Simulation Study on the Influence of Input Parameters on the Characteristics of SOFC Stack

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***Abstract* - In this paper we develop a MATLAB/Simulink model of SOFC (Solid Oxide Fuel Cell) stack, using: i) the mass conservation equation, ii) the electrochemical equation, iii) the state equation of ideal gas and iv) the thermodynamics formula. The output parameters of this model are voltage, power and temperature. The fuel of SOFC stack is hydrogen, and the oxidant is air. The study analyzes the main input parameters of hydrogen flow, air flow and the current step disturbance effect on the characteristics of SOFC, when the SOFC is working under the rated load. The effects are verified by simulating the developed model, so it can be used as reference in practice to adjust the parameters of SOFC stack.**

Keywords: SOFC stack; Mathematical model; Step disturbance; Characteristic simulation; Analysis of the results.

I. INTRODUCTION

In twenty-first century, energy shortage and environmental pollution have become very important issues of the whole world. Therefore, technology of developing efficient, clean new energy power has attracted more and more attention. Fuel cell is developed in this case as a new type of power generation technology. It uses the method of converting chemical energy of the fuel (hydrogen) directly into electrical energy without combustion, and isn't limited by Kano cycle. This method can improve power generation's efficiency; reduce the pollutants emission and reduce pollution on environment [1].

According to different types of electrolyte, fuel cell can be divided into Proton Exchange Membrane Fuel Cell (PEMFC), Phosphoric Acid Fuel Cell (PAFC), Molten Carbonate Fuel Cell (MCFC) and SOFC etc. [2]. The main structure of SOFC is solid, which not only avoids the electrolyte flow problem but makes the structure more compact. The reaction temperature of up to 1000℃ can make the cell a highly energy conversion efficient system, and its exhaust gas can be reused in CCHP system to improve energy utilization efficiency.

SOFC is a complex matrix including flow, heat transfer, mass transfer, electrochemical reactions and other kinds of phenomena. So establishing the dynamic mathematical model of SOFC stack has great significance in helping us understand characteristics of the system and finding factors affecting power output. In this article, a dynamic model of the SOFC stack is developed by MATLAB/Simulink and a study is made on the effect on the temperature of the stack and output power when changing the load, the fuel flow and the air flow.

II. PRINCIPLE OF SOFC

SOFC is a kind of high temperature fuel cell. And it can convert chemical energy directly into electrical energy. SOFC single cell consists of three parts: anode, cathode and electrolyte. And because SOFC should operate at temperatures from 600to1000℃, the electrolytes need to use ceramic materials with high temperature stability. The process of converting chemical energy into electrical energy of SOFC is equivalent to the inverse process of water electrolysis. In the process of electrode reaction, fuel and oxygen have oxidation and reduction reaction respectively. And exchange the electrons at the same time. Then the electrons go back to cathode by external circuit [3]. In the operating process of SOFC, it needs to continuously provide fuel and oxidant into batteries and discharge exhaust gas after reaction. In this study, the fuel of anode is hydrogen and the oxidant of cathode is air.

In the process of electrochemical reaction of fuel and air of SOFC, electrons move in external circuit and form current to generate power. And the conductive body of SOFC generally is oxygen ion. In the circuit, the anode of the cell is the negative pole and the cathode is the positive pole. The reaction process of SOFC is oxygen in the air has reduction reaction in the cathode to produce the oxygen ion, which is conductor of electrolyte. It arrives on the anode through electrolyte. In the anode, Hydrogen reacts with oxygen ion into water, and release electrons. Then electrons go back to cathode and form current [4].

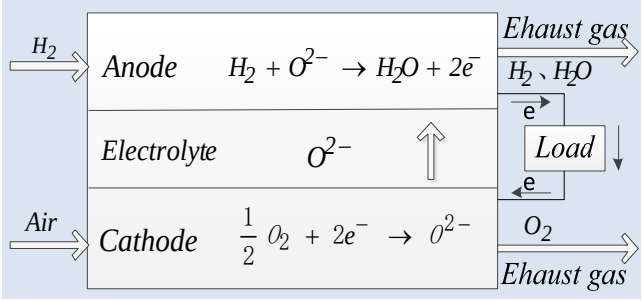


Figure.1. Electrochemical reaction principle of SOFC.

III. MODEL OF SOFC STACK

Usually the Output voltage of single SOFC is only about 1V [5], so the power is limited. In order to get higher voltage and power, many single cells need to be piled up to form the SOFC stack. SOFC power generation system, except SOFC stack, also consists of some other equipment and auxiliary devices such as fuel processing system, power regulator and load etc.

