

# Research on the Performance Modeling Method of Proton Exchange Membrane (PEMFC)

Zhenhao Liu, Binbin Sun, Lin Sun, Pengwei Wang and Wentao Li

**Abstract**—How to shorten the PEMFC development cycle is one of the key concerns of the PEMFC industry at present. Among them, developing a high-precision and high-efficiency PEMFC performance analysis platform is an important method to accelerate the PEMFC development progress. In this paper, from the PEMFC reaction mechanism and engineering development experience, we firstly analyze the mechanism and mathematical modeling of PEMFC reactor, and establish the voltage sub-model, cathode runner sub-model, anode runner sub-model and membrane hydration sub-model. Then, the performance analysis of the core components of the cathode system, such as air compressor, intercooler, humidifier and backpressure valve, was carried out, and a sub-model of each component was established. Further, the mathematical model of the anode system including the hydrogen circulation pump and the pressure regulating valve is studied and established. In addition, the core components of radiator, cooling water pump and thermostat are analyzed mechanically, and the PEMFC hydrothermal management system model is established. Finally, the established PEMFC model was experimentally verified. The results show that the constructed mathematical model for PEMFC performance analysis can accurately simulate the PEMFC working process and output reasonable numerical results with the error within 5%.

**Index Terms**—PEMFC, stack modeling, cathode system modeling, anode system modeling, hydrothermal management system modeling

## I. INTRODUCTION

Under the common vision of global carbon neutrality, with the proposal of the national "dual carbon" major strategy, electrification has become an important carrier for

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the automobile industry to achieve low-carbon goals, and it is also an important direction for the high-quality development of my country's automobile industry [1]. The development of zero-carbon emission PEMFC is currently the high ground of technological competition in the automotive industry, and it is also the core measure to implement the national "dual carbon" strategy [2]. However, the high development cycle and high development cost are still common problems in the current PEMFC industry, and it is also one of the important factors restricting its rapid development [3]. Therefore, how to shorten the PEMFC development cycle and reduce the development cost is of great significance to promote the development of the PEMFC industry [4].

The development of new PEMFC products involves parameter design and matching selection of core components, system integration design, design and calibration of control parameters, etc. [5,6]. If the above-mentioned design is carried out by the experimental method, it will cause the problems of long development cycle and high development cost, which will restrict the development of PEMFC [7]. Therefore, it is important to design and develop a high-precision and high-efficiency PEMFC performance analysis platform to support the development process of parameter matching, integrated design and control of PEMFC core components to accelerate the development of PEMFC [8,9].

Modeling method of PEMFC stack performance analysis model is mainly an empirical method [10,11]. The modeling process of this method is relatively simple. It does not need to consider the internal reaction mechanism of the fuel PEMFC stack. It only needs to conduct a large number of experiments on the selected PEMFC, and obtain the external characteristic curve fitting equation of the PEMFC according to the experimental data to describe the PEMFC. This method can usually reflect the performance of the selected PEMFC well, but cannot describe other types of PEMFCs well [10]. In addition, the empirical modeling method cannot represent the internal reaction of the battery, which is not conducive to the optimization of the internal structure of the PEMFC [11]. Modeling around PEMFC auxiliary systems is limited to a single cathode, anode or hydrothermal management system, and there is a lack of integrated modeling of the entire auxiliary system [12].

The overview describes the development of a high-precision and high-efficiency PEMFC performance analysis platform to shorten the PEMFC development cycle. The first part of this paper focuses on the PEMFC stack modeling method. The mechanism analysis and modeling method of the cathode subsystem are discussed in detail in the second part of the paper. The anode subsystem is analyzed in the third part of the paper and its mathematical

model is developed based on it. The PEMFC hydrothermal management subsystem model is presented in the fourth part. Finally, the performance verification and simulation analysis of the developed model are presented in the fifth part.

## II. PEMFC STACK MODELING

### A. Voltage Model

During the PEMFC reaction, electrons and hydrogen ions are generated, the former mainly in the anode and cathode, and the latter mainly in the electrolyte, so that a charge layer is generated between the cathode and the electrolyte, similar to the charge layer in a capacitor, and this phenomenon is called "double charge layer". Because of the capacitive nature of the "charge layer", the activation and polarization voltages do not change immediately with the change of current, as in the case of ohmic voltage, but have a certain hysteresis for the change of current when the current of the PEMFC changes abruptly. As shown in Figure 1, the equivalent circuit of PEMFC with proton exchange membrane is given.

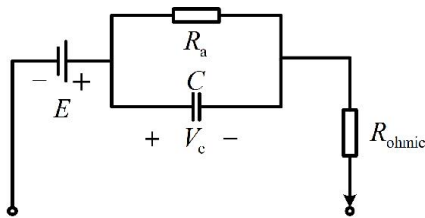


Fig. 1 Equivalent circuit diagram of fuel cell

The dynamic characteristics of PEMFC can be expressed by the following formula

$$\frac{du_a}{dt} = \frac{I}{C} - \frac{u_a}{\tau} \quad (1)$$

Where,  $u_a$  represents the total polarization over voltage, and the value is the sum of the activation over voltage and the concentration over voltage;  $\tau$  it represents the time constant,  $I$  is the current, and  $C$  is the capacitance.

$$R_a = \frac{V_{act} + V_{conc}}{I} \quad (2)$$

$$\tau = CR_a = C \left( \frac{V_{act} + V_{conc}}{I} \right) \quad (3)$$

Where,  $R_a$  is the equivalent resistance, the  $V_{act}$  table is the activation polarization voltage, and the table is  $V_{conc}$  the concentration polarization voltage.

