# Voltage modeling and simulation analysis of proton exchange membrane fuel cell

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**Abstract** Hydrogen energy as one of the key points of the 21st century energy reform, with clean, efficient and safe characteristics, proton exchange membrane fuel cells to hydrogen energy as an energy source, by governments and car companies focus on. Based on the working principle of proton exchange membrane fuel cell, the voltage model of fuel cell is established in MATLAB/Simulink software environment, including open circuit voltage model, three polarization model and actual voltage model. Based on this model, the influence of working temperature and working pressure on output voltage is explored.

**Keywords** Proton exchange membrane fuel cell; Modeling; Simulation analysis

## 1. Research status

Fuel cell is a device that directly converts chemical energy into electrical energy, which is not limited by Carnot Cycle and has high power generation efficiency. It is known as the fourth generation power generation technology after hydropower, thermal power and nuclear power [1], and fuel cell has a high specific energy and a wide range of fuels, so it has great potential for application in the automotive industry. In 1842, Grove developed the first fuel cell, and the fuel cell has since entered the stage of history. [2] The output characteristics of proton exchange membrane fuel cells can be analyzed and the output performance of the system can be improved. Fuel cell model can be divided into mechanism model and empirical model [3]. The empirical model can reflect the performance of fuel cell to a certain extent, and the modeling is simpler than the mechanism model. Empirical models include Amphlett model [4], Pukrushpan model [5] and Pathapati model [6]. Based on Pukrushpan model, open circuit voltage model, activation voltage loss model, ohm voltage loss model, concentration voltage loss model and actual output voltage model are established in this paper. Input different system parameters and conduct simulation analysis to explore the influence of working temperature and working pressure on output voltage to improve the output performance of the system.

## 2. PEMFC voltage modeling

The output voltage of the fuel cell directly reflects the performance of the reactor, which is affected by temperature, pressure, mass flow of the reactants and other factors. There are activation polarization, ohmic polarization and concentration polarization inside the fuel cell, and the existence of the three kinds of polarization is the reason why the actual voltage of the fuel cell is lower than the theoretical voltage [7].

### 2.1 Open Circuit Voltage

The Gibbs free energy of the reactants is converted into the output electrical energy of the fuel cell, taking into account the influence of the partial pressure of each gas and the stack temperature. The open circuit voltage can be expressed by the Nernst equation as:The Gibbs free energy of the reactants is converted into the output

electrical energy of the fuel cell, taking into account the influence of the partial pressure of each gas and the stack temperature. The open circuit voltage can be expressed by the Nernst equation as:

$$V_{rev} = -\left(\frac{\Delta H}{nF} - \frac{T_{st}\Delta S}{nF}\right) + RT\ln\left(\frac{P_{H_2}P_{O_2}^{0.5}}{P_{H_2O}}\right)$$
(1)

Where: $\Delta H$ represents the enthalpy generated by the reaction; $n$ Represents the number of moles of electrons transferred; $T_{st}$ Indicates the stack temperature; $F$ Denotes Faraday's constant; $F$ :The difference in entropy between the product and the reactant; $R$ Represents the ideal gas constant; $P_{H_2}$ Hydrogen partial pressure; $P_{O_2}$ Oxygen partial pressure; $P_{H_2O}$ Represents the saturation pressure of generated water vapor. The standard value of entropy change in thermodynamics is brought into Equation 2.2, and according to the energy balance between reactants and products [40]:

$$V_{rev} = 1.229 - 0.85\times10^{-3}\left(T_{st} - 298.15\right)$$
$$+4.3085\times10^{-5}T_{st}\left[\ln\left(P_{H_2}\right) + \frac{1}{2}\ln\left(P_{O_2}\right)\right]$$
(2)

## 2.2 Activation Polarization

The activation voltage loss is caused by the need to consume a certain amount of energy in order to overcome the reaction activation energy barrier in the process of electron transfer. The activation polarization phenomenon is related to temperature and current density. In the normal operation of fuel cell, the loss of cathode and anode is inevitable. The activation loss occurring at the cathode and anode can be expressed using Butler-Volmer as:

$$V_{act} = V_{act,ca} + V_{act,an}$$
(3)

Where: $V_{act,ca}$ represents the activation voltage loss occurring at the cathode, and $V_{cat,an}$ represents the activation voltage loss occurring at the anode.

