Study on data-driven PEMFC humidity mechanism soft-sensing model

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Abstract. Proton exchange membrane fuel cell (PEMFC) has a special closed structure, whose humidity cannot be measured directly. This paper selects the diffusion model as the modelling and analysis basis of the humidity mechanism soft-sensing based on the experimental research object. After the study of the basic principles of the diffusion model, a one-dimensional data-driven proton exchange membrane fuel cell humidity mechanism soft-sensing model is analysed and completed. At last, the actual experimental data drives the humidity mechanism soft-sensing model and the predicted output error based on the humidity mechanism soft-sensing model can be controlled within 3%. The output results verify the effectiveness of the humidity mechanism soft-sensing model.

1. Introduction
Proton exchange membrane fuel cell (PEMFC) is essentially an "inverse" device for water electrolysis [1-2]. As the "fuel", hydrogen enters and reaches the anode of the battery through a gas channel on the bipolar plate. As the "oxidant", oxygen or air enters and reaches the cathode of the battery through the air channel on the bipolar plate. Through the action of the catalyst, the hydrogen and oxygen molecules form water by electrochemical reaction respectively, and at the same time, the reaction release electrical energy and heat. The product of fuel cell is water, heat and electric energy, so that it will not pollute the environment, and it is a very clean energy.

When the fuel cell is operating, it needs to work under a certain humidity condition. The water content of the PEM polymer film will directly affect the voltage output. The proton conductivity of the polymer PEM depends on its internal water content, and the unhealthy humidity status of the film, which includes “dry” and “flooded”, will have negative effects on the performance of the fuel cell [3].

This paper selected the diffusion model as the modeling and analysis basis of the humidity mechanism soft-sensing based on the experimental research object [4]. After studying the basic principles of the diffusion model, then a one-dimensional data-driven proton exchange membrane fuel
cell humidity mechanism soft-sensing model was analyzed and completed. At last, the actual experimental data drove the humidity mechanism soft-sensing model. And the predicted output error based on the humidity mechanism soft-sensing model can be basically controlled within 3%. And which verify the effectiveness of the humidity mechanism soft-sensing model.

2. Humidity mechanism model experiment and soft measurement analysis

The operating principle of proton exchange membrane fuel cell is shown in figure 1. It has a special closed structure, whose humidity cannot be measured directly. As the only product of electrochemical reaction, the fuel cell generates water at the cathode by combining hydrogen and oxygen under the action of catalyst [5]. The water in PEMPC is usually in the form of gas and liquid. In addition to the water generated at the cathode through the electrochemical reaction, it should also contain the water brought in by the humidified reaction gas input at the cathode and anode. Proton exchange membrane is the core element of PEMFC. It provides a pathway for protons to migrate and transport from the anode to the cathode. However, proton transport process is carried out in the form of hydrated ions, so the membrane should have the right amount of moisture humidity.

![Figure 1. The operating principle of proton exchange membrane fuel cell](image)

Currently, there are many researches on water management models of proton exchange membrane, but most of them are realized around convection and transfer model, dust flow model, statistical mechanics model and diffusion model [6]. And all these models assume that the fuel cell system is stable, adiabatic, and one-dimensional.

In the preliminary work of this paper [7-8], four kinds of humidity mechanism models of various proton exchange membranes were analyzed and compared. And typical assumptions were compared, and conclusions and deficiencies of each model were analyzed. The results show that the diffusion model assumes that water is in equilibrium in the gas phase and the membrane phase, the membrane is uniformly wet and completely saturated with water, and the water dissolved in the membrane is mainly generated in the cathode by the electroinduced drag migration and electrochemical reaction. It is consistent with the actual situation of proton exchange membrane fuel cell operating state. Therefore, the research object in this paper is more suitable for applying the diffusion model.

2.1. Hypothesis of humidity mechanism model

In this paper, according to the basic idea of diffusion model, the basic mechanism model of water management of proton exchange membrane fuel cell is established by taking the diffusion model as the prototype mechanism. In all concrete analysis, some established hypothesis condition should be followed, which is shown in table 1.
2.2. Soft-sensing model analysis of humidity mechanism

In this paper, the rectangular coordinate system is used to build the soft-sensing model. In the proton exchange membrane, the direction from anode to cathode is defined as the X direction, and all parameters are set to change in the X direction, thereby a one-dimensional moisture diffusion mechanism model is established.