### B. Cathode runner model

The cathode channel model describes the changes in the composition of the air entering the reactor cathode during the flow, including the mass flow rate and pressure changes of oxygen, nitrogen and water vapor, etc. Assumptions are made for the cathode flow channel model, one is that all gases are considered to be ideal gases. Second, the temperature of the cathode and the reactor are the same, and the excess heat

generated by the reactor can be dissipated in time. Third, the cathode water vapor and liquid water are both present on the cathode side, and the PEMFC obeys the law of mass conservation, where the sum of all input masses is equal to the sum of all output masses, and the mass change of each substance inside the cathode can be expressed by the following equation:

$$\begin{cases} \frac{dn_{O_2,ca}}{dt} = m_{O_2,ca,in} - m_{O_2,ca,out} - m_{O_2,cons} \\ \frac{dn_{N_2,ca}}{dt} = m_{N_2,ca,in} - m_{N_2,ca,out} \\ \frac{dn_{w,ca}}{dt} = m_{v,ca,in} - m_{v,ca,out} + m_{v,ca,gen} + m_{v,member} - m_{l,ca,out} \end{cases} \quad (4)$$

Where,  $n_{O_2,ca}$ ,  $n_{N_2,ca}$ ,  $n_{w,ca}$ , represent the mass of oxygen, nitrogen and water at the cathode, respectively (kg);  $m_{O_2,ca,in}$ ,  $m_{v,ca,in}$  represent the mass flow of oxygen, nitrogen and water vapor at the cathode inlet ( $kg \cdot s^{-1}$ );  $m_{O_2,ca,out}$ ,  $m_{v,ca,out}$ , represent the oxygen, nitrogen and water vapor at the  $m_{N_2,ca,out}$  cathode outlet, respectively. Water vapor mass flow ( $kg \cdot s^{-1}$ );  $m_{v,ca,gen}$ , represents the generated water vapor mass flow ( $kg \cdot s^{-1}$ );  $m_{v,member}$  represents the exchange membrane transmission water mass flow ( $kg \cdot s^{-1}$ );  $m_{l,ca,out}$  represents the cathode outlet water mass flow ( $kg \cdot s^{-1}$ ).

As the reaction process continues, the cathode water vapor gradually accumulates and finally generates liquid water. The maximum water vapor mass  $n_{v,ca,max}$  is:

$$n_{v,ca,max} = \frac{P_{sat} V_{ca}}{R_v T} \quad (5)$$

Where,  $V_{ca}$  represents the cathode volume ( $m^3$ );  $R_v$  represents the water vapor gas constant.

Then the mass of water vapor and liquid water in the cathode is:

$$\begin{aligned} n_{w,ca} \leq n_{v,ca,max} &\Rightarrow n_{v,ca} = n_{v,ca}; n_{l,ca} = 0 \\ n_{w,ca} > n_{v,ca,max} &\Rightarrow n_{v,ca} = n_{v,ca,max}; n_{l,ca} = n_{w,ca} - n_{v,ca,max} \end{aligned}$$

The partial pressure of each substance in the cathode can be expressed by the following formula:

$$P_{i,ca} = \frac{n_{i,ca} R_i T}{V_{ca}} \quad i = O_2, N_2, H_2O \quad (6)$$

Where,  $P_{i,ca}$  represents the partial pressure of the cathode material (kPa);  $n_{i,ca}$  represents the mass of the cathode material (kg);  $R_i$  represents the material gas constant.

The internal pressure of the cathode is equal to the sum of the partial pressures of the gases:

$$P_{ca} = P_{O_2,ca} + P_{N_2,ca} + P_{v,ca} \quad (7)$$

The molar mass of the air at the cathode inlet and inside the cathode is:

$$\begin{cases} M_{a,ca,in} = y_{O_2,ca,in} M_{O_2} + (1 - y_{O_2,ca,in}) M_{N_2} \\ M_{a,ca} = y_{O_2,ca} M_{O_2} + (1 - y_{O_2,ca}) M_{N_2} \end{cases} \quad (8)$$

Where,  $M$  represents the molar mass of the corresponding substance ( $\text{kg}\cdot\text{mol}^{-1}$ );  $y_{O_2,ca,in}$ ,  $y_{O_2,ca}$  represents the mole fraction of air at the cathode inlet and inside the cathode.

The air mole fraction at the inlet is constant, and the internal mole fraction is expressed as:

$$y_{O_2,ca} = \frac{P_{O_2,ca}}{P_{a,ca}} \quad (9)$$

Where,  $P_{a,ca}$  represents the dry air pressure (kPa).

The humidity ratio of the cathode inlet to outlet gas is:

$$\begin{cases} \omega_{ca,in} = \frac{M_v}{M_{a,ca,in}} \frac{P_{v,ca,in}}{P_{a,ca,in}} \\ \omega_{ca,out} = \frac{M_v}{M_{a,ca}} \frac{P_{v,ca}}{P_{a,ca}} \end{cases} \quad (10)$$

Where,  $\omega_{ca,in}$ ,  $\omega_{ca,out}$  represents the humidity ratio of the cathode inlet and outlet gas; represents the cathode inlet and outlet dry air partial pressure (kPa);  $P_{a,ca,in}$ ,  $P_{a,ca}$  represents the cathode inlet and outlet water vapor partial pressure (kPa).

The expression for the partial pressure of water vapor and air at the cathode inlet is:

$$\begin{cases} P_{v,ca,in} = \phi_{ca,in} P_{sat}(T) \\ P_{a,ca,in} = P_{ca,in} - P_{v,ca,in} \end{cases} \quad (11)$$

The mass flow rates of air, water vapor, oxygen and nitrogen at the cathode inlet and outlet are:

$$\begin{cases} m_{a,ca,in} = \frac{1}{1 + \omega_{ca,in}} m_{ca,in} \\ m_{a,ca,out} = \frac{1}{1 + \omega_{ca,out}} m_{ca,out} \\ m_{v,ca,in} = m_{ca,in} - m_{a,ca,in} \\ m_{v,ca,out} = m_{ca,out} - m_{a,ca,out} \end{cases} \quad (12)$$

$$\begin{cases} m_{O_2,ca,in} = \chi_{O_2,ca,in} m_{a,ca,in} \\ m_{O_2,ca,out} = \chi_{O_2,ca} m_{a,ca,out} \\ m_{N_2,ca,in} = (1 - \chi_{O_2,ca,in}) m_{a,ca,in} \\ m_{N_2,ca,out} = (1 - \chi_{O_2,ca}) m_{a,ca,out} \end{cases} \quad (13)$$