$$V_{act,ca} = \frac{RT_{st}}{n\alpha_{ca}F}\ln\left(\frac{i}{i_{0,ca}}\right)$$
(4)

Where: $\alpha_{ca}$ represents the cathode charge transfer coefficient, the magnitude of which depends on the activation energy barrier; $i_{0,ca}$ Represents the cathode exchange current density;

$$V_{cat,an} = \frac{RT_{st}}{n\alpha_{an}F}\ln\left(\frac{i}{i_{0,an}}\right)$$
(5)

Where: $\alpha_{an}$ represents the anode charge transfer coefficient; $i_{0,an}$ Represents the anode exchange current density;

The temperature and pressure of the fuel cell are variable, so the effective exchange current density can be calculated by:

$$i_0 = i_0^{ref}a_cL_c\left(\frac{P_r}{P_r^{ref}}\right)^{\gamma}\exp\left[-\frac{E_c}{RT}\left(1 - \frac{T_{st}}{T_{ref}}\right)\right]$$
(6)

Where: $i_0^{ref}$ represents the reference current density per unit catalytic area; $a_c$ Represents specific surface area of catalyst; $L_c$ Represents catalyst load; $P_r$ Represents the local pressure of the reaction gas; $P_r^{ref}$ Indicates the reference pressure (e.g. 101.25kPa); $\gamma$ Pressure correlation coefficient; $E_c$ Denotes activation energy; $T_{ref}$ Indicates the reference temperature (for example, 298.15K).

The exchange current density reflects the activity of the electrode surface. The higher the exchange current density, the more active the electrode surface, and the lower the activation energy barrier to be overcome by charge transfer. The hydrogen reaction rate of the anode is fast, and the exchange current density is large, which is much higher than that of the cathode, and the difference is 5 to 6 orders of magnitude. For this reason, when calculating the activation voltage loss, the anode is usually ignored and only the cathode is considered.

## 2.3 Ohmic polarization

There are two main reasons for the ohmic voltage loss, one is the resistance of proton transfer by the electrolyte, the other is the resistance of electron transfer by the conductive element. The energy consumed to overcome these two parts of resistance is ohm overvoltage loss, according to Ohm's law, ohm voltage loss is equal to the product of resistance and current density:

$$V_{ohm} = i\left(R_i + R_e\right) = iR_{ohm} \tag{7}$$

Where: $i$ indicates current density; $R_i$ Represents proton resistance; $R_e$ Represents electronic resistance; $R_{ohm}$ Ohm internal resistance.

The ohm internal resistance is related to the temperature of the reactor and the humidity of the proton exchange membrane. A large number of research results show that the ohm internal resistance is a function of the conductivity of the membrane:

$$R_{ohm} = \frac{t_m}{\sigma_m} \tag{8}$$

Where: $t_m$ indicates the thickness of the film; $\sigma_m$ Represents the conductivity of the film.

The conductivity of the exchange film can be calculated according to the following formula:

$$\sigma_m = b_1 \exp\left[b_2\left(\frac{1}{303} - \frac{1}{T}\right)\right] \tag{9}$$

Where: $b_2$ represents constant; $b_1$ Is a function of membrane water content:

$$b_1 = b_{11}\lambda_m - b_{12} \tag{10}$$

Where: $b_2$ indicates the membrane water content; $b_1$ represents the empirical constant.

## 2.4 Concentration polarization

Concentration polarization is mainly caused by the concentration difference caused by the rapid consumption of reactants. The concentration voltage loss can be expressed as:

$$V_{conc} = -c \ln\left(1 - \frac{i}{i_L}\right) \tag{11}$$

Where: $c$ represents a constant, usually obtained by experience; $i_L$ Represents the limiting current density

As can be seen from the above formula, when the current density approaches the limit current density, the concentration voltage loss increases significantly. Therefore, concentration polarization usually occurs in the region of high current density, and greatly affects the output voltage of the fuel cell.

The limiting current density can be expressed as follows:

$$i_L = \frac{nFC_B D}{\delta} \tag{12}$$

Where: $C_B$ represents the concentration of reactants; $D$ Represents diffusion coefficient; $\delta$ Represents the diffusion distance.

