A Comparative Study of SIMULINK 1D Dynamic Model and FLUENT 3D Model for PEMFC Faults Diagnosis

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Abstract—**According to the different research platforms of PEMFC (Proton Exchange Membrane Fuel Cell) faults diagnosis, experimental diagnostics and mathematical modeling are employed in the characterization and determination of fuel cell performance. The methods based on mathematical modeling are promised on establishing a suitable model, which is capable to reflect the physical properties of actual fuel cell stack as accurate as possible. Further, a scientific and reasonable PEMFC model is also indispensable for the system performance analysis, design, control, and optimization. Generally, PEMFC auxiliary system adopts a lumped parameter model to provide the boundary conditions of stack, such as current demand, gas flow rate, pressure, and temperature. As PEMFC stack needs to be embedded particular faults in a specific time and space position, it necessitates adopting a distributed parameter model in one dimensional (1D), two dimensional (2D) or three dimensional (3D). In this paper, a comparative analysis is carried out between a diagnostic one dimensional dynamic model by MATLAB/SIMULINK and a diagnostic three dimensional distributed parameter model based on FLUENT. Also, the diagnostic results in specific faults are studied.**

Index Terms—**SIMULINK 1D dynamic model; PEMFC; FLUENT 3D model; Faults Diagnosis**

I. INTRODUCTION

The study of PEMFC diagnosis can be classified into the methods based on experimental diagnostics and mathematical modeling. The methods based on experimental diagnostics have the drawbacks of high experimental cost, complex operation conditions, poor stability, and the requirements of certain precision instruments. Also, due to the fuel cell manufacturing process, the big errors possibly exist in experimental data. Thus, the research of this paper is model-based. Establishing a scientific and reasonable PEMFC model is indispensable for the system performance analysis, design, control, optimization and faults diagnosis. Additionally, the advantages of a theoretical method are that the results have universality and the various influencing factors are clearly visible. Mathematical modeling is a theoretical basis of guiding the experiment research and verifying a new numerical calculation method [1].

The diagnostic approaches based on mathematical modeling are promised on establishing an appropriate model. Besides, the typical faults types can be embedded in specific positions of the model. Then, identify the faults by using a relevant digital signal processing method. Further, the contrast experiments are taken to make the corresponding methods validation, and finally reach the purpose of fuel cell faults diagnosis. Currently, according to the relationship between model parameters and spatial positions, the fuel cell models can be divided into lumped parameter model and distributed parameter model; according to the dimension, the fuel cell models can be divided into 0D, 1D, 2D, and 3D model.

For the researches of distributed parameter models, Zhou Su et al. [2] built a 1D stack model which can reflect the single cell difference, and detailedly analyzed the dynamic characteristics of important parameters (temperature, water content and output voltage, etc.) in special conditions (such as starting, braking and idling, etc.); By a 2D model, Sun W et al. [3] studied the the influences of flow channel length/width changes on the reaction in cathode catalyst layer; Using a 3D model, Wang C Y et al. [4] studied the the influences of straight channel, cross channel, and S-shaped channel on fuel cell performance; By building a 3D PEMFC stack model, Zhai S et al. [5] analyzed the influences of interior temperature distribution on voltage non-uniformity from the mechanism. For the researches of PEMFC faults diagnosis, Karimi G et al. [6] studied the cathode 'flooding' phenomenon in fuel cell stack; Kadyk T et al. [7,8] studied the dynamic characteristics in different conditions (such as anode CO poisoning, membrane dehydration, and flooding) when a non-linear frequency is superimposed. Pei, the author of this paper, et al. [9] studied the typical faults identification and classification (such as temperature fault, membrane dehydration fault, and inlet flow inefficiently supplying fault) of a PEMFC system based on a semi-empirical distributed parameter stack model.py.