Where,  $\chi_{O_2,ca,in}$ ,  $\chi_{O_2,ca}$  represents the oxygen mass fraction at the cathode inlet and inside the cathode. Its specific expression is as follows:

$$\begin{cases} \chi_{O_2,ca,in} = \frac{y_{O_2,ca,in} M_{O_2}}{y_{O_2,ca,in} M_{O_2} + (1 - y_{O_2,ca,in}) M_{N_2}} \\ \chi_{O_2,ca} = \frac{y_{O_2,ca} M_{O_2}}{y_{O_2,ca} M_{O_2} + (1 - y_{O_2,ca}) M_{N_2}} \end{cases} \quad (14)$$

The mass flow rate of oxygen and water vapor involved in

the reaction inside the stack is:

$$\begin{cases} m_{O_2,cons} = \frac{IM_{O_2}}{4F} \\ m_{v,ca,gen} = \frac{IM_v}{2F} \end{cases} \quad (15)$$

### C. Anode runner model

The anode flow channel model describes the changes of each component of hydrogen fuel entering the anode of the reactor during the flow process, including the mass flow rate of hydrogen and water vapor, pressure changes, etc. First, reasonable assumptions are made for the anode channel model. First, all gases are considered as ideal gases. Second, the anode and the reactor are at the same temperature, and the excess heat generated by the reactor can be dissipated in time. Third, the anode water vapor and liquid water are both present on the anode side. The change in mass of each substance inside the anode can be expressed by the following equation:

$$\begin{cases} \frac{dn_{H_2,an}}{dt} = m_{H_2,an,in} - m_{H_2,an,out} - m_{H_2,cons} \\ \frac{dn_{w,an}}{dt} = m_{v,an,in} - m_{v,an,out} + m_{v,number} - m_{l,an,out} \end{cases} \quad (16)$$

Where,  $n_{H_2,an}$ ,  $n_{w,an}$  represent the mass flow of hydrogen and water at the anode, respectively (kg);  $m_{H_2,an,in}$ ,  $m_{v,an,in}$  represent the mass flow of oxygen and water vapor at the anode inlet, respectively ( $\text{kg}\cdot\text{s}^{-1}$ );  $m_{H_2,an,out}$ ,  $m_{v,an,out}$  represent the mass flow of hydrogen and water vapor at the anode outlet ( $\text{kg}\cdot\text{s}^{-1}$ ), respectively;  $m_{l,an,out}$  Indicates the mass flow rate of the anode outlet water ( $\text{kg}\cdot\text{s}^{-1}$ ).

Over time, water vapor will gradually accumulate inside the anode, and liquid water will be formed when the water vapor reaches saturation. The maximum water vapor mass of the anode  $n_{v,an,max}$  is:

$$n_{v,an,max} = \frac{P_{sat} V_{an}}{R_v T} \quad (17)$$

Where,  $V_{an}$  represents the cathode volume ( $\text{m}^3$ ).

Then the mass of water vapor and liquid water in the anode is:

$$\begin{aligned} n_{w,an} \leq n_{v,an,max} &\Rightarrow n_{v,an} = n_{v,an}; n_{l,an} = 0 \\ n_{w,an} > n_{v,an,max} &\Rightarrow n_{v,an} = n_{v,an,max}; n_{l,an} = n_{w,an} - n_{v,an,max} \end{aligned}$$

The partial pressure of each substance in the anode can be expressed by the following formula:

$$P_{i,an} = \frac{n_{i,an} R_i T}{V_{an}} \quad i = H_2, H_2O \quad (18)$$

Where,  $P_{i,an}$  represents the partial pressure of the anode material (kPa);  $n_{i,an}$  represents the mass of the anode material (kg).

The internal pressure of the anode is equal to the sum of the partial pressures of the gases:

$$P_{an} = P_{H_2,an} + P_{v,an} \quad (19)$$

The humidity ratio of anode inlet to outlet gas is:

$$\begin{cases} \omega_{an,in} = \frac{M_v}{M_{H_2}} \frac{P_{v,an,in}}{P_{an,in}} \\ \omega_{an,out} = \frac{M_v}{M_{H_2}} \frac{P_{v,an}}{P_{H_2,an}} \end{cases} \quad (20)$$

Where,  $\omega_{an,in}$ ,  $\omega_{an,out}$  represents the humidity ratio of the anode inlet and outlet gas;  $P_{an,in}$ ,  $P_{H_2,an}$  represents the anode inlet gas partial pressure and anode hydrogen partial pressure (kPa);  $P_{v,an,in}$ ,  $P_{v,an}$  represents the cathode inlet and outlet water vapor partial pressure (kPa).

The partial pressures of water vapor and hydrogen at the anode inlet are expressed as:

$$\begin{cases} P_{v,an,in} = \phi_{an,in} P_{sat}(T) \\ P_{H_2,an,in} = P_{an,in} - P_{v,an,in} \end{cases} \quad (21)$$

The hydrogen and steam mass flows at the anode inlet and outlet are:

$$\begin{cases} m_{H_2,an,in} = \frac{1}{1 + \omega_{an,in}} m_{an,in} \\ m_{H_2,an,out} = \frac{1}{1 + \omega_{an,out}} m_{an,out} \\ m_{v,an,in} = m_{an,in} - m_{H_2,an,in} \\ m_{v,an,out} = m_{an,out} - m_{H_2,an,out} \end{cases} \quad (22)$$

When a chemical reaction occurs inside the stack, the hydrogen mass flow involved in the reaction is:

$$m_{H_2,cons} = \frac{IM_{H_2}}{2F} \quad (23)$$

#### D. Membrane hydration model

The transfer of water across the exchange membrane exists in two main forms. One is that during the reaction, hydrogen ions moving from the anode to the cathode must combine with water molecules and pass through the exchange membrane, this form is called "electroosmotic migration". The second is that the reaction process will produce water, resulting in more water on the cathode side compared to the anode side, thus forming a concentration gradient, and the water on the cathode side will move to the other side, this form is known as "counter-diffusion". In the modeling of the water on the exchange membrane to make the following assumptions, the exchange membrane and the water inside the stack are in the ideal state, and the water in the exchange membrane and the stack are uniformly distributed, then the two forms of water transfer can be expressed by the following equation:

$$\begin{cases} N_{v,osm} = n_d \frac{i}{F} \\ N_{v,diff} = D_w \frac{dc_v}{dy} \end{cases} \quad (24)$$

Where,  $N_{v,osm}$ ,  $N_{v,diff}$  represents the water transfer amount on the exchange membrane caused by "electroosmotic migration" and "reverse diffusion" ( $\text{mol} \cdot \text{s}^{-1}$ );  $n_d$  represents the electroosmotic coefficient;  $D_w$  represents the water diffusion coefficient;  $c_v$  represents the water concentration ( $\text{mol} \cdot \text{cm}^{-3}$ ).

