

A Dynamic Model and Simulation for Describing the Transient Phenomena in a Small PEM Fuel Cell System

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Abstract: Mathematic model is an efficient tool to understand and analyze fuel cell system, and studies on modeling are important to the development and research of the proton exchange membrane fuel cells (PEMFC) technology. In this paper, we will introduce a dynamic model for describing the transient phenomena in a PEM Fuel Cell System. This model can predict the transient response of cell voltage, reactant flow rate and pressure. SIMULINK is used for the simulation of the model and the transient response of the system to step changes in the load current and the reactant flow rate are presented. The simulation results are analyzed and compared to benchmark results and there is a good agreement between tests and simulations. It shows that this model is useful for the optimal design and real-time control of PEM fuel cell systems.

Keywords: Proton Exchange Membrane Fuel Cells (PEMFC); transient phenomena; dynamic modeling; control and simulation.

1. INTRODUCTION

Fuel cells operate like a battery by converting the chemical energy from the reactants into electricity. They offer a highly efficient and environmentally friendly option for energy conversion. They are widely regarded as commercial stationary power generation, residential applications and transportation technologies, especially in ground vehicle applications.

In order to use the fuel cell system in an effective way, mathematical models of the fuel cell are necessary. The model capable of predicting transient dynamics will be useful to prescribe internal design modifications and the subsequent design and analysis of model-based control systems.

Despite a large number of publications on fuel cell modeling, there are few suitable for control studies. Some publications have been seen in the literature on steady-state fuel-cell modeling^[1-2]. These studies are mostly based on empirical equations or the electrochemical reactions inside the fuel cell. In recent years, some scholars have studied the dynamic modeling of fuel cell with emphasis on the electrical terminal characteristics^[3-4]. Moreover, a few publications^[5-6] focused on the dynamics of the air supply system and their influence on the fuel cell system behavior. Though Pukrushpan^[7] proposed a fuel cell system-level dynamic model by incorporating the dynamic property of fluid flow through anode and cathode channels, it has neglected the effects of charge double layer capacitance.

Building on these modeling studies and the experiment results on the fuel cell testbench of our laboratory, a fuel cell system-dynamic model capable of

describing transient phenomena is introduced in this paper which includes the main dynamic aspects: the effective of temperature, fluid flow changes through channels and capacitor effect of charge double layer. The simulation result of this model shows good agreement with test results. This model is tested to be very useful for the optimal design and real-time control of PEM fuel cell systems.

2. TESTBENCH

The testbench described in this section was designed, constructed and demonstrated in a project by the Institute of Automation of Chinese Academy of Sciences. All the experiment results used in the model are based on this testbench.

The fuel cell testbench is consisted of air compressor, hydrogen tank, PEM fuel cell stack, humidifier, electrical load and all kinds of sensors (Fig.1).



Fig.1 Testbench

The PEM fuel cell stack is made up of 24 cells with an active area of 160cm^2 . Under optimal conditions with regard to pressure, humidity, reactants flow and temperature the electrical output capability of the stack is 1KW. The cells are electrically connected in series. In the cathode, the air entering the cathode channel is controlled by a gas mass flow meter. Similarly, the hydrogen entering the anode channel is also controlled by a gas mass flow meter.

3. SYSTEM DYNAMIC MODEL

The dynamic model mainly includes gas mass flow meter sub-model, fuel cell stack sub-model, charge double layer capacitance sub-model and flow dynamic of the anode channel and cathode channel. Since the response of the stack temperature is relatively slow ($\sim 10^2$ s), the temperature is considered in this model. Temperature effects can be modeled in a separate model and should be handled by a separate controller.

3.1 Gas mass flow meter model

In this PEMFC system we use two gas mass flow meters to control the inlet mass flow rate of the air and hydrogen respectively. The relation between the gas flow rate and the input voltage of mass flow meter is one-order inertia type, that is:

$$W_{air} = \frac{k_1}{\tau_1 s + 1} v_{air}; \quad W_{H_2} = \frac{k_2}{\tau_2 s + 1} v_{H_2} \quad (1)$$

where k_1, k_2 are proportional constants and τ_1, τ_2 are time constants, v_{air} and v_{H_2} are given voltage of the flow meter of air and hydrogen.

3.2 Fuel cell stack model

PEM fuel cell is electrochemical devices that convert the chemical energy of a reaction directly into electrical energy. A schematic representation of a fuel cell with the reactant product gases and the ion conduction flow direction the cell is shown in Fig. 2.