### 2.5 Actual output voltage

The actual output voltage can be expressed as the theoretical voltage minus the voltage loss of various polarizations:

$$V = N_{cell}V_{cell} = N_{cell}\left(V_{rev} - V_{act} - V_{ohm} - V_{conc}\right) \tag{13}$$

Where: $V$ indicates the actual output voltage; $N_{cell}$ Represents the number of single fuel cells; $V_{rev}$ Represents the fuel cell open circuit voltage; $V_{act}$ Represents activation voltage loss; $V_{ohm}$ Ohmic voltage loss; $V_{conc}$ Represents the loss of concentration voltage.
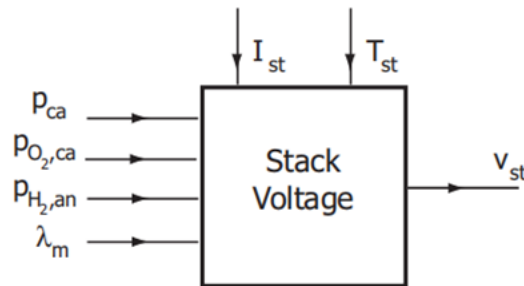


*Figure: 1  Stack voltage model block*

According to the above theoretical formula, the voltage model of proton exchange membrane fuel cell is established. Based on the voltage model of the fuel cell, the influence of different system parameters on the output voltage of the fuel cell is discussed by using the control variable method.

### 3. Analysis of influence of pressure and temperature on output voltage

### 3.1 Analysis of the influence of pressure on output voltage

FIG. 2 shows the simulation curve of activation overvoltage when the cathode pressure of the fuel cell changes from 1bar to 4bar at 80℃. As can be seen from the figure, when the current density is greater than 0.5A· cm-2, the maximum activation overvoltage from top to bottom is 0.478V, 0.429V, 0.395V, and 0.373V, respectively. It can be seen that the activation overvoltage decreases with the increase of cathode pressure. The reason is that when the pressure increases, the activation energy consumed by the reaction is reduced, which is conducive to the forward reaction. The curve interval from top to bottom gradually becomes smaller, indicating that the activation overvoltage is significantly reduced when the pressure is relatively small. On the contrary, the activation overvoltage decreases and weakens.
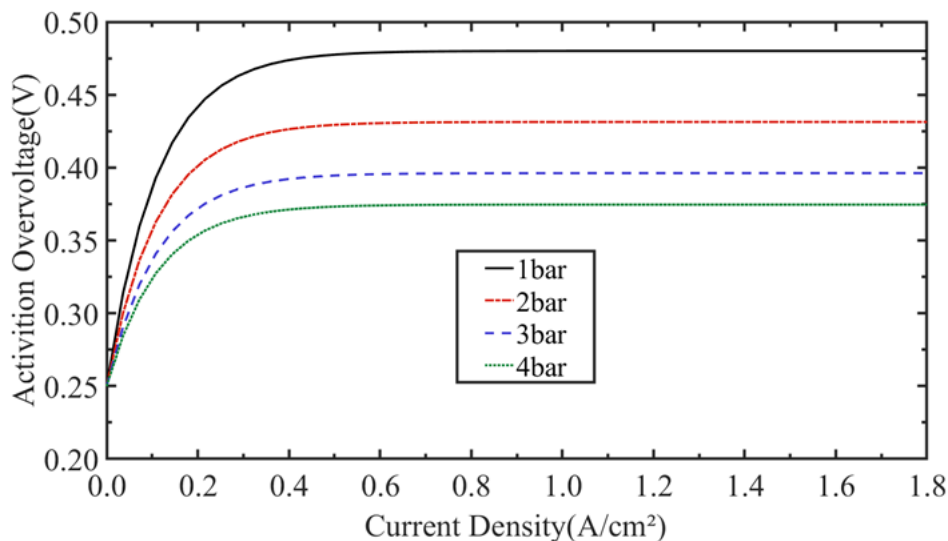