According to the above formula, the amount of water transferred through the exchange membrane is:

$$N_{v,member} = n_d \frac{i}{F} - D_w \frac{c_{v,ca} - c_{v,an}}{l} \quad (25)$$

Where,  $N_{v,member}$  represents the water transfer capacity on the exchange membrane ( $\text{mol} \cdot \text{s}^{-1}$ );  $c_{v,ca}$  and  $c_{v,an}$  represents the cathode and anode water concentrations ( $\text{mol} \cdot \text{cm}^{-3}$ );  $l$  represents the thickness of the exchange membrane (cm).

The total water mass flow through the exchange membrane is:

$$m_{v,member} = n_{cell} \cdot N_{v,member} \cdot M_v \cdot A \quad (26)$$

Where,  $A$  represents the effective area of the exchange membrane ( $\text{cm}^2$ ).

The expression formula of water concentration in cathode and anode is:

$$\begin{cases} c_{v,ca} = \frac{\rho_{m,dry} \lambda_{ca}}{M_{m,dry}} \\ c_{v,an} = \frac{\rho_{m,dry} \lambda_{an}}{M_{m,dry}} \end{cases} \quad (27)$$

Where,  $\rho_{m,dry}$  represents the density of the exchange membrane when drying ( $\text{kg} \cdot \text{cm}^{-3}$ );  $M_{m,dry}$  represents the molar mass of the membrane when drying ( $\text{kg} \cdot \text{mol}^{-1}$ );  $\lambda_{ca}$ ,  $\lambda_{an}$  represents the water content of the exchange membrane on the cathode side and the anode side.

The water content in the exchange membrane is related to the relative humidity of the membrane, which can generally be expressed by the following formula:

$$\lambda_i = \begin{cases} 0.043 + 17.81a_i - 39.85a_i^2 + 36.0a_i^3, & 0 < a_i \leq 1 \\ 14 + 1.4(a_i - 1), & 1 < a_i \leq 3 \end{cases} \quad (28)$$

Where,  $\lambda_i$  represents the water content at  $a_i$  different locations; represents the activation coefficient of water at different locations, where  $a_m = (a_{ca} + a_{an}) / 2$

The activation coefficient of water is equal to:

$$a_i = \frac{P_{v,i}}{P_{sat}} \quad i = m, ca, an \quad (29)$$

Where,  $P_{v,i}$  represents the water vapor pressure at different positions (kPa);  $P_{sat}$  represents the saturated water vapor pressure (kPa).

The electro-osmotic coefficient and the water-diffusion coefficient can be expressed by the following equations:

$$\begin{cases} n_d = 0.0029\lambda_m^2 + 0.05\lambda_m - 3.4 \times 10^{-19} \\ D_w = D_\lambda \exp\left(2416\left(\frac{1}{303} - \frac{1}{T}\right)\right) \end{cases} \quad (30)$$

Where,  $D_\lambda$  represents the diffusion coefficient of the exchange membrane, and the specific calculation method is as follows:

$$D_\lambda = \begin{cases} 10^{-6}, & \lambda_m < 2 \\ 10^{-6}(1+2(\lambda_m-2)), & 2 \leq \lambda_m \leq 3 \\ 10^{-6}(3-1.67(\lambda_m-3)), & 3 < \lambda_m \leq 4.5 \\ 1.25 \times 10^{-6}, & 4.5 < \lambda_m \end{cases} \quad (31)$$

### III. MODELING OF THE CATHODE SYSTEM

#### A. Air compressor model

The air compressor inputs compressed air into the stack, the inlet is the ambient pressure, the air compressor pressure is controlled by the motor speed, and the dynamic analysis of the air compressor is carried out. According to the mechanism method, the air compressor model is obtained as:

$$J_{cp} \frac{d\omega_{cp}}{dt} = \tau_{cm} - \tau_{cp} \quad (32)$$

Where,  $J_{cp}$  the moment of inertia of the air compressor ( $\text{kg} \cdot \text{m}^2$ );  $\omega_{cp}$  the angular velocity of the air compressor ( $\text{rad} \cdot \text{s}^{-1}$ );  $\tau_{cm}$  the motor torque ( $\text{N} \cdot \text{m}$ );  $\tau_{cp}$  the air compressor torque ( $\text{N} \cdot \text{m}$ ).

The above hollow compressor and air compressor motor torque can be calculated according to the following formula:

$$\begin{cases} \tau_{cp} = \frac{c_{Air} T_{amb} m_{Air}}{\eta_{cp} \omega_{cp}} \left( \lambda_{comp}^{\frac{k-1}{k}} - 1 \right) \\ \tau_{cm} = \frac{\eta_{cm} k_t}{R_{cm}} (u_{cm} - k_v \omega_{cp}) \end{cases} \quad (33)$$

Where,  $\eta_{cp}$ ,  $\eta_{cm}$  represent the efficiency of the air compressor and the motor of the air compressor;  $k_t$ ,  $k_v$  and  $R_{cm}$  represent the motor parameters of the air compressor;  $u_{cm}$  represents the input voltage of the air compressor motor.