To simplify the model, it uses hydrogen as fuel and air as oxidant of the SOFC stack. The operation process of SOFC needs stable output voltage. So the output voltage of the stack is an output parameter of the model. In process of the stack, too high temperature will make the material life decline; affect the output voltage and power of the stack. So the temperature of stack is also an output parameter of the model. In summary, this SOFC stack is a dynamic model using hydrogen flow rate and air flow rate as input parameters, output voltage, output power and temperature of the stack as output parameters. .

A. Modeling of Each Part of SOFC Stack

SOFC stack model consists of four interconnected sub modules: anode flow model, cathode flow model, electric characteristic model and temperature characteristic model of stack [6~8]. And these four modules are associated and coupled, and jointly determine the output voltage and power of stack.

In the process of SOFC stack modeling, in order to simplify the model, some assumptions are made as follows:

(1) All of the gas is an ideal gas and meet the state equation of ideal gas;

(2) The stack temperature is uniform. It means that the temperature of anode and cathode channels is equal to the temperature of stack;

(3) The distribution of components in the stack is uniform, and partial pressure of each component is the same;

(4) The temperature and mole fraction when gas flowing out the stack are the same with inside;

(5) The stack doesn't change heat with outside, and its entrance and exit are adiabatic boundary.

The model of anode flow channel shows the situation of fuel flow in stack. In the anode flow, hydrogen and vapor are mainly substances, and the mass conservation is mainly about these two substances. According to the law of mass conservation, when the fuel through the anode channel, the relationship between entrance velocity $\dot{n}_{in,an}$ and exit velocity $\dot{n}_{out,an}$ of fuel flow is as follows:

$$\dot{n}_{out,an} = \dot{n}_{in,an} - \dot{n}_{H_2}^r + \dot{n}_V^r \tag{1}$$

In this expression, $\dot{n}_{H_2}^r$ and $\dot{n}_V^r$ are consumption of hydrogen and generation of vapor in the reaction process respectively. Their calculation formulas are as follows:

$$\dot{n}_{H_2}^r = 2K_r I = \dot{n}_V^r \tag{2}$$

In the above formula, K_r is a constant, whose value is calculated by $N/4F$. N is the number of single cell in the stack, and $F(96486\,C/mol)$ is Faraday Constant.

Molar flow state equations of anode:

$$\frac{dn_{H_2,an}}{dt} = \dot{n}_{H_2,an,in} - \dot{n}_{H_2,an,out} - \dot{n}_{H_2}^r \tag{3}$$

$$\frac{dn_{V,an}}{dt} = \dot{n}_{V,an,in} - \dot{n}_{V,an,out} + \dot{n}_V^r \tag{4}$$

According to the state equation of ideal gas, the hydrogen pressure$P_{H_2,an}$ and vapor pressure$P_{V,an}$ can be calculated.

According to the above mathematical model, simulation model of anode flow channel is developed on the MATLAB/Simulink platform. As shown in Fig. 2, it is the whole simulation model of anode flow channel. There are two subsystem models: hydrogen subsystem model and vapor subsystem model. In this model, the input variables are fuel flow, current I of SOFC and the temperature T of stack, and the output variables are hydrogen pressure$P_{H_2,an}$, vapor pressure$P_{V,an}$ and hydrogen and vapor output velocity.

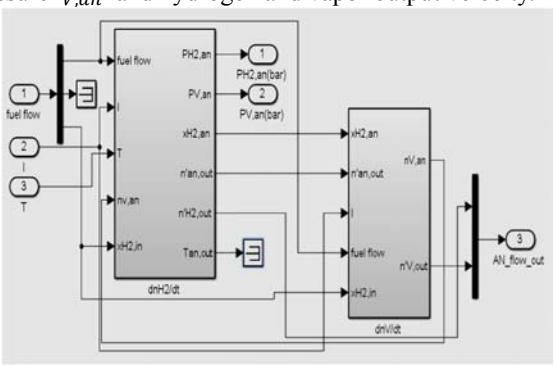


Figure. 2 The simulation model of anode flow channel

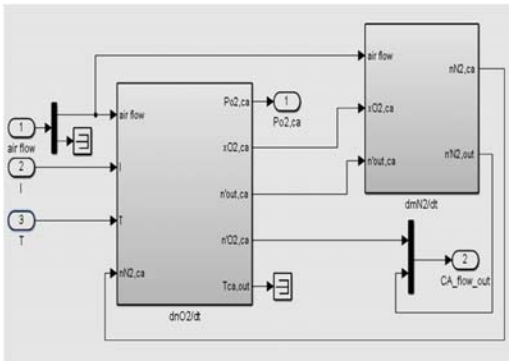


Figure. 3 The simulation model of cathode flow channel

Similar to the anode flow channel, the cathode flow is mainly the mass conservation of oxygen and nitrogen. Similarly, according to the law of mass conservation, the relationship between entrance velocity $\dot{n}_{in,ca}$ and exit velocity $\dot{n}_{out,ca}$ of the air flow in the cathode flow channel is as follows:

