Water Flooding Fault Management of PEMFC Based on Grey Prediction and Digital Twin

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Abstract

In view of the difficulty in predicting the water flooding fault of proton exchange membrane fuel cell (PEMFC), the flooding fault management of PEMFC was carried out based on grey system theory and five-dimensional digital twin framework. Firstly, the collected PEMFC anode gas pressure drop data are processed, and the extracted sample data are used to construct the original grey prediction sequence. The analysis shows that the grey prediction model can maintain a high accuracy both under normal condition and when there is flooding. In order to realize the fault management of PEMFC, the water flooding fault identification and self-healing strategy of PEMFC were determined based on the five-dimensional digital twin model, so as to realize the predictive maintenance of PEMFC for water flooding fault.

***Keywords**: Grey prediction, PEMFC, flooding fault, digital twin, mitigation strategies, predictive maintenance*

I. Introduction

In view of the energy and climate problems, "peak carbon dioxide emissions " and " carbon neutrality" have gradually attracted people's attention [1, 2]. In the energy and transportation industries, fuel cells are regarded as a "zero carbon emission" energy source [3]. Proton Exchange Membrane Fuel Cell (PEMFC) has been widely used in on-board Fuel cells due to its advantages of high energy efficiency, quick start in cold state and relatively low operating temperature [4, 5]. At present, many car enterprises, such as Toyota, Hyundai, SAIC and so on have developed a real car or test car. However, its internal reaction mechanism is complex, online fault diagnosis is difficult, and its life is difficult to predict, which leads to the slow commercialization progress [6]. Water flooding is one of the common failures in the operation of fuel cell. A small range of water flooding will affect the output power of fuel cell, while a long-term serious water flooding will cause irreversible damage to the fuel cell. At present, most of the monitoring strategies for flooding are after the occurrence of flooding, at which time the fuel cell may have been affected. Therefore, the prediction and self-healing strategies for PEMFC flooding faults are of great importance for extending the life of PEMFC and its commercial process [7]. Therefore, based on the theory of grey prediction and the method of Digital Twin, this paper will study the prediction and self-healing strategy of PEMFC flooding fault.

II. Grey Prediction Theory

Gray Model theory is a theory between "white Model" and "black Model". For uncertain problems, some information can be obtained through analysis, but the information is not enough for accurate mathematical modeling to carry out quantitative analysis, which is a kind of gray system [8]. Although the accurate quantitative relationships in water flooding fault evolution mechanism of the fuel cell can be solved by certain electrochemical and fluid dynamics analysis, however, in the actual reaction process, there are too many influencing parameters, and the quantitative relationship only conforms to the specific operating conditions. Therefore, it is impossible to carry out real-time monitoring due to the large amount of calculation during online monitoring. Therefore, for this

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gradually evolving flooding fault, this paper introduces the grey system theory, through the small sample to realize the flooding trend analysis, so as to realize the water flooding prediction.

2.1 Classical grey model

The classical grey model $GM(1,1)$ is mostly applicable to sample events without mutation [9]. Since the flooding of PEMFC is a gradual development process, the classical grey model is used to build the grey prediction model. The original sequence is constructed by collecting data on a regular basis:

$$x^{(0)} = (x^{(0)}(1), x^{(0)}(2) \cdots\cdots x^{(0)}(n)) \tag{1}$$

Accumulated generating operation (AGO) on $x^{(0)}$ and a new sequence $x^{(1)}(k)$ is obtained, where the k represents the first k items in (1).

Determine the background value:

$$z^{(1)}(k) = 0.5x^{(1)}(k) + 0.5x^{(1)}(k-1), k = 2,3,4\cdots \tag{2}$$

$GM(1,1)$ grey model and $GM(1,1)$ whitening equation are:

$$x^{(0)}(k) + az^{(1)}(k) = b \tag{3}$$

$$\frac{dx^{(1)}}{dk} + ax^{(1)} = b \tag{4}$$

Where, k is the sampling time series, a is the development coefficient, and b is the gray model action quantity. The values of the three can be calculated by the least square method, specifically as follows:

Define

$$Y = (x^{(0)}(2), x^{(0)}(3), \cdots, x^{(0)}(n))^T \tag{5}$$

$$u = (a,b)^T \tag{6}$$

$$B = \begin{bmatrix} -z^{(1)}(2) & 1 \\ -z^{(1)}(3) & 1 \\ \vdots & \vdots \\ -z^{(1)}(n) & 1 \end{bmatrix} \tag{7}$$

Then

$$Y = Bu \tag{8}$$

Using least square method

$$\tilde{u} = (a, \tilde{b})^T = (B^T B)^{-1} B^T Y \tag{9}$$

The prediction results of the grey model are as follows:

$$x^{(1)}(k+1) = (x^{(0)}(1) - \frac{b}{a})e^{-ak} + \frac{b}{a} \tag{10}$$

The prediction set of the event is obtained after inverse accumulated generating operation (IAGO):

$$x^{(0)}(k+1) = x^{(1)}(k+1) - x^{(1)}(k), k = 1, 2, 3, \cdots, n \tag{11}$$

2.2 Grey prediction model test

As the grey prediction model is a data-based method, it is unnecessary to fully consider the real quantitative relationship, so it is necessary to evaluate the quality of the grey prediction model to determine whether the grey prediction model is applicable. The main test methods include residual test, variance ratio test and small probability test [10].

(1) Residual test

The original sequence and the grey prediction sequence are used to make a difference to get the prediction residual sequence:

$$\begin{aligned} \varepsilon^{(0)} &= (\varepsilon_1, \varepsilon_2, \varepsilon_3, \cdots, \varepsilon_n) \\ &= \left\{ x^{(0)}(i) - x^{(0)}(i) \right\}, i = 1, 2, 3, \cdots, n \end{aligned} \tag{12}$$

$$Q = \frac{1}{n} \sum_{k=1}^{n} \frac{\varepsilon_k}{x^{(0)}(k)} \tag{13}$$

(2) Variance ratio test

Variance ratio $C = \frac{S_\varepsilon^2}{S_x^2}$, the ratio of residual sequence variance to original sequence variance is used to evaluate the model accuracy level.

(3) Small probability test

The method of probability statistics and residual error are used to evaluate the small probability events:

$$p = P\left\{ \left| \varepsilon_k - \bar{\varepsilon} \right| < 0.6745 S_1 \right\} \tag{14}$$

Where, S_1 is the standard deviation of the original sequence, 0.6745 is the radius of the confidence interval when the confidence level is 50%.

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The corresponding evaluation indexes of the three test methods are shown in Table 1.

Table 1 Accuracy test index of grey prediction model

Level	Residual test Q	Variance ratio test C	Small probability test p
1	< 0.01	< 0.35	> 0.95
2	< 0.05	< 0.50	< 0.80
3	< 0.10	< 0.65	< 0.70
4	> 0.20	> 0.80	< 0.60

III. Prediction of Flooding Trend Based On Grey Model

The water flooding of fuel cell is a complex and gradual process. The efficient operation of PEMFC cannot be achieved without a certain humidity on the membrane. However, excessive water content will cause water flooding, which will affect the output efficiency and even damage the fuel cell. For a long time, scholars have been trying to explore the characteristics of water flooding fault monitoring parameters. Restrepo et al. [5] made a detailed review on the use of e electrochemical impedance spectroscopy(EIS) method to monitor the changes of PEMFC impedance and the discrimination of water flooding state. However, when using electrochemical impedance spectroscopy to monitor fuel cells, peripheral devices are needed, which is not conducive to online monitoring and predictive maintenance of equipment. Pei et al. [11] used the gas pressure drop to monitor the flooding state, while Song [12] conducted a large number of experiments on the anode gas pressure drop and divided the development of cell flooding into four periods. Thus, the development of water flooding can be judged by the anode gas pressure drop, and good results have been achieved. Because the flooding process of PEMFC is a gradual process without abrupt change, it is feasible to predict the flooding trend based on grey prediction and anode pressure drop.