The total efficiency  $\eta_T$  of the air compressor is the product of the motor efficiency and the compression efficiency of the air compressor:

$$\eta_T = \eta_{cm} \cdot \eta_{cp} \quad (34)$$

The outlet temperature of the air compressor can be calculated according to formula; the actual power of the air compressor  $W_{comp}$  is:

$$W_{comp} = \tau_{cp} \omega_{cp} \quad (35)$$

The relationship between the flow, speed and pressure ratio  $m_{cp} = f(\omega_{cp}, \lambda_{comp})$  of the air compressor is established according to the MAP map of the air compressor.

To make the air compressor modeling more realistic, the inlet air mass flow rate and the air compressor speed are corrected for:

$$\begin{cases} m_{cp,in} = \frac{m_{Air} \sqrt{\theta}}{\delta} \\ N_{cp,r} = \frac{N_{cp}}{\sqrt{\theta}} \end{cases} \quad (36)$$

Where,  $m_{cp,in}$  represents the corrected air compressor inlet mass flow ( $\text{kg} \cdot \text{s}^{-1}$ );  $N_{cp,in}$ ,  $N_{cp,r}$  are represents the rotational speed before and after correction (rpm);  $\theta$  represents the temperature correction coefficient, its value  $T_{amb}/298$ ;  $\delta$  represents the pressure correction coefficient, its value  $P_{amb}/101325$ .

#### B. Intercooler model

Assume that the air entering the intercooler is an ideal gas and that its mass flow rate does not change and the gas pressure does not change after passing through the intercooler. The change in temperature changes the humidity of the air flowing through it, so that the relative humidity of the air exiting the intercooler is:

$$\phi_{cooler,out} = \frac{P_{cooler,out} P_{v,amb}}{P_{amb} P_{sat}(T_{cooler,out})} = \frac{P_{cooler,out} \phi_{amb} P_{sat}(T_{amb})}{P_{amb} P_{sat}(T_{cooler,out})} \quad (37)$$

Where,  $\phi_{cooler,out}$  represents the relative humidity at the outlet of the intercooler (%);  $P_{cooler,out}$  represents the air pressure at the outlet of the intercooler (kPa);  $P_{sat}(T)$  represents the saturation pressure of water vapor at this temperature (kPa);  $\phi_{amb}$  represents the relative humidity of the air in the atmosphere (%).

The partial pressure of air and water vapor at the outlet of the intercooler is:

$$\begin{cases} P_{Air,cooler} = P_{cooler,out} - P_{v,cooler} \\ P_{v,cooler} = \phi_{cooler,out} P_{sat}(T_{cooler,out}) \end{cases} \quad (38)$$

Where,  $P_{Air,cooler}$  represents the partial pressure of dry air (kPa);  $P_{v,cooler}$  represents the partial pressure of water vapor (kPa).

The mass flow of air and water vapor at the outlet of the intercooler is:

$$\begin{cases} m_{Air,cooler} = \frac{1}{1 + \omega_{cooler}} m_{cooler,in} \\ m_{v,cooler} = m_{cooler,in} - m_{Air,cooler} \end{cases} \quad (39)$$

Where,  $m_{Air,cooler}$  is the mass flow of dry air ( $\text{kg} \cdot \text{s}^{-1}$ );  $m_{v,cooler}$  represents the mass flow of water vapor ( $\text{kg} \cdot \text{s}^{-1}$ );  $\omega_{cooler}$  represents the water content of the gas in the intercooler.

The gas water content in the intercooler can be expressed as:

$$\begin{cases} \omega_{\text{cooler}} = \frac{M_v P_{v,\text{cooler}}}{M_{\text{Air,cooler}} P_{\text{Air,cooler}}} \\ M_{\text{Air,cooler}} = y_{\text{O}_2} M_{\text{O}_2} + (1 - y_{\text{O}_2}) M_{\text{N}_2} \end{cases} \quad (40)$$

Where,  $M_{\text{Air,cooler}}$  is the molar mass of air in the intercooler ( $\text{g}\cdot\text{mol}^{-1}$ );  $M_{\text{O}_2}$  is the molar mass of oxygen,  $M_{\text{N}_2}$  is the molar mass of nitrogen.

### C. Humidifier model

It is assumed that the intercooler humidification water is used from the reactor cathode outlet and its temperature is equal to the reactor internal temperature and the air temperature entering the reactor is equal to the reactor temperature. Therefore, it is assumed that the temperature does not change during the humidification process of the intercooler, only the water content of the air changes, and the air flow and pressure also change. The mass flow of air after passing through the humidifier  $m_{\text{hum,out}}$  is:

$$m_{\text{hum,out}} = m_{\text{Air,cooler}} + m_{v,\text{hum}} + m_{v,\text{cooler}} \quad (41)$$

The gas pressure after passing through the intercooler  $P_{\text{hum,out}}$  can be expressed by the following formula:

$$\begin{cases} P_{\text{hum,out}} = P_{\text{cooler,out}} + P_{v,\text{hum}} \\ P_{v,\text{hum}} = \phi_{\text{hum}} P_{\text{sat}}(T_{\text{hum}}) \end{cases} \quad (42)$$

Where, it  $\phi_{\text{hum}}$  is the relative humidity in the intercooler.

The humidifier is connected to the reactor cathode inlet, and the relationship between the humidifier outlet and the reactor cathode inlet air is as follows:

$$\begin{cases} \phi_{\text{hum}} = \phi_{\text{ca,in}} \\ P_{\text{hum,out}} = P_{\text{ca,in}} \\ m_{\text{hum,out}} = m_{\text{ca,in}} \end{cases} \quad (43)$$

### D. Back pressure valve model

The gas and liquid water flow at the cathode outlet pass through the humidifier. Assuming that the liquid water flows through the humidifier and is completely discharged, only gas enters the backpressure valve. If the temperature of the back pressure valve is constant, the gas mass flow  $m_{\text{bp,in}}$  into the back pressure valve is:

$$m_{\text{bp,in}} = m_{\text{ca,out}} \frac{1 - \omega_{v,\text{ca,out}}}{1 - \omega_{v,\text{amb}}} \quad (44)$$

Where,  $\omega_{v,\text{ca,out}}$ ,  $\omega_{v,\text{amb}}$  represent the water vapor content in the cathode outlet and the atmosphere.