Table 1. Hypothesis conditions of humidity mechanism model

| No. | Postulated conditions |
|-----|-----------------------|
| 1   | The proton exchange membrane is completely hydrated. |
| 2   | The capillary phenomenon is ignored. |
| 3   | Regardless of the configuration of water, both liquid and gaseous water are considered as water molecules in gaseous form. |
| 4   | There is electroneutral in the membrane. |
| 5   | Fuel agent and oxidant gas are ideal pure gas. |
| 6   | The solubility of H2 and O2 in the flow channel and gas diffusion layer in the liquid water is neglected. |
| 7   | The bidirectional nature of water flow is not considered, and the water flows in one direction. |
| 8   | The battery temperature inside the battery is constant and evenly distributed. |
| 9   | The thickness of the diffusion layer is not considered. |
| 10  | The pressure of anode and cathode are uniform and equal distribution. |

From the water balance process of proton exchange membrane fuel cell, and according to the electroinduced drag migration, concentration difference reverse diffusion and pressure migration, there are:

\[
W_{\text{in}}^a - W_{\text{out}}^a = -W_{\text{drag}} + W_{\text{diff}} + W_{\text{pres}}
\]  

(1)

Where, \(W_{\text{in}}^a\) is anode humidifying water; \(W_{\text{out}}^a\) is the water which expelled from the anode in gaseous form; \(W_{\text{drag}}\) is the water of the electroinduced drag migration; \(W_{\text{diff}}\) is concentration difference reverse diffusion water; \(W_{\text{pres}}\) is the water coursed by pressure migration.

In the electroinduced drag migration process, there is:

\[
W_{\text{drag}} = n_d \frac{i A}{F}
\]  

(2)

If the activity of water is denoted as \(\alpha_w\), the electroosmosis coefficient can be calculated as:

\[
n_d = \begin{cases} 
0.0049 + 2.02\alpha_w - 4.53\alpha_w^2 + 4.09\alpha_w^3, & \alpha_w \leq 1 \\
1.59 + 0.159(\alpha_w - 1), & 3 \geq \alpha_w > 1 \\
16.8 \times \frac{2.5}{22}, & \alpha_w > 3
\end{cases}
\]  

(3)

In the concentration difference reverse diffusion process, there are:

\[
\begin{cases} 
W_{\text{diff}} = D_w \frac{\partial C_w^m}{\partial x} A \\
W_{\text{pres}} = n_d \frac{i}{F} - D_w \nabla C_w^m - C_w^m \frac{K_w}{\mu} \nabla P_w
\end{cases}
\]  

(4)

The diffusion coefficient \(D_w\) is:
$D_n = \begin{cases} 
[(0.0049 + 2.02\alpha_w - 4.53\alpha_w + 4.09\alpha^2_w)\times10^{+4}]\exp\left[\frac{241(1.1\alpha_w - 1)}{306}\right], & \alpha_w \leq 1 \\
[\left[1.59 + 0.159(\alpha_w - 1)\right]\times10^{-6}]\exp\left[\frac{241(1.1\alpha_w - 1)}{306}\right], & 3 \geq \alpha_w > 1 \\
[16.8\times10^{-6}]\exp\left[\frac{241(1.1\alpha_w - 1)}{306}\right], & \alpha_w > 3 
\end{cases}$

(5)

Take $\rho_m$ as the density of the membrane, and the unit is $kg \cdot cm^{-1}$; $EW$ is the molar mass of the membrane, and the unit is $g \cdot mol^{-1}$, then the water concentration in the membrane is expressed as:

$$C_w = \frac{D_w}{EW} \lambda$$

(6)

Set $\lambda$ as the water content of proton exchange membrane, then the water content of proton exchange membrane can be expressed as:

$$\lambda = 0.043 + 17.81\alpha_w - 39.85\alpha^2_w + 36.0\alpha^3_w$$

(7)

3. Humidity mechanism model and results analysis

According to the previous analysis and research of this paper, the basic humidity mechanism model of fuel cell is finally determined, as shown in figure 2.

