymer electrolyte membrane fuel cells; flow-field design; water management, temperature field.

1. Introduction

Polymer exchange membrane fuel cells (PEMFCs) have been considered as one of the best solutions for the energy crisis and environmental pollution due to the reason that they produce fewer harmful emissions and are more efficient in comparison with the Carnot efficiency of heat engines [1-2]. Nowadays, they have become more and more popular in applications because of their self-starting at low temperatures, very high power density and simple operation [2].

A typical PEMFC includes seven main components: Anode and cathode bipolar plate (BP), gas diffusion layer (GDL) at the anode and cathode side, anode and cathode catalyst layers, and membrane as shown in Fig. 1 [3]. In PEMFCs operating process, heat and water are formed from electrochemical reactions between hydrogen and oxygen, this process creates electrical energy. The fundamental operation of a PEMFC is as follows: the catalyst oxidizes fuel (hydrogen) into positively charged ions and a negatively charged electrons at the anode side, and thank to the special design of membrane, ions can pass through it; however the electrons cannot. In addition, the free electrons travel through a wire creating the electric current. The formed water is transferred along the channels as well as in the direction perpendicular to the MEA [4]. As we know the products of these processes are heat and water, which affect again fuel cell performance. Consequently, it is necessary to enhance the thermal and water management in order to improve fuel cell operating characteristics. Thermal management is required to remove the heat and prevent overheating and dehydration of the membrane. Proper water management will maintain high electrical conductivity of the membrane and avoid water flooding in fuel cells.

To optimize operating temperature in the operating process of fuel cells, a simulation using computational fluid dynamics (CFD) is the cheap and effective method, which will help to understand the mechanisms inside the fuel cell, aid in data analysis, and identify limiting parameters without wasting a lot of time and cost in the experiment.

The purpose of this research is to evaluate the fuel cell performance when it operates with different operating temperature. To investigate, a simulation of a 3-D fuel cell models based on serpentine flow fields focusing on the effect of the temperature were built and evaluated. The operating temperature varies from 60^0C to 80^0C.

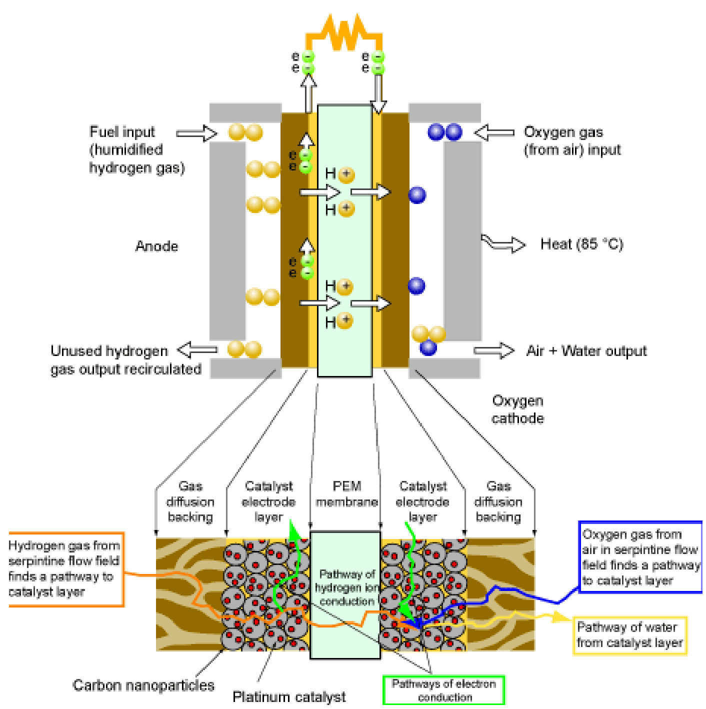

Fig. 1. Principles of PEMFC with proton exchange membranes.

2. Simulation model description

In this research, the numerical work is consumed that it operates on a steady state, multi-phase phenomena, and 3-dimensional mass transfer model, including heat transfer aspects of a PEMFC. Comsol software based on version 5.2 was used to model and simulate PEMFCs. The computational domain of the simulation model composes of two bipolar plates, the anode and the cathode gas channels, the anode and the cathode gas diffusion layers (GDLs), and MEA on active area of 121 cm^2. Its parameter characteristics are listed in Table 1 and Table 2.