II. DIAGNOSTIC SIMULINK 1D DYNAMIC MODEL AND SIMULATION

The variables of lumped parameter model are uniform in the system and unrelated with space position. For steady state, the equations are algebraic. For dynamic, they are ordinary differential equations. PEMFC auxiliary system can be found by the lumped parameter model. For distributed parameter model, at least one variable must relate to spatial location. For steady state, the model uses ordinary differential equations with space independent variable. For dynamic, they are partial differential equations with space and time independent variables. Due to the requirements of embedding typical faults at a specific time and space position, fuel cell stack simulation mainly uses the distributed parameter model.

A PEMFC dynamic distributed parameter model is established, which the stack has 60 cells divided into 15 modules and each module contains 4 cells with no performance difference. Each single cell of the model has 5 control volumes: collector, cooling channel, anode gas channel, MEA+GDL and cathode gas channel.

According to the temperature dynamical equation, mass conservation equation, pressure drop/initial flow equation, and single cell voltage equation as shown in equation (1-4)

$$\sum m_{i,k}^{r} Cp_{i,k}^{r} \cdot \frac{dT_{i,k}}{dt} = Q_{i,k}^{M} + Q_{i,k}^{amb} + Q_{i,k}^{ex} + S_{i,k} \qquad (1)$$

$$Mm^{j} \frac{dn_{i,k}^{j}}{dt} = M_{i,k}^{j\_in} - M_{i,k}^{j\_out} - M_{i,k}^{j\_re} \qquad (2)$$

$$\Delta P = K^{'} q_{0}[(\frac{1-e^{-\alpha l_{c}}}{\alpha}) + \sum_{i=0}^{m} 2 l_{e} e^{-\frac{i\alpha l_{c}}{m+1}}] \qquad (3)$$

$$E_{i} = E_{i}^{0} + \eta_{i}^{c} - \eta_{i}^{a} - \eta_{i}^{ohm} \qquad (4)$$

Where Q^{M} represents the heat caused by material flow, Q^{amb} represents the heat generated by heat exchange between control volume and air, Q^{ex} represents the heat generated by heat exchange between adjacent control volumes, Cp is specific heat capacity, m is mass and S is a source item; $n_{i,k}^{j}$ represents the component molar weight of a single cell, j represents H2,O2,N2 or H2O, $M_{i,k}^{j\_in}$ represents the inlet mass velocity of each component, $M_{i,k}^{j\_out}$ represents the outlet mass velocity of each component, $M_{i,k}^{j\_re}$ represents the reaction velocity of reactive gas; ΔP represents the pressure drop when fluid runs through the channel, K is frictional drag coefficient, q_0 is initial volume flow, α is fluid consumption ratio constant, lc is the length of single cell channel, le is local resistance equivalent length; Ei is single cell voltage, E_{i}^{0} is ideal open-circuit voltage, η_{i}^{c} is cathode polarization voltage, η_{i}^{c} is anode polarization voltage and η_{i}^{ohm} is Ohms voltage.

In view of the key equations upon, a PEMFC stack model is built up by MATLAB/SIMULINK, as shown in Fig.1. The PEMFC dynamic distributed parameter model provides a basis of diagnosis.

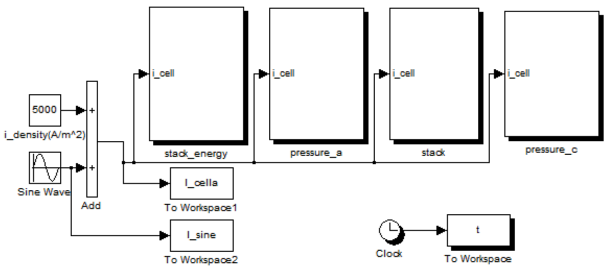

Figure 1. PEMFC stack model schematic diagram.

III. DIAGNOSTIC FLUENT 3D DISTRIBUTED PARAMETER MODELING AND SIMULATION

According to the mass conservation equation, momentum conservation equation, component conservation equation, energy conservation equation, and source term equation as shown in equation (5-9), a 3D PEMFC stack model is built up by Gambit & Fluent, as shown in Fig.2.