Where, "F-H2" is the hydrogen flow rate, "P-H2" is the hydrogen pressure, "$P_{sat}$" is the saturated vapor pressure of water, determined by the reaction process,"P-O2" is the air pressure,"F-O2"is the air flow rate, and "I" is the working current. By adjusting the values of each input, the average water content output value "RH" described by the humidity mechanism model can be obtained. In this paper, when conducting soft-sensing research based on the mechanism model, the values of relevant parameters are shown in table 2.
Table 2. The values of relevant parameters

| No. | The parameter name       | The parameter value |
|-----|--------------------------|---------------------|
| 1   | The hydrogen flow rate   | 0.15 l/s            |
| 2   | The hydrogen pressure    | 700bar              |
| 3   | The air pressure         | 4 standard atmospheric pressure |
| 4   | The air flow rate        | 0.75 l/s            |
| 5   | The running current value| 30A                 |

The FuelCon Evaluator-C test platform is used as the hardware platform, the TrueData-EIS analyzer is used as the test tool, and the FuelWork software is used as the test software. According to the time sequence, the test data is obtained, and then the simulation data of the mechanism model is compared and analyzed. The experiment data comparison table is shown in table 3.

Table 3. The comparison table of the measured output data and the test data

| Time(s) | Test data | Output data | Time(s) | Test data | Output data |
|---------|-----------|-------------|---------|-----------|-------------|
| 0.00    | 0         | 0           | 3.60    | 0.530     | 0.536       |
| 0.20    | 0.156     | 0.134       | 3.80    | 0.538     | 0.536       |
| 0.40    | 0.195     | 0.167       | 4.00    | 0.531     | 0.536       |
| 0.60    | 0.225     | 0.200       | 4.20    | 0.526     | 0.536       |
| 0.80    | 0.242     | 0.219       | 4.40    | 0.535     | 0.536       |
| 1.00    | 0.264     | 0.245       | 4.60    | 0.542     | 0.536       |
| 1.20    | 0.291     | 0.283       | 4.80    | 0.546     | 0.536       |
| 1.40    | 0.324     | 0.333       | 5.00    | 0.532     | 0.536       |
| 1.60    | 0.363     | 0.371       | 5.20    | 0.538     | 0.536       |
| 1.80    | 0.395     | 0.400       | 5.40    | 0.529     | 0.536       |
| 2.00    | 0.431     | 0.421       | 5.60    | 0.540     | 0.536       |
| 2.20    | 0.458     | 0.443       | 5.80    | 0.536     | 0.536       |
| 2.40    | 0.491     | 0.476       | 6.00    | 0.524     | 0.536       |
| 2.60    | 0.509     | 0.486       | 6.20    | 0.536     | 0.536       |
| 2.80    | 0.526     | 0.513       | 6.40    | 0.525     | 0.536       |
| 3.00    | 0.541     | 0.526       | 6.60    | 0.534     | 0.536       |
| 3.20    | 0.538     | 0.532       | 6.80    | 0.538     | 0.536       |
| 3.40    | 0.536     | 0.536       | 7.00    | 0.530     | 0.536       |

According to table 3, the soft-sensing simulation results of the humidity mechanism model are obtained, as shown in figure 3. Where, the dotted line is the output value of the mechanism model, and the solid line is the actual test data.

Figure 3. Soft-sensing simulation results of humidity mechanism model

Figure 4. The Soft-sensing simulation test results error curve
Shown as table 3 and figure 5, after the fuel cell operating, the output results of mechanism model based on soft-sensing consistent with the test data curve. The error is within 2%, and most of them in less than 1%. However, the local data has appeared in the large deviation, especially in the early stages of beginning, whose maximum error closed nearly to 3%. The soft-sensing simulation test results error is shown in figure 4. This may be due to the uneven distribution of the gas at the beginning. And the final output of humidity is only 0.532, which may be caused by the small test current used in the mechanism model soft-sensing analysis.

4. Conclusions

In this paper, the humidity mechanism soft-sensing establishment and simulation results of a data-driven proton exchange membrane fuel cell are analyzed and studied. The specific works are as follows:

(1) According to the experimental research object, the diffusion model is selected as the modeling and analysis basis of the humidity mechanism soft-sensing.

(2) According to the basic principles of the diffusion model, a one-dimensional humidity mechanism soft-sensing model was designed and completed.

(3) According to the analysis of actual experimental data, the humidity mechanism soft-sensing model was driven and the predicted output error based on the humidity mechanism soft-sensing model can be basically controlled within 3%. The analysis results of measured data verify the effectiveness of the humidity mechanism soft-sensing model.

However, the design of this paper is under a lot of assumptions and conditions, the actual proton exchange membrane fuel cell humidity mechanism will be more complex and difficult, and worthy of being studied and explored continually.

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