Two groups of experiments were set up, which were PEMFC running under normal condition and flooding fault. The anode gas pressure drop data is monitored and sampled every 100S, with a total of 18 sampling points collected, so as to construct the original series of anode gas pressure drop, and predict the flooded state by combining the grey prediction algorithm. The results of grey prediction are shown in Fig 1, and the residuals between the grey prediction series and the original series are shown in Fig 2, in which points 1-18 are sample sets, and the sample data come from [12] and 19-28 are prediction sets.

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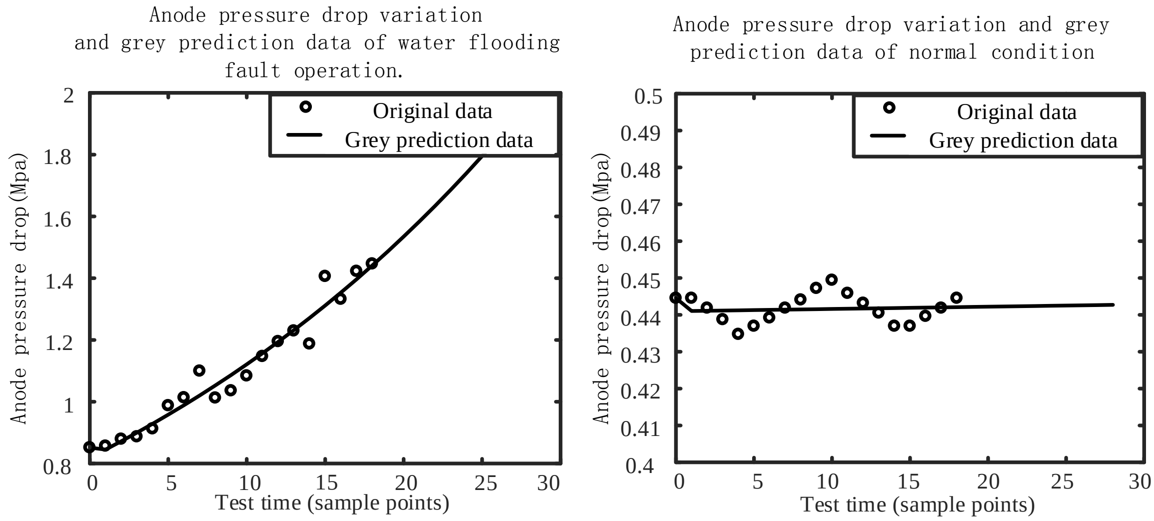