*Figure 2:  Activation overvoltage at different cathode pressure at 80°C*

Fig. 3 shows the concentration overvoltage simulation curve of the fuel cell cathode pressure changing from 1bar to 4bar at 80℃. The simulation results show that with the increase of cathode pressure, the concentration overvoltage decreases, especially when the pressure is from 1bar to 2bar. This is because as the cathode pressure increases, the pressure and concentration of the reactants also increase, and the consumed reactants can be quickly replenished.
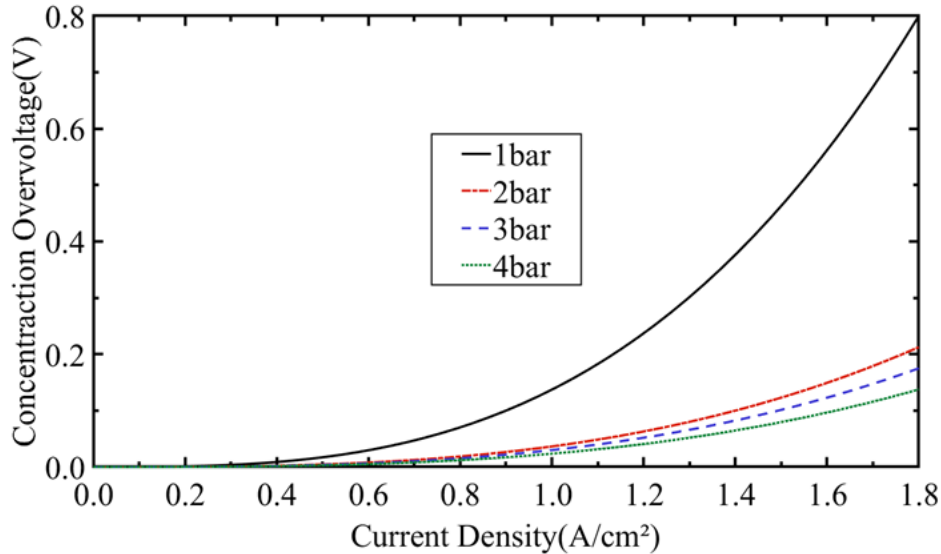


*Figure: 3  Concentration overvoltage at different cathode pressure at 80°C*

Figure 4 shows the simulation curve of the ohm overvoltage at 80℃ when the cathode pressure of the fuel cell changes from 1bar to 4bar. The ohmic overvoltage is the product of the current density and the internal resistance of the fuel cell, so a change in cathode pressure does not affect the ohmic overvoltage. So the simulation curves overlap.
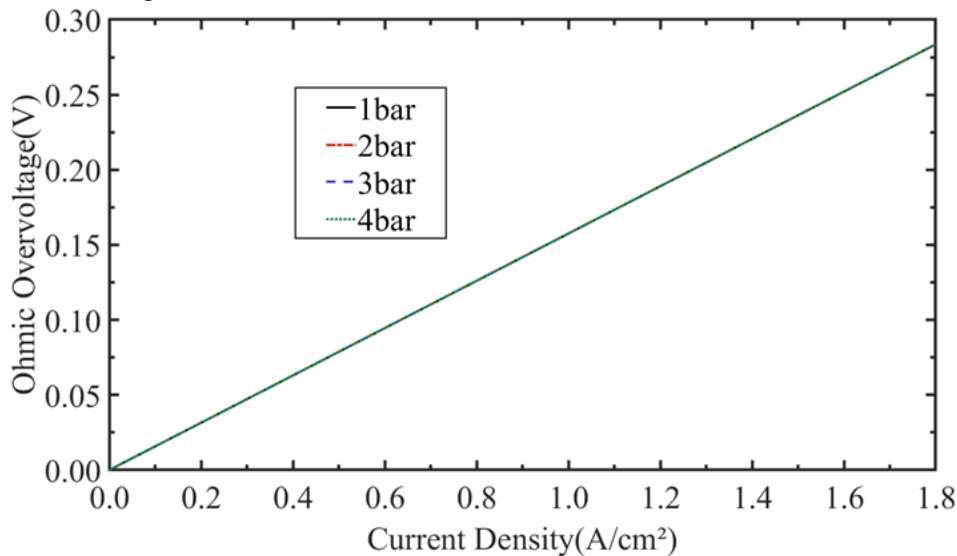