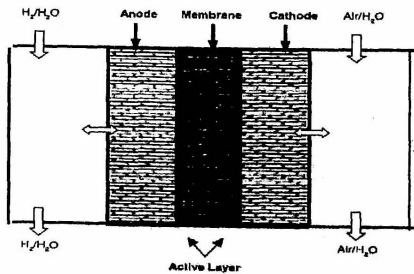
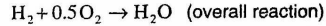
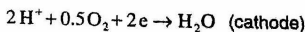
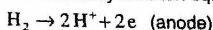


Fig.2 A PEM fuel cell

The chemistry reaction equations are:



One typical feature in fuel cell modeling is the prediction of the cell current-voltage relation referred to as the polarization curve. A parametric model of PEMFC developed by Amphlett [8] is used here. The basic expression for the voltage for a single cell is:

$$V_{cell} = E_{Nernst} + v_{act} + v_{ohmic} \quad (2)$$

In the above equation:

$$E_{Nernst} = 1229 - (8.5 \times 10^{-4})(T_a - 298.15) + 43.08 \times 10^{-5} * T_a * \ln(P_{H_2} * 0.5 P_{O_2} / P_{H_2O}) \quad (3)$$

v_{act} is the activation loss or activation overvoltage which is a result of the need to cause electron transfer and to break and form chemical bonds in the anode and cathode. Its steady value is:

$$\eta_{act} = \xi_1 + \xi_2 T_{st} + \xi_3 T_{st} (\ln(I)) + \xi_4 T_{st} (\ln(C_{O_2})) \quad (4)$$

where the parameters ξ_i in the above equation can be obtained from testbench experiment, T_{st} is the stack temperature and C_{O_2} is defined by the Henry's law:

$$C_{O_2} = P_{O_2} / (5.08 \times 10^6 * \exp(-498/T_{st})) \quad (5)$$

where P_{O_2} is the partial pressure of the oxygen. v_{ohm} is Ohmic polarization is resulted from resistance to electron transfer in the graphite collector plates and graphite electrodes plus resistance to proton transfer in the solid polymer membrane. This can be expressed using Ohm's law:

$$v_{ohm} = -I \times R_{ohm} \quad (6)$$

where I is the stack current, and:

$$R_{ohm} = t_m / \sigma_m \quad (7)$$

t_m is the membrane thickness and σ_m is a function of membrane water content, λ_m and fuel cell temperature:

$$\sigma_m = b_1 \exp(b_2 (1/303 - 1/T_{st})) \quad (8)$$

$$b_1 = (b_3 \lambda_m - b_4) \quad (9)$$

λ_m varies between 0 and 14, which is equivalent to the relative humidity of 0% and 100%, respectively. b_i is usually determined empirically.

3.3 Charge double layer capacitance

In this model we consider the effect of charge double layer capacitance to the voltage dynamics. In most of the existing dynamic models such effect has not been taken into consideration. The effect of charge double layer capacitance is to make the change of

stack voltage can't follow up the change of stack current in time. The equivalent circuit is shown in Fig.3:

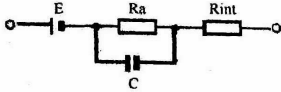


Fig.3. Electrical equivalent of stack voltage

A differential equation that describes such effect is:

$$dv_{act}/dt = I/C - v_{act}/R_{act}/C \quad (10)$$

$$R_{act} = \eta_{act}/I \quad (11)$$

where C depends on electrical permittivity, actual surface area of the electrode and the separation of the plates.

3.4 Anode flow model

The anode mass flow model represents the hydrogen flow behavior inside the anode of the fuel cell stack (Fig.4).

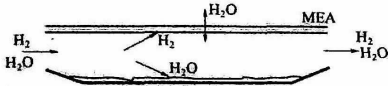


Fig.4 Anode mass flow

Using the energy conservation and ideal gas law we have:

$$\frac{dP_{H_2}}{dt} = \frac{R_{H_2} T_{st}}{V_{an}} (W_{H_2,in} - W_{H_2,used} - W_{H_2,out}) \quad (12)$$

$$\frac{dP_{H_2O,an}}{dt} = \frac{R_{H_2O} T_{st}}{V_{an}} (W_{H_2O,an,in} - W_{H_2O,an,out}) \quad (13)$$

where P_{H_2} and $P_{H_2O,an}$ are partial pressure of the hydrogen and water in the anode respectively and $W_{H_2,used}$ is the mass flow rate of oxygen reacted:

$$W_{H_2,used} = M_{H_2} \times \frac{NI}{2F} \quad (14)$$

where M_{H_2} is the molar mass of hydrogen and F is Farady const.