Table 1. Fuel cell geometrical dimensions

No	Component	Length (mm)	Width (mm)	Thickness (mm)
1	Gas diffusion layer	110	110	0.5
2	Catalyst Layer	110	110	0.03
3	Membrane	110	110	0.1
5	Bipolar plate	60	60	10

Table 2. Properties and parameters in this numerical study

No	*Parameters*	*Value*	*Unit*
1	Porosity after compressed	150	%
2	Diffusion adjustment	100	%
3	GDL thermal conductivity	0.34	W/m·K
4	Membrane thermal conductivity	0.15	W/m·K
5	Membrane density in dry condition	4.0	g/cm^3
6	Cathode exchange current density	5	A/cm^2
7	Cathode transfer coefficient	0.65	
8	Anode exchange current density	10000	A/cm^2
9	Anode transfer coefficient	200	

For enhancing the computational accuracy of the simulation process, the grid cells were created by equalizing the node connectivity in each component and by using flexible meshes. The convergence criteria for the mass balance and energy balance are 0.1% with a maximum residual tolerance of 1E-05 [5, 6].

3. The governing equation and boundary conditions

3.1. Governing Equations

The equations used in this work is based on the mass conservation, Navier-stokes equations, transport equations of species, energy equation, and water phase change mode, and so on. Some assumptions were applied in this research as mentioned below:

- Catalyst layers were assumed to be an ultra-thin layer as integrate parts of the system;
- Water liquid is not formed in the flow channels;
- Oxygen and hydrogen would not dissolve in water

Model equations are:

- *The continuity equation is*

$$\frac{\partial(\varepsilon\rho)}{\partial t} + \nabla\cdot(\varepsilon\rho u) = 0 \qquad (1)$$

- *For the two-phase mixture in the gas channel, the Maxwell-Stefan mass transport equation was used*

$$F_i = \sum_{i\neq j} \zeta_{i,j} x_j (u_i - u_j) \qquad (2)$$

Where, F_i is the driving force on I, at a given T and p, $F_i = -\frac{RT}{x_i}\frac{dx_i}{dz}$, $\zeta_{i,j}$ is the friction coefficient between i and j, x_j is mole fraction of j. u is velocity.

- *For the multiphase mixture flow in the GDL, Darcy's Law was used for momentum transport modelling*

$$\frac{\partial(\rho u)}{\partial t} + \nabla\cdot(\rho u u) = -\nabla P + \nabla\cdot(\nabla \mu u) - \frac{\mu}{K}(\varepsilon u) \qquad (3)$$

3.2. Boundary Condition

The boundary conditions need to be defined for the Fuel Cell and Electrolysis simulation based on your problem specification [7]. The boundary conditions for anode Inlet and cathode inlet include mass flow rate, temperature, direction specification method, direction specification method, mass fraction, and water saturation. For pressure outlets, realistic backflow conditions will be defined. Next, set the boundary conditions for the terminal anode and cathode including its temperature and electric potential. These boundary conditions will affect directly to the operation of Fuel Cells system. This research focuses on the effect of changing of temperature and mass fractions in inlets on the water management which is the main parameter influencing essentially to Fuel Cells performance.