*Figure: 4  Ohmic overvoltage with different cathode pressure at 80°C*

Figure 5 shows the polarization curve of the fuel cell at 80℃ when the cathode pressure changes from 1bar to 4bar. The polarization curve simulation results show that the fuel cell voltage increases with the increase of cathode pressure. When the current density is 0.9A· cm-2, the voltage change from 1bar to 2bar is about 4 times that of the cathode pressure from 2bar to 3bar. It shows that increasing the pressure when the pressure is small has an obvious effect on increasing the fuel cell voltage.
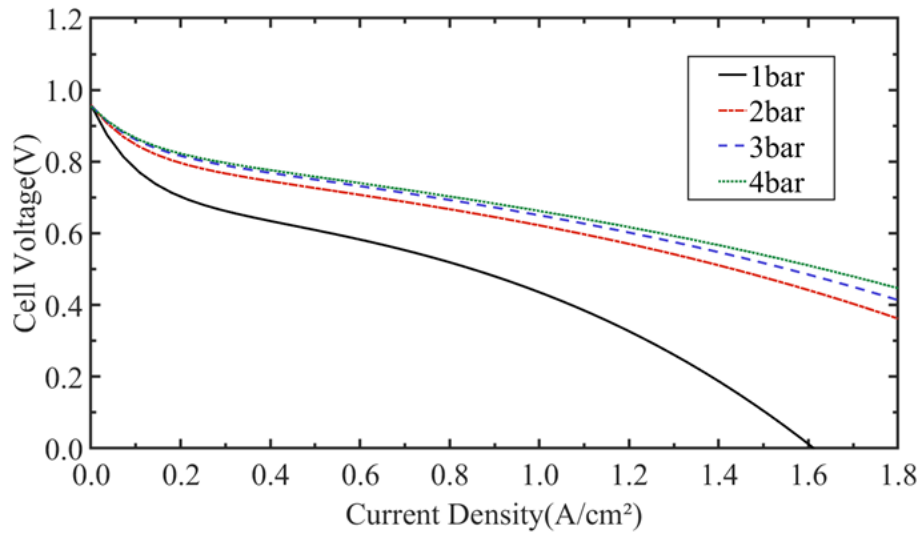
*Figure: 5  Polarization curve with different cathode pressure at 80°C*

**3.2 Analysis of the influence of temperature on output voltage**

Figure 6 shows the simulation curve of activation overvoltage when the fuel cell temperature changes from 25℃ to 100℃ at a cathode pressure of 2.5bar. The simulation results show that the fuel cell activation overvoltage decreases with the increase of operating temperature. This is mainly because the increase of temperature promotes the forward progress of electrochemical reaction, and the decrease of activation energy leads to the decrease of activation overvoltage.
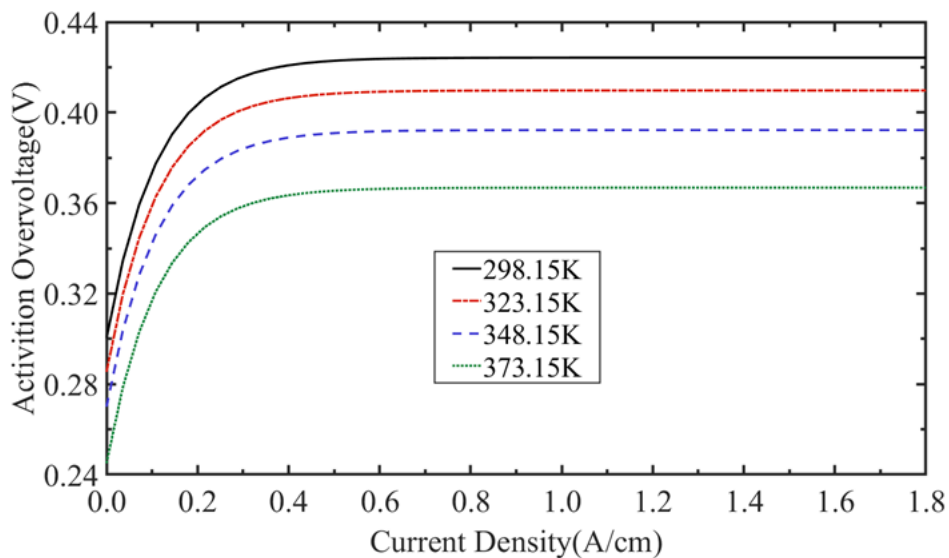