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \vec{u}) = 0 \qquad (5)$$

$$\frac{\partial(\rho \vec{u})}{\partial t} + \nabla(\rho \vec{u}\vec{u}) = \nabla(\mu \nabla \vec{u}) + S_{\vec{u}} \qquad (6)$$

$$\frac{\partial(\rho Y_{i})}{\partial t} + \nabla(\rho \vec{u} Y_{i}) = \nabla \cdot (D_{i} \nabla Y_{i}) + S_{Y_{i}} \qquad (7)$$

$$\frac{\partial(\rho T)}{\partial t} + \nabla \cdot (\rho \vec{u} T) = \nabla(\frac{k}{C_{p}} \nabla T) + S_{T} \qquad (8)$$

$$S_{\vec{u}} = -\frac{\mu}{K} \vec{u} \qquad (9)$$

Where ρ represents the density, is the velocity vector, μ is the coefficient of viscosity, S is the source item, Y_i is the component mass fraction, k is the thermal conductivity, C_p is the isobaric heat capacity; K is the permeability coefficient.

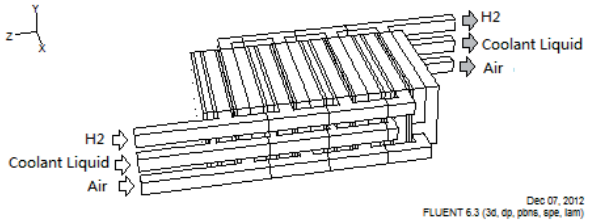

Figure 2. 3D PEMFC model based on FLUENT

The structural, physical property and operating parameters of the 3D distributed parameter model is as shown in Table 1. The 4-cells model employs Fuel Cell Modules in Fluent software and its dynamic boundary conditions and embedded faults are solved by UDF (User-Defined Function). UDF programming must use C language, and its internal communication with Fluent module must through predefined macro to achieve [10].

IV. RESULTS AND COMPARATIVE ANALYSIS

The research of faults diagnosis is based on AC polarography, which the input current is superimposed by an AC small signal with specific pattern and the system response will be analyzed [11]. Further, by signal processing, the signal features will be extracted and identified to diagnose the faults.

Using the 1D dynamic model, several typical faults, such as temperature fault, membrane dehydration fault, and inlet flow inefficiently supplying fault, have been classified. The comparison of stack voltages and their linearity is as shown in Figure 3. According to the simula-

TABLE I.
STRUCTURAL, PHYSICAL PROPERTY AND OPERATING PARAMETERS

Structural Parameters: Width/ Height/Length (mm)	Value	Physical Property and Operating Parameters	Value
Terminal Plate	20/10/2	Excess Coefficient: anode/cathode	2
Channel	20/6/2	Temperature (K) :anode/cathode	353
GDL	20/10/0.3	Inlet Pressure (atm) :anode/cathode	2
Catalyst Layer	20/10/0.01	Open-circuit Voltage (V)	1.147
PEM	20/10/0.04	Conductivity(S/m) PEM/GDL/Catalyst Layer	1×10^{-16}/5000/5000/ 3.5×10^{7}
Single Cell	20/10/8.66	Reference Current Density(A/m^3) Anode/Cathode	$1\times10^{9}/3\times10^{3}$
		Diffusion Coefficient (m^2/s) H2/H2O/O2	$1.1\times10^{-4}/7.35\times10^{-5}/3.2\times10^{-5}$
		Coefficient of Resistance($1/m^2$) GDL/Catalyst Layer	5.68×10^{10}

tion results, the output voltages under faulty conditions are different from normal operation, combined with the range of their linearity, the faults can be judged (the linear slope: trouble-free stack: - 0.0154, temperature fault: - 0.0305, membrane dehydration fault: - 0.037, inlet flow inefficiently supplying: 0.0535), however, the fault types cannot be identified hereby.

Further, based on the stack voltages from 18 simulation experiments for 3 faults types, combining the Wavelet Packet Analysis Method, a characteristic quantity named Ne (Normalized Energy Value) is constructed in different faults, as shown in Figure 4. By setting the ranges of (0.333-0.33304), (0.3329-0.333), three typical faults (temperature fault, membrane dehydration fault, and inlet flow inefficiently supplying fault), which are produced by SIMULINK 1D model, can be distinguished.