4. Result and discussion

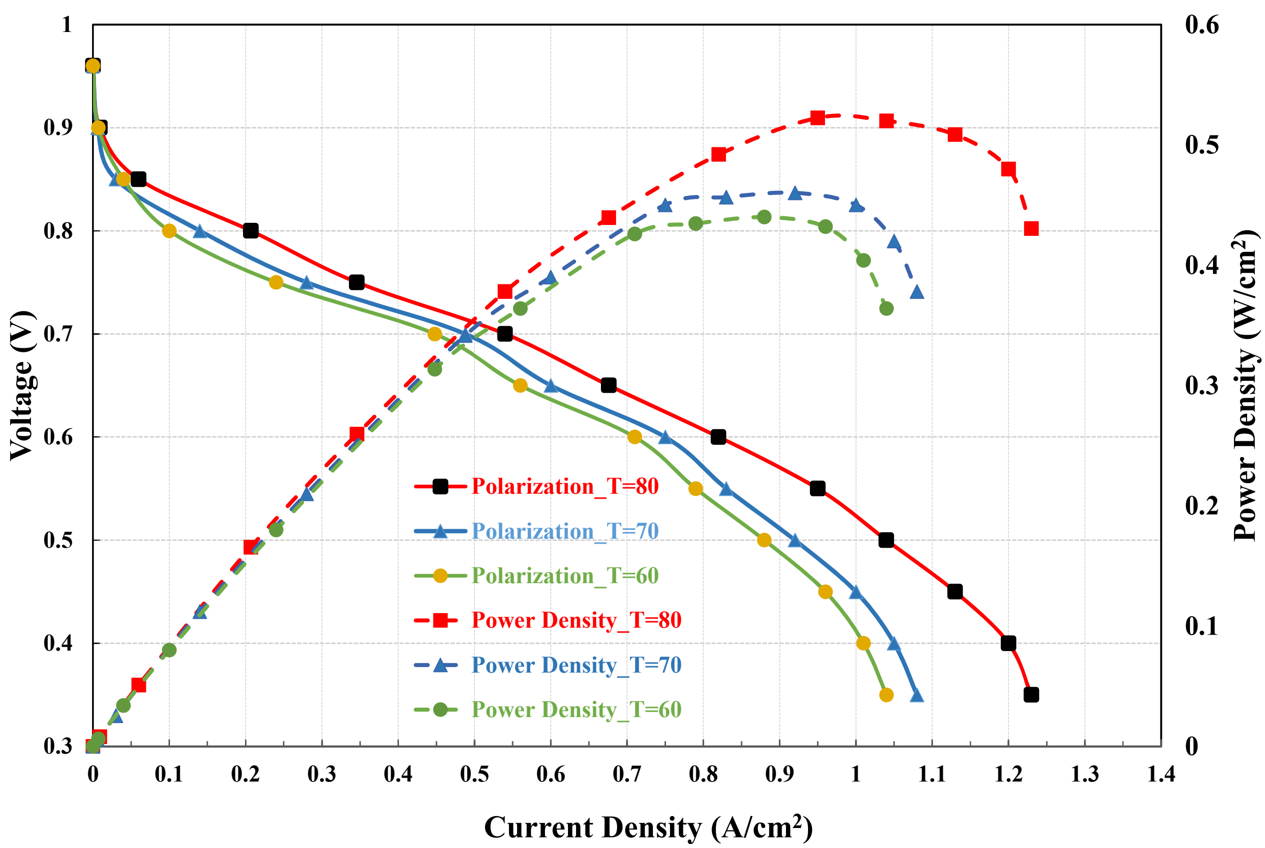

Fig. 2. Comparison of fuel cell performance with different operating temperatures

The temperature of fuel cell work is directly related to water content in the membrane and the catalyst layers, which plays an important factor for enhancing PEM fuel cell performance. The resulting restrictions for the thermal management make proper fuel cell temperature control essential in order to maintain proper humidification and guarantee optimal performance. Fig. 2 shows the Comparison of fuel cell performance with different operating temperatures. We can see that temperature affects directly fuel cell performance. At 60^0C, the fuel cell performance is lowest since the liquid is formed too much at low temperature; the water flooding will happen. This leads to instant increase in mass transport losses, particularly at the cathode. The transport rate of the reactants to the catalyst active sites is significantly reduced. And, Excess water blocks the pores of the GDL and thus prevents the reactants from reaching the catalysts. If the water content is too low conductivity decreases, leading to higher ionic resistance and larger ohmic losses [8], which results in a substantial drop in cell potential and thus a temporary power loss. Consequently, the fuel cell performance was enhanced when the operating temperature increased from 60^0C to 70^0C, especially, it reached to maximum value at 80^0C. The simulation results also showed that when continuing increasing the operating temperature, the fuel cell performance is reduced due to the dry membrane happens. Many previous studies also showed that the dry cell operation over a long time can cause serious and irreversible damage to the membrane.

5. Conclusion

The operating temperature of fuel cells is an important parameter strongly affects to the fuel cell performance. In this research, a 3-D CFD PEMFC model has been used to study the effect of temperature on the transport phenomena in a single fuel cell. This model can be used as an effective CFD tool for fuel cell development to reduce cost in fuel cell design and optimization. The optimization of operating temperature and humidity of inlet gases will enhance fuel cells performance and long-life. The results of this research also showed that when operating at 80^0C, the fuel cell performance can be optimized corresponding to the fuel cell configuration and boundary conditions of this research. It is recommend that the optimized operating temperature process should be conducted for each fuel cell configuration.

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