$$\dot{n}_{out,ca} = \dot{n}_{in,ca} - \dot{n}_{O_2}^r \tag{5}$$

In this expression, $\dot{n}_{O_2}^r = K_r I$ is the consumption of oxygen in the reaction.

Molar flow state equations of cathode:

$$\frac{dn_{O_2,ca}}{dt} = \dot{n}_{O_2,ca,in} - \dot{n}_{O_2,ca,out} - \dot{n}_{O_2}^r \tag{6}$$

$$\frac{dn_{N_2,ca}}{dt} = \dot{n}_{N_2,ca,in} - \dot{n}_{N_2,ca,out} \quad (7)$$

According to the state equation of ideal gas, the oxygen pressure $P_{O_2,ca}$ and nitrogen pressure $P_{N_2,ca}$ can be calculated.

According to the above mathematical model, the simulation model of cathode flow channel is developed. As shown in Fig. 3, it is the whole simulation model of cathode flow channel. There are two subsystem models: oxygen subsystem model and nitrogen subsystem model. In this model, the input variables are air flow, current I of SOFC and the temperature T of stack, and output variables are oxygen pressure $P_{O_2,ca}$, the output velocity of oxygen and nitrogen.

According to the reference [9] and [10], the output voltage of SOFC can be represented as

$$E = NE_N - E_{ohmic} - E_{act} - E_{con} \quad (8)$$

In the above formula, N is the number of cell in the SOFC stack; E is the output voltage of SOFC; E_N is Nernst voltage; E_{ohmic} is ohm polarization voltage; E_{act} is activation polarization voltage; E_{con} is concentration polarization voltage. They can be calculated by

$$E_N = E_0 + \frac{RT}{2F} ln\left(\frac{P_{H_2,an} \times P_{O_2,ca}^{1/2}}{P_{H_2O,an}}\right) \quad (9)$$

$$E_{ohmic} = r(T)I = \left\{r_0 exp\left[\alpha\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]\right\} I \quad (10)$$

$$E_{act} = a + blogI \quad (11)$$

$$E_{con} = -\frac{RT}{nF} ln\left(1 - \frac{I}{I_L}\right) \quad (12)$$

In the above formula, $E_0 = 1.18V$is the standard potential; $R(8.314\, kJ/(kmol \cdot K))$ is gas constant; T is temperature of cell working process; $r_0 = 0.126\Omega\ \alpha = -2870K$ and $T_0 = 973K$ are the constant of cell. $a = 0.05$ and $b = 0.11$ is respectively Tafel constant and Tafel slope; $n = 2$ is the number of electronic Moore in the electrochemical reaction; $I_L = 350A$ is the limit current value of concentration polarization loss.

According to the above mathematical model and Simulink model of each part, the electric characteristic model of SOFC is developed. Fig. 4 is the electric characteristic model of SOFC.

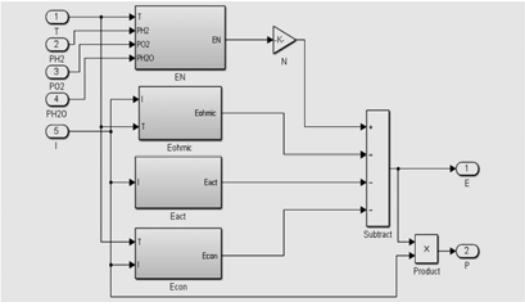


Figure. 4 The electric characteristic model of SOFC

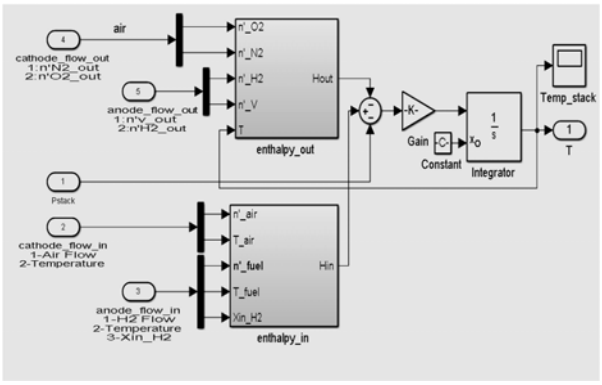


Figure. 5 The temperature model of SOFC

To simplify the stack temperature characteristic model, we assume that the temperature of stack is uniform, and the stack is insulated. It means that the stack does not exchange heat with the outside. The heat in stack is mainly the heat of inflow gas, outflow gas and the power produced by electrochemical reaction. Thus, the enthalpy balance equation of stack is as follows:

$$AC_p \frac{dT}{dt} = \dot{H}_{in} - \dot{H}_{out} - P_{stack} \quad (13)$$

In this equation P_{stack} is the power of SOFC stack, and the expressions of input enthalpy $\dot{H}_{in}$ and output enthalpy $\dot{H}_{out}$ are as follows:

$$\dot{H}_{in} = \dot{n}_{air,in}h_{air,in} + \dot{n}_{H_2,in}h_{H_2,in} + \dot{n}_{V,in}h_{V,in} \quad (14)$$

$$\dot{H}_{out} = \dot{n}_{O_2,out}h_{O_2,out} + \dot{n}_{N_2,out}h_{N_2,out} + \dot{n}_{H_2,out}h_{H_2,out} + \dot{n}_{V,in}h_{V,out} \quad (15)$$

All kinds of gas enthalpy in above expressions are related to temperature. According to the references, Table 1 is the formulas of gas enthalpy.

TABLE 1 CALCULATION FORMULAS OF GAS ENTHALPY

Gas species	The approximate calculation formula of enthalpy(J/mol)
H_2	$h_{H_2} = -0.9959 \times 10^4 + 30.73T$
H_2O	$h_{H_2O} = -25.790 \times 10^4 + 42.47T$
O_2	$h_{O_2} = -1.2290 \times 10^4 + 35.12T$
N_2	$h_{N_2} = -1.059 \times 10^4 + 31.4T$
Air	$h_{air} = -1.0947 \times 10^4 + 32.5T$

According to the above mathematical model, the temperature model of SOFC is developed, as shown in Fig. 5.

B. 2.2 Model and Simulation of SOFC Stack System

According to the mathematical model of each part, the Simulink model of SOFC stack power generated system is developed combining with the thermodynamic parameters of fuel and air, as shown in Fig. 6. The main parameters of the stack model in this paper are as shown in Table 2.

TABLE2 MAIN PARAMETERS OF SOFC STACK MODEL

Parameters	Value
The input velocity of hydrogen(mol/s)	0.746
The input velocity of air(mol/s)	3.10
The temperature of gas before entering stack(K)	923.15
The cell number of stack	384
Hydrogen humidity	2%

Using the stack parameters and the simulation model of SOFC stack system, the electrical characteristic studied in this paper is as shown in Fig. 7.

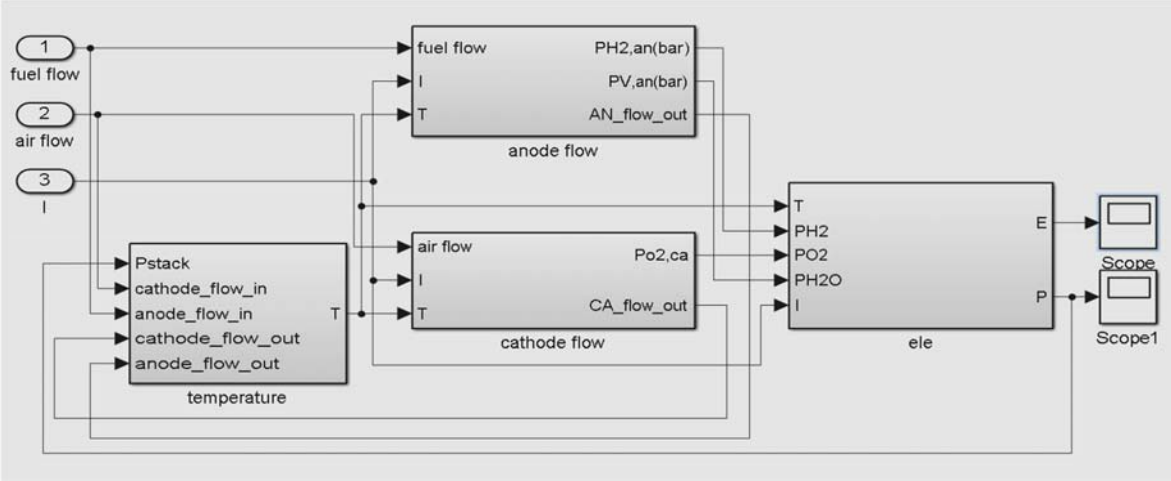


Figure. 6 The model of SOFC stack system.