*Figure: 6  Activation overvoltage with different temperature at 2.5bar*

Figure 7 shows the concentration overvoltage simulation curve of the fuel cell temperature changing from 25℃ to 100℃ at a cathode pressure of 2.5bar. The simulation results show that the fuel cell concentration overvoltage increases slightly with the increase of operating temperature. Because concentration polarization is closely related to the concentration of reactants, the increase of temperature only makes the distribution of reactants more uniform, and the effect on concentration is not obvious.
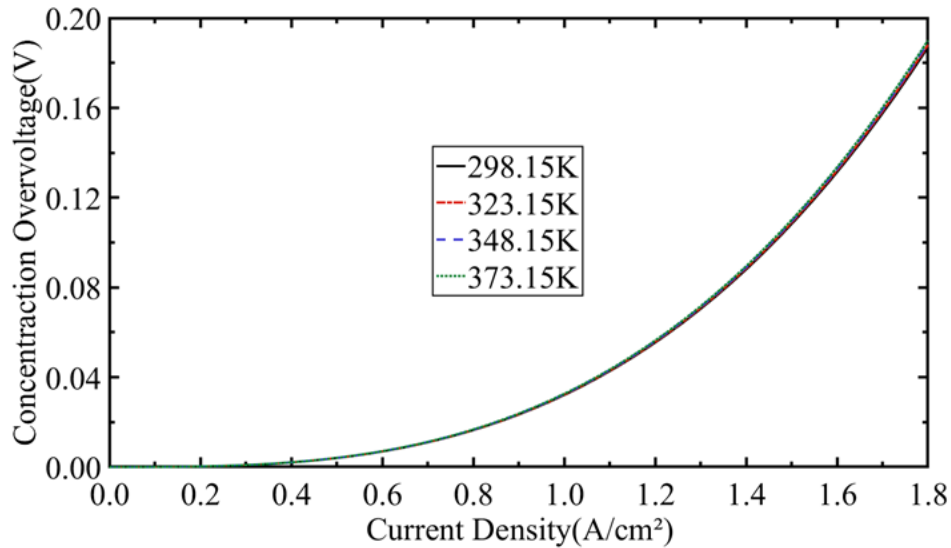
*Figure: 7 Concentration overvoltage with different temperature at 2.5bar*

Figure 8 shows the ohm overvoltage simulation curve of the fuel cell temperature changing from 25℃ to 100℃ under the working pressure of 2.5bar. The simulation results show that the ohm overvoltage of the fuel cell decreases with the increase of operating temperature. The ohmic internal resistance in the fuel cell is a function of the conductivity, and the conductivity is related to temperature, so when the exchange film thickness is determined, the conductivity increases with the increase of temperature, and the ohmic internal resistance decreases, resulting in the decrease of ohmic overvoltage.
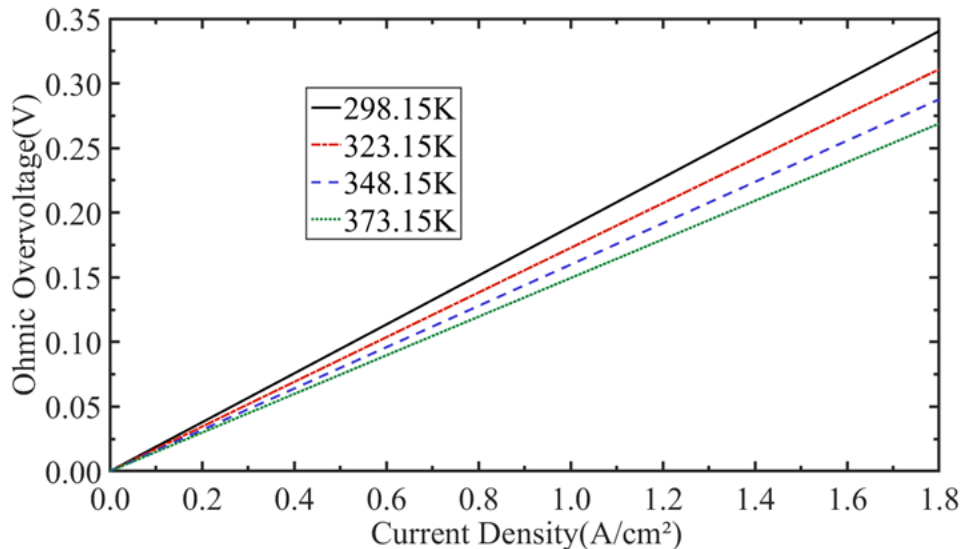