Fig 1: Results of grey prediction

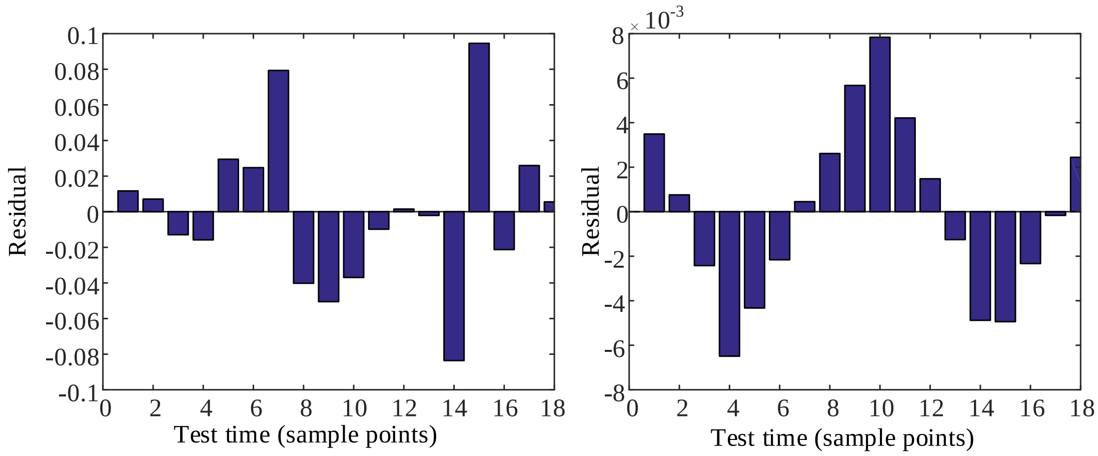

Fig 2: Residuals between the grey prediction sequence and the original sequence

The above test method is used to test the data of operation under normal state and water-flooding fault respectively. When operating under normal state, data are as follows: $Q_1 = 0.0069, M_1 = 0.4814, p_1 = 0.7206$ .When there is flooding, the data are as follows: $Q_2 = 0.0258, M_2 = 0.2124, p_2 = 1$. According to the accuracy test index of gray prediction model, the three indexes of gray prediction accuracy are Grade 1, Grade 2 and Grade 2 in normal state, and Grade 1 in case of flooding. Therefore, the gray prediction accuracy is relatively high in both cases and the results are credible.

IV. Water Flooding Fault Management Based on Digital Twin

4.1 Prediction of water flooding fault

Through experiments, Song et al. [12] found that the flooded process was divided into "proper period", "humid period", "transitional period" and "flooded period". Based on these four stages, the pressure drop of PEMFC in the experiment was divided into four regions, as shown in Fig 3, and the prediction process was shown in Fig 4.

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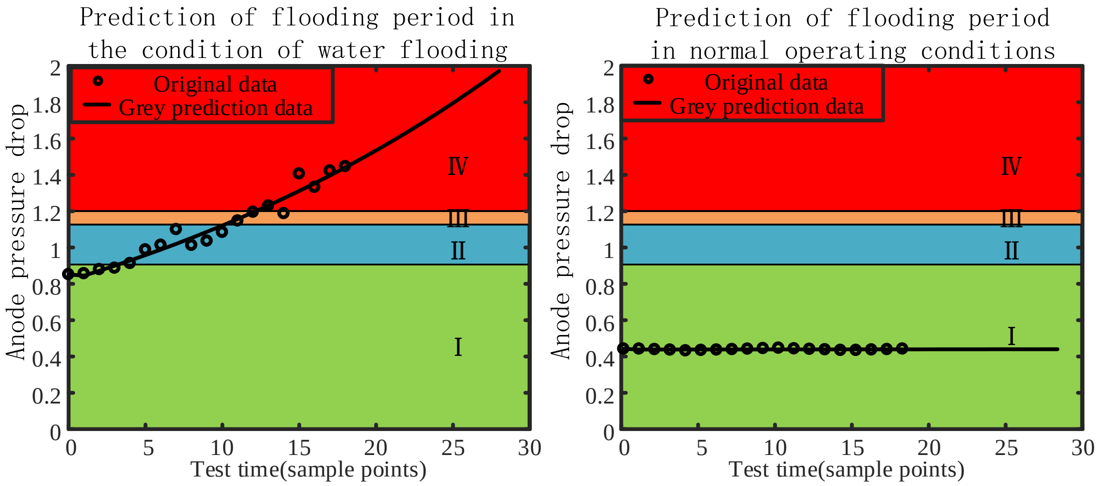