Using the stack parameters and the simulation model of SOFC stack system, the electrical characteristic studied in this paper is as shown in Fig. 7.

According to the above parameters and the stack model formulas, a simulation program of SOFC stack is programmed in MATLAB. After running the program, a three-dimensional figure is obtained. Its independent variables are current and temperature, and the dependent variable is the stack voltage. Fig. 8 shows the simulation results.

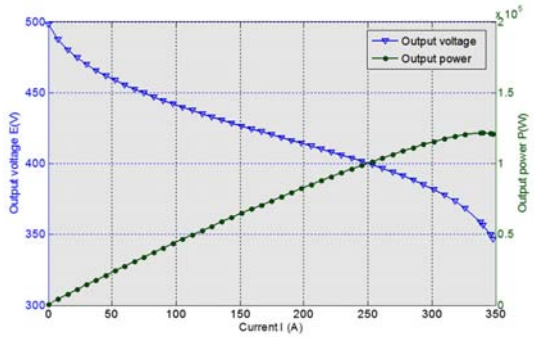


Figure. 7 E-I and P-I curve of stack

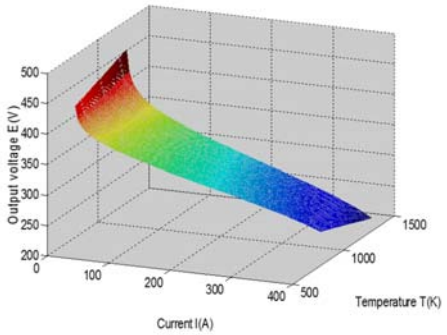


Figure. 8 The three-dimensional figure of stack voltage with different temperature and current distribution

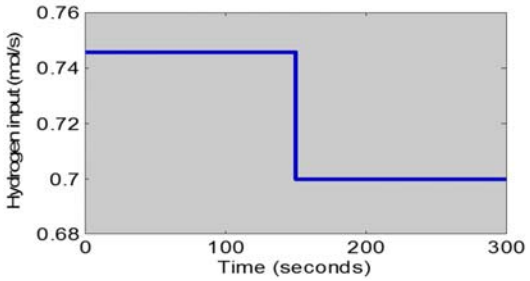
IV. THE INFLUENCE OF INPUT PARAMETERS ON THE SOFC STACK

From the modeling process of SOFC stack, we can know that the hydrogen input, air input and load current are important parameters of SOFC. Changing any one of them, it will influence on every parts of the model. And the output characteristics of SOFC will be changed.

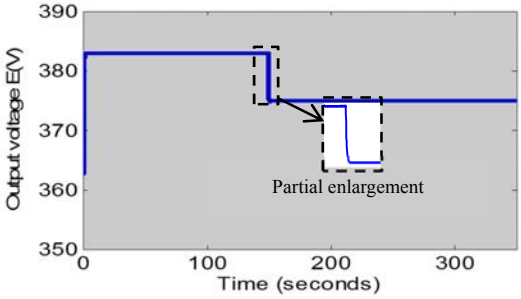
A. The Influence of Hydrogen Input Changes on System

First, the rated input parameters of the system are hydrogen input of $0.746mol/s$, air input of $3.10mol/s$ and stack load current of $300A$. After the system running stable, the hydrogen input has a tiny step disturbance at 150s. Hydrogen input steps down from $0.746mol/s$ to $0.7mol/s$. The air input and load current keep unchanged. We can

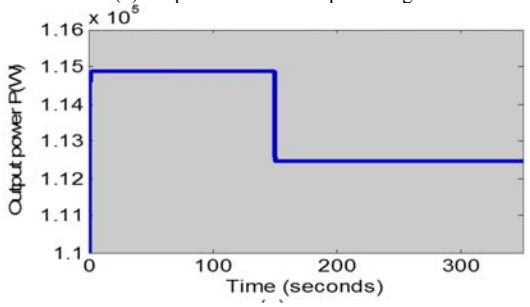
observe the changes of output parameters. The simulation results are shown in Fig. 9.