3.5 Cathode flow model

Similar to the anode flow model, the cathode mass flow model represents the air flow behavior inside the cathode of the fuel cell stack (Fig.5).

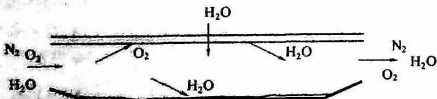


Fig.5 Cathode mass flow

Three state equations are developed by continuity of the mass flow of oxygen, nitrogen and water:

$$\frac{dP_{O_2}}{dt} = \frac{R_{O_2} T_{st}}{V_{ca}} (W_{O_2,in} - W_{O_2,used} - W_{O_2,out}) \quad (15)$$

$$\frac{dP_{N_2}}{dt} = \frac{R_{N_2} T_{st}}{V_{ca}} (W_{N_2,in} - W_{N_2,out}) \quad (16)$$

$$\frac{dP_{H_2O,ca}}{dt} = \frac{R_{H_2O} T_{st}}{V_{ca}} (W_{H_2O,ca,in} + W_{H_2O,produced} - W_{H_2O,ca,out}) \quad (17)$$

where P_{O_2} , P_{N_2} and $P_{H_2O,ca}$ are partial pressure of the oxygen, nitrogen and water in the cathode respectively; $W_{O_2,used}$ is the mass flow rate of oxygen reacted and $W_{H_2O,produced}$ is the mass flow rate of water generated in fuel cell reaction:

$$W_{O_2,used} = M_{O_2} \times \frac{NI}{4F} \quad (18)$$

$$W_{H_2O,produced} = M_{H_2O} \times \frac{NI}{2F} \quad (19)$$

3.6 Humidity affection

Humidity management is crucial for operation of PEM fuel cell and for optimization of the output power. Flooding of the fuel cell due to excess water production blocks the gas transport towards the catalyst particles of the electrodes. On the other hand, drying of the membrane leads an increase of resistive losses and a decrease of outpour power. The flow rate of the water entering the cathode can be calculated by the equation:

$$W_{H_2O,ca,in} = \frac{M_{H_2O} P_{H_2O,ca,in}}{M_{H_2O} P_{H_2O,ca,in} + M_{air} P_{air,in}} W_{air,in} \quad (20)$$

Where $W_{H_2O,ca,in}$ is the mass flow rate of water entering the cathode and $W_{air,in}$ is the flow rate of the air entering the cathode, $P_{H_2O,ca,in}$ is given as:

$$P_{H_2O,ca,in} = \phi_{ca} P_{sat}(T_{ca,in}) \quad (21)$$

where ϕ_{ca} is the relative humidity, $P_{sat}(T_{ca,in})$ is vapor saturation pressure, which is a function of temperature.

4. MODEL VALIDATION AND SIMULATION

The dynamic model of the fuel cell system described above is simulated in Matlab's SIMULINK environment. Appendix. B Fig.11 Shows the SIMULINK simulation blocks. The parameters used in the modelling are listed in the Appendix. A Table1. The Simulation results of the model and the test results at

two situations are listed below:

1) Stack current is changed from 10A to 40A at 5s and from 40A to 20A at 10s, Where $v_{air} = 2.5V$ and $v_{H_2} = 2V$.

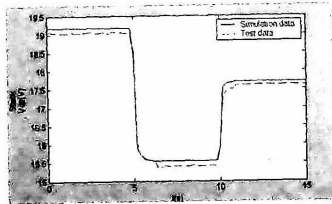


Fig. 6 Stack volt response

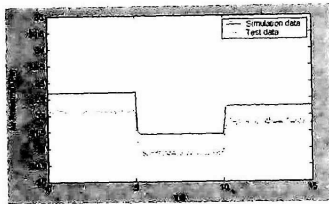


Fig. 7 Air pressure response

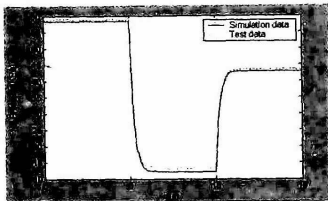


Fig.8 Hydrogen pressure response

2) v_{air} is changed from 2.5V to 3.0V at 5s and from 3.0V to 2.2V at 10s and at the same time v_{H_2} is changed from 0.8V to 1.0V at 5s and from 1.0V to 0.7V at 10s, where stack current $i=0A$.