Fig3: Prediction of flooding period

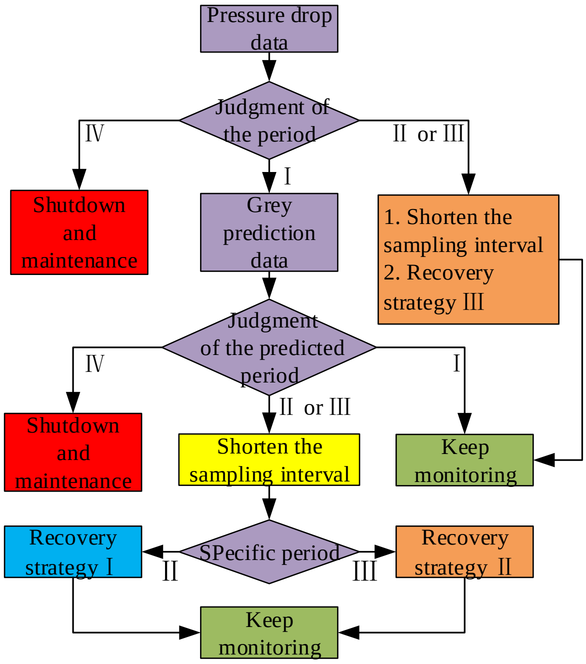

Fig4: Flooding fault diagnosis and prediction process

4.2 Recovery strategy of flooding fault

The PEMFC can be self-healing by controlling the components of its system in the event of minor flooding failures [13]. The composition of PEMFC assembly is shown in Fig 5. There are many researches on self-healing of PEMFC flooding fault. The common methods are pulse exhaust, increasing the temperature of the stack and reducing the power of humidifier. According to the four stages of flooding, the severity of flooding is distinguished. In the proper period, the humidity on the membrane is suitable, the electron transmission rate is the highest, and the working efficiency of PEMFC is also the highest; During the humid period, the humidity on the membrane is high, but there is still no droplet aggregation in the flow channel, and the working efficiency of PEMFC begins to decline, but it is not obvious; During the transitional period, droplets that can be blown away are formed in the flow channel, and liquid aggregation also occurs in the gas diffusion layer (GDL) and microporous layer (MPL), and the polarization curve of PEMFC is greatly deviated, and the output power decreases; During the flooding period, water masses are formed in the flow channel, and PEMFC may be damaged if it continues to work.

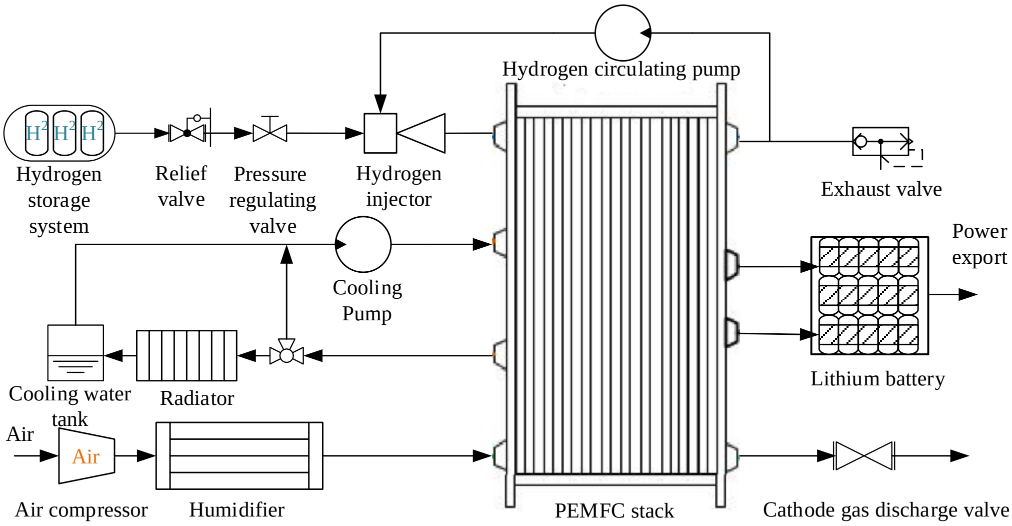

Fig 5: Schematic diagram of PEMFC system components

And different failure recovery strategies are set, specifically:

Recovery strategy Ⅰ: The humidifier stops working and reducing the power of the cooling system to increase the temperature of the PEMFC stack.

Recovery strategy Ⅱ: On the basis of recovery strategy I, the control is improved by the control of the anode side valve to improve the anode gas excess coefficient.

Recovery strategy Ⅲ: Pulse exhaust is carried out to purge water droplets in the flow passage, and recovery strategy II is implemented at the same time.

4.3 Construction of water flooding fault management model based on digital twin

Tao et al. [14] proposed a five-dimensional digital twin model that includes physical entity(PE), virtual entity(VE), digital twin data(DD), service system(SS) and connection(CN). In the process of development, the concept of digital twin has been gradually applied to different fields, among which a relatively important part is predictive maintenance of equipment [15, 16]. The water flooding management model based on digital twin can be constructed for monitoring prediction and recovery strategy of water flooding fault in PEMFC. Each part is as follows:

PE: PEMFC system, which uses sensors to collect basic physical parameters.