The advantages of diagnosis by SIMULINK 1D simulation are: 1) easily build the PEMFC system model with auxiliary system, which can strongly reflect the dynamic characteristics of system response; 2) the simulation process is relatively fast (simulation time: 120 s, the running time will be 0.5 hour). The drawbacks of the simulation are: 1) the PEMFC stack can hardly be embedded the faults in mechanism; 2) the results of the faults identification are a little bit less obvious, which is as shown in Figure 4.

In the meantime, by the simulation results of FLUENT 3D distributed parameter model, not only the polarization curve, pressure drop and voltage & current maps can be obtained for relevant diagnostic studies, but also the space distributions of various vital parameters (such as temperature, current density, the fractions of hydrogen, water, and oxygen) can be displayed and studied. As Figure 5 shows, they are the voltage distributions at cathode current plates for every single cell. The range of voltage values is from 4.5V to 8.5V. The distribution is non uniform and the voltages along the edge are higher than in the middle position. By our research and refer to reference [12], This distribution is caused by 'Skin Effect', that is when the alternating current (ac) through the conductor, current density/voltage is not uniform distribution in the cross sectional area, but tend to the edge of the plate, thus, the voltage values at the edge are greater than the values in the intermediate position. This kind of skin effect has a significant impact on fuel cell performance and lifetime.

Generally, the FLUENT distributed parameter model is mainly used for the research in steady state. Through the development of UDF, the author etc. compiled the dynamic boundary conditions and internal physical parameters in order to embed faults, such as cathode gas