The ratio of the outlet to inlet pressure of the back pressure valve is:

$$\lambda_{\text{bp}} = \frac{P_{\text{amb}}}{P_{\text{bp,in}}} \quad (45)$$

Where,  $\lambda_{\text{bp}}$  represents the pressure ratio of the  $P_{\text{bp,in}}$  back pressure valve, which represents the inlet pressure of the back pressure valve (kPa).

The backpressure valve can be regarded as a nozzle with variable outlet area, which can be modeled using the nozzle model. The gas flow form at the outlet of the backpressure valve will vary according to the inlet and outlet pressure ratios, which is sub-critical flow when the pressure ratio is large, and critical flow when the pressure ratio is small, and the specific mass flow at the outlet of the back pressure valve  $m_{\text{bp,out}}$  is:

$$m_{\text{bp,out}} = \begin{cases} \frac{\theta_{\text{bp}} C_D A_{\text{bp}} P_{\text{bp,in}}}{\sqrt{RT}} \lambda_{\text{bp}}^{\frac{1}{k}} \sqrt{\frac{2k}{k-1} \left(1 - \lambda_{\text{bp}}^{\frac{k-1}{k}}\right)}, & \lambda_{\text{bp}} > \left(\frac{2}{k+1}\right)^{\frac{k}{k-1}} \\ \frac{\theta_{\text{bp}} C_D A_{\text{bp}} P_{\text{bp,in}}}{\sqrt{RT}} \sqrt{k} \left(\frac{2}{k+1}\right)^{\frac{k+1}{2(k-1)}}, & \lambda_{\text{bp}} \leq \left(\frac{2}{k+1}\right)^{\frac{k}{k-1}} \end{cases} \quad (46)$$

Where,  $\theta_{\text{bp}}$  represents the opening of the  $C_D$  back pressure valve, which represents the flow correction coefficient of the  $A_{\text{bp}}$  back pressure valve, which represents the outlet area of the back pressure valve.

The pressure of the gas entering the back pressure valve is:

$$\frac{dP_{\text{bp,in}}}{dt} = \frac{RT}{V_{\text{bp}} M_{\text{bp}}} (m_{\text{ca,out}} - m_{\text{bp,out}}) \quad (47)$$

Where,  $V_{\text{bp}}$  represents the volume of the cathode outlet pipeline ( $\text{m}^3$ )

## IV. MODELING THE ANODE SYSTEM

### A. Hydrogen circulating pump model

The function of the hydrogen circulation pump has been introduced above. The hydrogen circulation pump is connected to the anode outlet of the stack. Assuming that the gas entering the hydrogen circulation pump is of, the same nature as the anode outlet gas, and the inlet pressure is equal to the anode outlet pressure, the hydrogen circulation pump The mass flow is:

$$m_{\text{Hcp}} = m_{\text{bl}} \frac{\sqrt{T_{\text{Hcp}} / T_{\text{ref}}}}{P_{\text{Hcp}} / P_{\text{ref}}} \quad (48)$$

Where,  $m_{\text{Hcp}}$  represents the mass flow rate of the hydrogen circulating pump outlet ( $\text{kg}\cdot\text{s}^{-1}$ );  $m_{\text{bl}}$  represents the mass flow rate of the circulating pump under standard conditions ( $\text{kg}\cdot\text{s}^{-1}$ );  $T_{\text{Hcp}}$  represents the gas temperature entering the circulating pump (K);  $T_{\text{ref}}$  represents the reference temperature, whose value is 288 K;  $P_{\text{Hcp}}$  indicates the gas pressure (kPa) entering the hydrogen circulation pump;  $P_{\text{ref}}$  indicates the reference pressure, which is the standard atmospheric pressure.

The rotational angular velocity of the hydrogen circulating pump can be expressed by the following formula:

$$\omega_{\text{Hcp}} = \frac{\omega_{\text{bl}}}{\sqrt{T_{\text{Hcp}} / T_{\text{ref}}}} \quad (49)$$

Where,  $\omega_{Hcp}$  represents the rotational angular velocity of the circulating pump ( $\text{rad}\cdot\text{s}^{-1}$ );  $\omega_{bl}$  represents the rotational angular velocity of the circulating pump under standard conditions ( $\text{rad}\cdot\text{s}^{-1}$ ).

Standard hydrogen circulating pump has a dimension of 1 parameter  $\psi_{bl}$  and the correction parameter  $\phi_{bl}$  is expressed by the following formula:

$$\begin{cases} \psi_{bl} = \frac{c_{an} T \left[ \left( \frac{P_{Hcp,out}}{P_{Hcp,in}} \right)^{\frac{k-1}{k}} - 1 \right]}{1/2 U_{bl}^2} \\ \phi_{bl} = \frac{m_{Hcp}}{\pi/4 \rho_{an} d_{bl}^2 U_{bl}} \end{cases} \quad (50)$$

Where,  $\rho_{an}$  represents the anode outlet gas density ( $\text{kg}\cdot\text{m}^{-3}$ );  $d_{bl}$  represents the diameter of the circulating pump rotor (m);  $U_{bl}$  represents the top speed of the rotor blades  $U_{bl} = (d_{bl} \omega_{Hcp}) / 2$ .

The dynamic model of the hydrogen circulation pump can be expressed by the following formula:

$$J_{bl} \frac{d\omega_{bl}}{dt} = \tau_{bm} - \tau_{bl} \quad (51)$$

Where,  $J_{bl}$  represents the moment of inertia of the circulating pump ( $\text{kg}\cdot\text{m}^2$ );  $\omega_{bl}$  represents the angular velocity of the circulating pump ( $\text{rad}\cdot\text{s}^{-1}$ );  $\tau_{bm}$  represents the motor torque ( $\text{N}\cdot\text{m}$ );  $\tau_{cp}$  represents the circulating pump torque ( $\text{N}\cdot\text{m}$ ).