*Figure: 8 Ohmic overvoltage with different temperature at 2.5bar*

Figure 9 shows the polarization curve of the fuel cell temperature changing from 25℃ to 100℃ under the working pressure of 2.5bar. The polarization curve simulation results show that the voltage drop of the fuel cell increases with the increase of operating temperature when the pressure is constant. This is mainly because the temperature increases, the open circuit voltage increases, the activation overvoltage and the ohmic overvoltage decrease, and the concentration overvoltage is almost constant, which increases the output voltage of PEMFC.
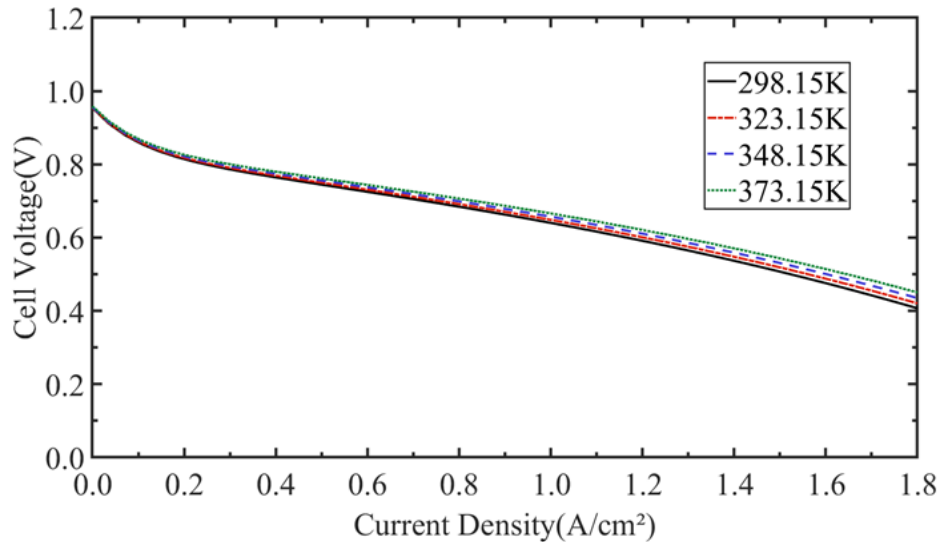
*Figure: 9  Polarization curve with different temperature at 2.5bar*

## 4 Conclusion

The simulation results show that:

1) the activation overvoltage and concentration overvoltage are affected by the change of cathode pressure, while the ohmic overvoltage is not affected by the change.

2) With the increase of cathode pressure, the output voltage of the fuel cell increases, so the appropriate increase of oxygen partial pressure is conducive to the improvement of the output performance of the fuel cell.

3) Changing the stack temperature affects the activation overvoltage and ohmic overvoltage, while the concentration overvoltage is less affected.

4) With the increase of the stack temperature, the output voltage of the fuel cell increases, especially when the current density is large and the temperature is low. Therefore, controlling the fuel cell temperature within a reasonable range is conducive to improving the output performance of the fuel cell.

## References

[1] Wang Huawen, Qi Guozhen. Research progress and industrialization of fuel cell technology [J]. Gaoqiao Petrochemical, 2005, 20(3):5.

[2] Haldane J B S. Daedalus or Science and the Future[M]. New York: EP Dutton, 1924.

[3] Clothing treasure, battery. Fuel Cell -- Principle, Technology and Application [M]. Chemical Industry Press, 2003.

[4] Amphlett J C, Mann R F, Peppley B A, et al. A model predicting transient responses of proton exchange membrane fuel cells [J]. Journal of Power sources, 1996, 61(1-2): 183-188.

[5] Pukrushpan J T, Peng H, Stefanopoulou A G. Control-oriented modeling and analysis for automotive fuel cell systems [J]. J. Dyn. Sys., Meas., Control, 2004, 126(1): 14-25.

[6] Pathapati P R, Xue X, Tang J. A new dynamic model for predicting transient phenomena in a PEM fuel cell system [J]. Renewable energy, 2005, 30(1): 1-22.

[7] Mench M M, Wang C Y, Thynell S T. An introduction to fuel cells and related transport phenomena [J]. International journal of transport phenomena, 2001, 3: 151-176.