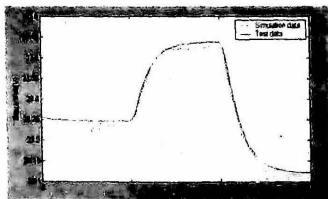


Fig.9 Stack volt response

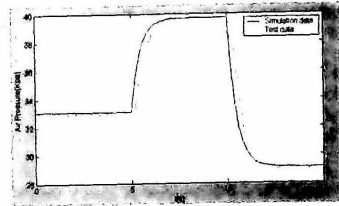


Fig.10 Air pressure response

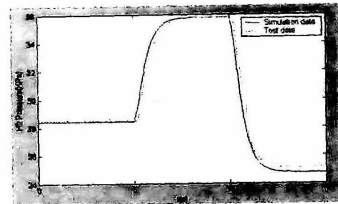


Fig.11 Hydrogen pressure response

5. CONCLUSIONS

A Dynamic model is proposed to simulate the transient phenomena in a PEMFC system. We have given complete equations to characterize the effects of mass flow meter dynamics, charge double layer capacitance, the flow and pressure dynamics in the anode and cathode and the affection of humidity. The dynamic model is implemented in MATLAB/SIMULINK^[9] environment. A series of simulation are carried out. The simulation results are in good agreement with our testbench results. This study enables us to predict PEMFC dynamic behavior under operating conditions, which give a good tool for optimization and control development.

APPENDIX. A

Table 1. Parameters used in the model

Symbol	Value	Symbol	Value
k_1	20	F	96485.3C/mol
k_2	4	t_m	$5.1 \times 10^{-5}m$
τ_1	0.44	b_2	350
τ_2	0.44	b_3	0.005139
T_{st}	338K	b_4	0.00326
ξ_1	-0.9484	N	24
ξ_2	0.00312	C	3F
ξ_3	-0.000187	V_{an}	$8.4 \times 10^{-6}m^3$
ξ_4	7.4×10^{-5}	V_{ca}	$8.4 \times 10^{-6}m^3$
M_{H_2}	$2.016 \times 10^{-3} \text{ kg/mol}$	M_{H_2O}	$18.02 \times 10^{-3} \text{ kg/mol}$
M_{O_2}	$32 \times 10^{-3} \text{ kg/mol}$	R_{O_2}	$259.8J/(kg \cdot K)$
R_{H_2}	$296.8J/(kg \cdot K)$		

APPENDIX. B

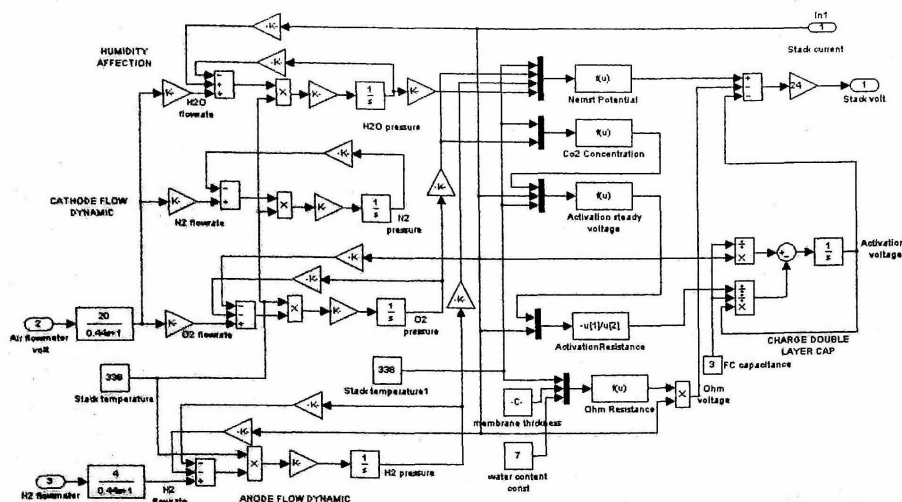


Fig.12 Fuel cell system simulation block

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