The power of the hydrogen circulating pump can be expressed by the following formula:

$$W_{Hcp} = \frac{\rho_{H_2} g H_p m_{Hcp}}{\eta_{bl} \eta_{bm}} \quad (52)$$

Where,  $\eta_{bl}$  and  $\eta_{bm}$  represent the efficiency (%) of the circulating pump and the circulating pump motor respectively.

In the above formula, the torque of the circulating pump and the circulating pump motor can be calculated according to the following formula:

$$\begin{cases} \tau_{bl} = \frac{c_{an} T m_{Hcp}}{\eta_{bl} \omega_{bl}} \left( \left( \frac{P_{Hcp,out}}{P_{Hcp,in}} \right)^{\frac{k-1}{k}} - 1 \right) \\ \tau_{bm} = \frac{\eta_{bm} k_{tl}}{R_{bm}} (u_{bl} - k_{v1} \omega_{bl}) \end{cases} \quad (53)$$

Where,  $k_{tl}$ ,  $k_{v1}$  and  $R_{bm}$  represent the parameters of the circulating pump motor;  $u_{bl}$  represents the input voltage (V) of the circulating pump motor.

### B. Model of pressure regulating valve

The pressure regulating valve is responsible for controlling the flow pressure into the anode hydrogen of the reactor, and its specific role has been introduced in the previous chapters. There are many types of pressure regulating valves, and in the

automotive PEMFC system more proportional regulating valves are used to regulate the hydrogen into the reactor. The principle of the proportional control valve is similar to that of the backpressure valve described above, and the proportional control valve is modeled by referring to the backpressure valve modeling process.

## V. MODELING OF WATER AND HEAT MANAGEMENT SYSTEM

### A. Radiator Model

The radiator is responsible for distributing the heat carried by the cooling water flowing through it to the environment. The temperature of the cooling water exiting the radiator can be expressed by the following equation:

$$\frac{dT_{rad,out}}{dt} = \frac{m_{cw} c_{water} (T_{rad,in} - k_{rad} T_{rad,out}) - Q_{rad,amb}}{\rho_{water} V_{rad}} \quad (54)$$

Where,  $T_{rad,in}$ ,  $T_{rad,out}$  represent the inlet and outlet temperature of the radiator (K);  $m_{cw}$  represents the mass flow of cooling water ( $\text{kg}\cdot\text{s}^{-1}$ );  $k_{rad}$  represents the heat transfer coefficient;  $Q_{rad,amb}$  represents the heat dissipation capacity of the cooling fan (W);  $V_{rad}$  represents the volume of the radiator ( $\text{m}^3$ ).

Heat sink and the environment for heat exchange mainly rely on cooling fans, cooling fans to accelerate the airflow on the surface of the heat sink to improve the efficiency of heat dissipation, the amount of cooling fan cooling is expressed as follows

$$Q_{rad,amb} = A_{rad} h_{rad} (T_{rad,in} - T_{amb}) \quad (55)$$

Where,  $A_{rad}$  represents the heat dissipation area of the radiator ( $\text{m}^2$ );  $h_{rad}$  represents the transfer coefficient of the cooling fan.

The expression of the cooling fan transfer coefficient is expressed by the fitting relation:

$$h_{rad} = -1.4495 m_{amb}^2 + 5.9045 m_{amb} - 0.1157 \quad (56)$$

Where,  $m_{amb}$  represents the air mass flow near the radiator.

The radiator power consumption power is expressed by the following formula:

$$W_{rad} = \frac{\rho_{Air} \eta_{fan} h_{rad} m_{amb}^3}{2\pi^3 r^6} \quad (57)$$

Where,  $\eta_{fan}$  represents the mechanical efficiency of the radiator fan (%), and  $r$  represents the radius of the radiator fan blade (m).

### B. Cooling water pump model

The cooling water pump is responsible for circulating the cooling water and is a very important component in the hydrothermal management system. Similar in structure to the hydrogen circulation pump, it consists of a pump head and a drive motor. When modeling the cooling water pump, refer to the hydrogen circulation pump modeling process.

C. Thermostat model

The thermostat is mainly responsible for the opening of the large and small circulation of cooling water, its structure is similar to the three-way valve, when the valve is fully closed, the cooling water flows completely through the small circulation; when the valve is fully open, the cooling water all flows through the large circulation; in the process of valve all open and all closed, the flow of cooling water flowing through the large circulation and small circulation is linearly related to the valve opening, which can be described by the following formula:

$$\begin{cases} m_{lc} = \theta_{ts} m_{cw} \\ m_{sc} = (1 - \theta_{ts}) m_{cw} \end{cases} \quad (58)$$

Where,  $m_{lc}$  represent the mass flow of cooling water ( $\text{kg} \cdot \text{s}^{-1}$ ) flowing to the large cycle;  $m_{sc}$  represent the mass flow of cooling water ( $\text{kg} \cdot \text{s}^{-1}$ ) flowing to the small cycle;  $\theta_{ts}$  represents the opening degree of the thermostat valve.

VI. PEMFC MODEL VALIDATION

Figure 2 shows the polarization curves of the single cell in the stack model and the experimentally measured polarization curves. From the figure, it can be seen that the polarization curves obtained by the model simulation and the experimental data are consistent with each other, and the error is small, within 3%. The voltage of the single cell decreases with the gradual increase of current density, and the rate of decrease is larger at the beginning and near the limit of current density, and smaller in the middle part. At the beginning, the voltage drop is mainly due to activation polarization loss. In the intermediate stage, the resistance loss caused by the internal resistance of the stack gradually increases. In the closing stage, the concentration polarization loss is rapidly increased by the difference in electrolyte concentration between the two ends of the electrode formed by the reaction.