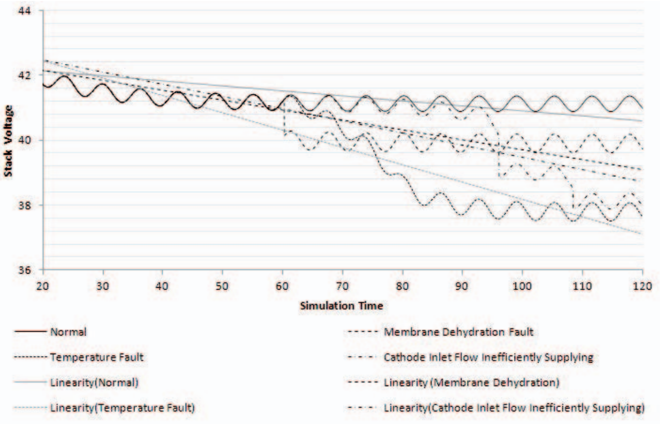

Figure 3. Comparison of Stack Voltages and their Linearity

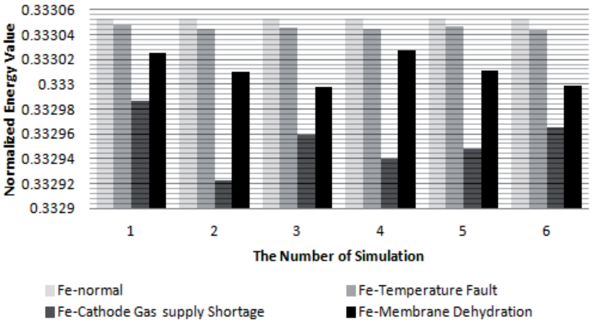

Figure 4. Comparison of Normalized Energy Values in Three Typical Faults

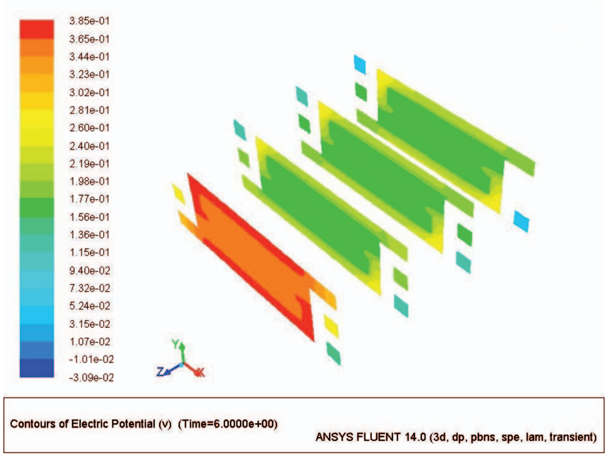

Figure 5. Voltages Distribution at Cathode Current Plates

supply shortage and the porosity setting of membrane, etc; Additionally, by changing the physical structure of the model, such as changing the thickness of the diffusion layer, the author etc. carried on the analysis of the relevant factors. As Figure 6 shows, in the fault of cathode gas supply shortage, the normal voltage and the fault voltage are evaluated, combined with the trend lines, the fault can be identified (the linear slope: trouble-free stack: 0.0018, inlet flow inefficiently supplying: 0.0004). Also, the output voltages from FLUENT 3D model and SIMULINK model are compared. The result shows that the voltage from SIMULINK model is excessively idealistic and the outputs from FLUENT model are more close to the real.

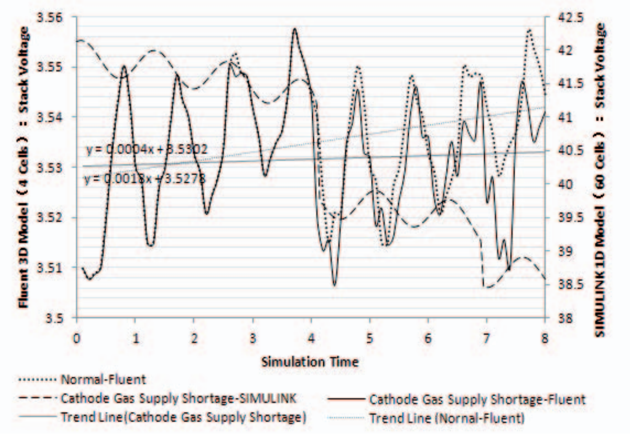

Figure 6. Stack Voltages Comparison in Cathode Inlet flow Inefficiently Supplying

According to the 3D distributed parameter model, the dehydration fault and the inlet flow inefficiently supplying fault have been studied. The advantages of diagnosis based on FLUENT 3D simulation are: 1) the faults caused by PEMFC physical property parameters, such as porosity, diffusivity of membrane etc., can be embedded in mechanism 2) the model provides sufficient space information and the physical quantities information varying with space. The drawbacks of the simulation are: 1) this type of models mainly aims at steady-state condition, however, most problems of dynamic boundaries are solved by UDF; 2) modeling and calculation process is complicated and the simulation duration is relatively long (Using a computer with Pentium(R)Dual-Core CPU:E5200 @ 2.5Hz & RAM:2.98GB, simulation time: 8 s, Step-length: 0.1s, iterations of each step: 400, the running time will be 45-50 hours.

V. CONCLUSION

The paper has compared the modeling methods and simulation process between a diagnostic 1D dynamic model by MATLAB/SIMULINK and a diagnostic 3D distributed parameter model based on FLUENT. Both of them have their own advantages and disadvantages respectively. Moreover, both of the stack voltage outputs in a specific fault have been comparatively analyzed. Accordingly, the conclusion is as follows: 1) For the modeling, the SIMULNK model is easier to be established and the faults are easier to be embedded; However, the FLUENT model can be embedded the faults in mechanism according to the physical property; 2) For the simulation Process, the dynamic response of the SIMULINK model is better and the simulation time is shorter, when the computational procedure of the FLUENT model is more complex and a computer with strong calculation ability is needed; 3) For the simulation and diagnosis results, as the results of the FLUENT model can preferably reflect the influences and conditions of physical factors, the results are more accord with reality.

For further works, a Diagnostic Collaborative Simulation Platform (COSIM), which synthesizes the benefits of SIMULINK dynamic model and FLUENT distributed parameter model, will be built. Additionally, combined with experimental data, a real-time faults diagnosis method using the COSIM will be put forward.

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