VE: PEMFC finite element model, which takes the basic physical parameters of the physical entity as boundary conditions to build a digital image of dynamic iteration with the physical entity.

DD: save data parameters in the process of running by physical entity and virtual entity.

SS: man-machine interaction, based on physical entity and virtual entity, diagnose flooding fault, use grey prediction to predict flooding fault, and adjust and control corresponding system components in physical entity according to preset self-healing strategy.

CN: mutual data connection between the first four parts.

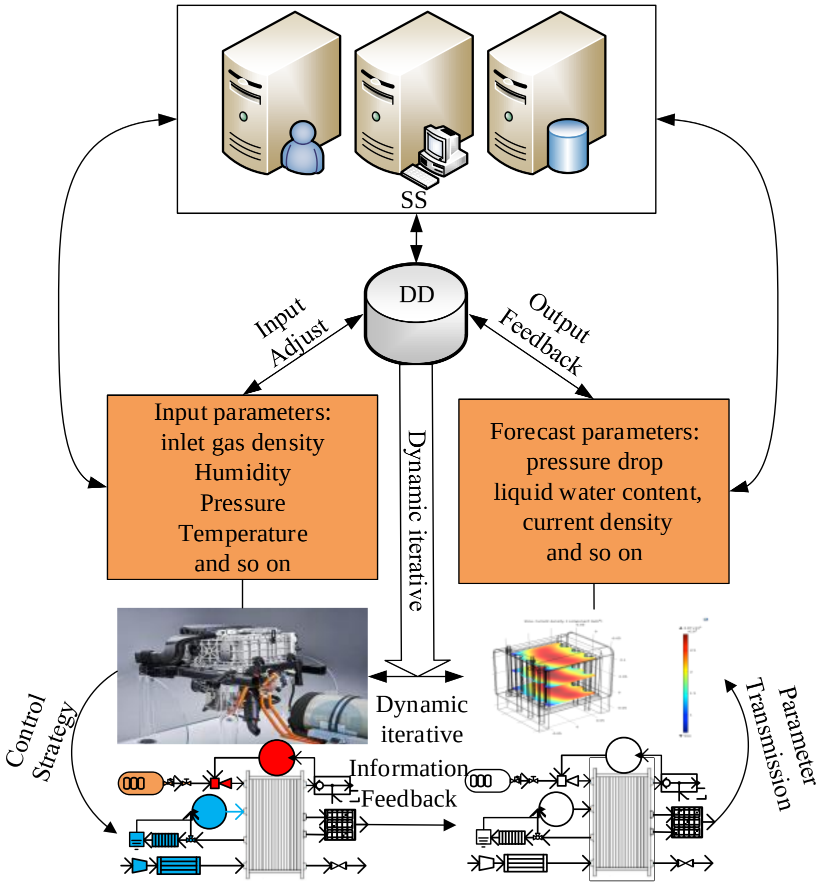

Fig 6: Flooding fault management model based on digital twin

V. Conclusion

In view of the problem that the water flooding fault of PEMFC seriously affects its operation life and is difficult to monitor online, the grey model is used to predict the anode gas pressure drop, and the PEMFC flooding fault management model based on grey prediction and digital twin is constructed by combining the framework of digital twin.

As the flooding process of PEMFC is a gradual process, through the evaluation of the grey prediction model, it can be concluded that the grey prediction model is able to maintain a high accuracy in the normal state and in the state of flooding fault occurrence, and can meet the requirement of flooding fault prediction. The analysis of the results has been shown in the figure

With the four stages of flooding development as the threshold, four regions are set. When the actual value and the predicted value fall into different areas, the digital twin service system chooses different recovery strategies, so as to realize the self-healing of PEMFC when it is slightly flooded and the emergency shutdown when it is seriously flooded.

The PEMFC flooding fault management model based on grey prediction and digital twin is different from the simple model-based or data-based fault monitoring method, and is more conducive to the implementation of online monitoring and fault prediction. However, under complex variable load conditions, the pressure drop change will no longer be a smooth gradual change process, and the use of the traditional grey prediction model will be limited to some extent, which needs further optimization.

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