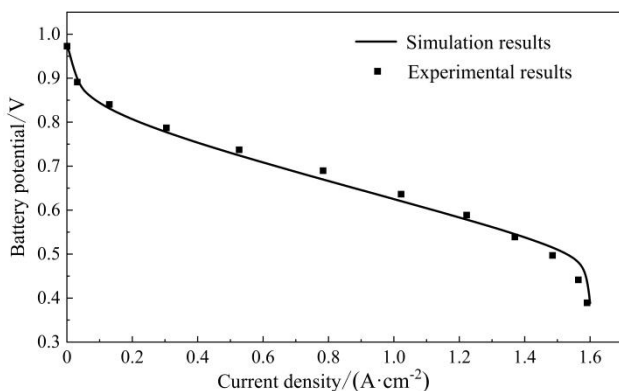


Fig. 2 Comparison of polarization curves between model and experiment

Figure 3 is the cell power density and cell efficiency curves of the stack model. It can be seen from the figure that with the increase of the current density, the power density of the battery first increases and then decreases, reaching a peak value of  $0.81 \text{ W} \cdot \text{cm}^{-2}$  when the power density is  $1.52 \text{ A} \cdot \text{cm}^{-2}$ , and then rapidly decreases. The change of the efficiency curve of the battery is similar to that of the polarization curve, the decline rate is larger at the beginning and the end stage,

and the decline rate in the middle part is smaller, from 83.87% to 35.77%. The cell efficiency is 54.82% under rated conditions, and the stack power density is  $0.66 \text{ W} \cdot \text{cm}^{-2}$ .

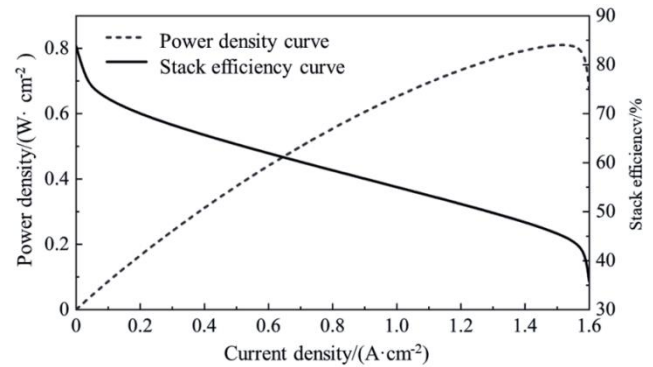


Fig. 3 Battery power density and efficiency curve

It can be seen from Figure 4 that the measured values of the output power and voltage of the stack are consistent with the simulated values, and the maximum errors are 3.6% and 4.1%, respectively. The error between the measured value and the simulated value of the power output by the system is within 5%. The output voltage of PEMFC decreases gradually with the increase of current, and decreases rapidly at the beginning, and then decreases more slowly, with the same trend as the first half of the polarization curve. Stack output power and system output power gradually increase with the increase of current, the system output power is always smaller than the stack output power, and the difference between the two gradually increased. The reason for this phenomenon is that the power output of the reactor has to be consumed by the auxiliary system, and the percentage of power consumed by the auxiliary system also increases gradually as the power increases.

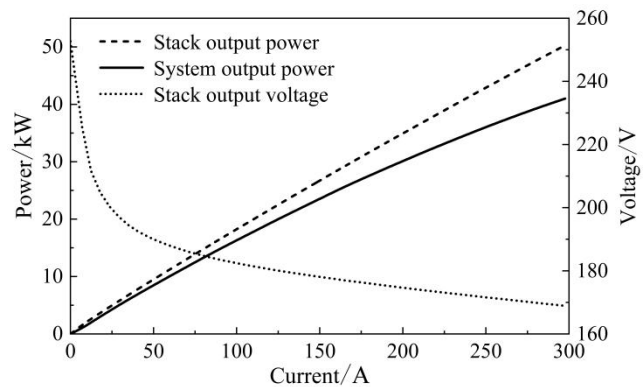


Fig. 4 Power and voltage curve of fuel cell

Figure 5 is a PEMFC system efficiency curve and hydrogen consumption rate curve. It can be seen from the figure that the maximum simulation errors of the PEMFC system efficiency and hydrogen consumption rate are 3.2% and 3.9%, respectively. With the increase of PEMFC efficiency, the system efficiency first sharply increased to a peak, and then decreased gradually. The highest efficiency of the system is 48.41 %, and the system efficiency is 39.78 % under rated conditions. The efficiency after simulation cannot meet the requirements of the system efficiency in Chapter 2, and the parameters of the PEMFC system need to be optimized. The hydrogen consumption rate increases



gradually with the increase of PEMFC power.

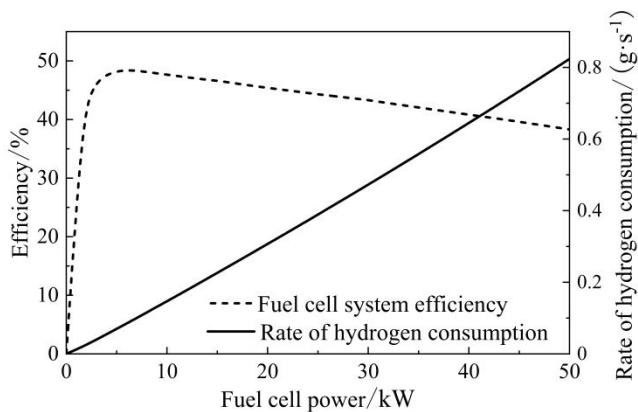


Fig. 5 Curve of fuel cell system efficiency and hydrogen consumption rate

## VII. CONCLUSION

In order to shorten the PEMFC development cycle and develop a high-precision and high-efficiency PEMFC performance analysis platform, this paper analyzes and mathematically models each subsystem and core component of PEMFC based on PEMFC mechanism analysis and empirical method. The reactor model includes voltage model, cathode and anode flow channel model, and membrane hydration model. The cathode subsystem model includes air compressor, intercooler, humidifier and backpressure valve core component models. Anode subsystem model includes hydrogen circulation pump, pressure regulating valve core component model. The hydrothermal management subsystem includes radiator, cooling water pump and thermostat core component models. On this basis, the established PEMFC model is validated and analyzed. The results show that the constructed mathematical model for PEMFC performance analysis can accurately simulate the PEMFC working process and output reasonable numerical results with the error within 5%, which meets the engineering development needs.

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