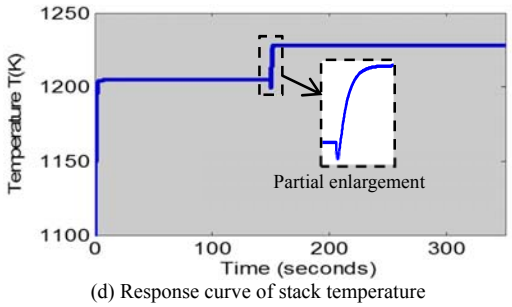
(a) Input curve of hydrogen



(b) Response curve of output voltage

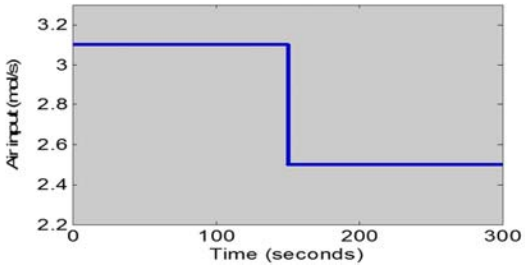


(c) Response curve of output power

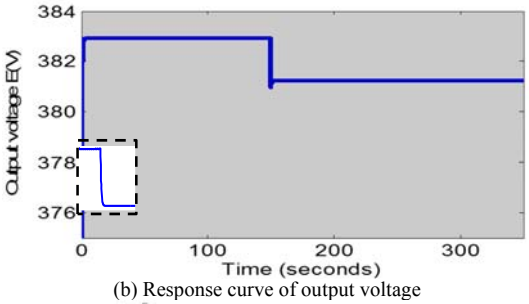


(d) Response curve of stack temperature

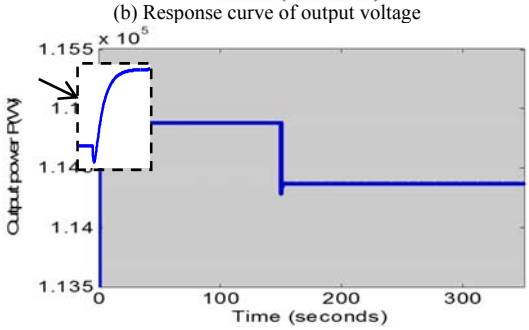
Figure. 9 Response curve of hydrogen step input



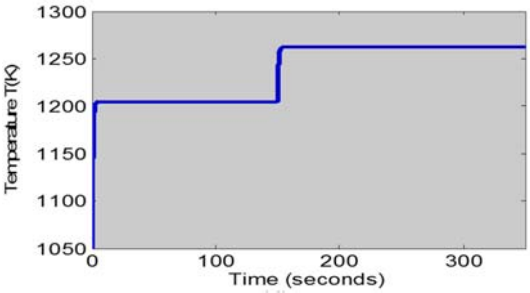
(a) Input curve of air



(b) Response curve of output voltage



(c) Response curve of output power



(d) Response curve of stack temperature

Figure. 10 Response curve of air step input

Observe curves in Fig. 9. With the hydrogen input decreasing 0.046 mol/s, the output voltage of stack decreases and the stack temperature rises. While the output voltage transition process is relatively faster than temperature. When hydrogen input decreasing, the load current not changes. Thus, the amount of hydrogen in the reaction has not changed. At this time, the change of partial pressure of hydrogen is mainly because of the imbalance of hydrogen input and output. The imbalance eventually affects the output voltage. The pressure imbalance recovers fast, so the transition process of voltage is fast. The reduction of hydrogen input is equivalent to reduction of cooling quantity, so the stack temperature rises. Because the cooling is a slow process, the transition process of stack temperature is relatively slow and almost no influence on voltage.

B. The Influence of Air Input Changes on System

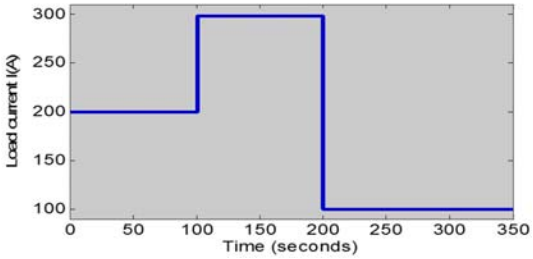
And the same as above, the system runs under the rated parameters. After the system running stable, the air input has a tiny step disturbance at 150s. Air input steps down from $3.10 mol/s$ to $2.50 mol/s$. The hydrogen input and load current keep unchanged.

Then, we can observe the changes of output parameters. The simulation results are shown in Fig. 10.

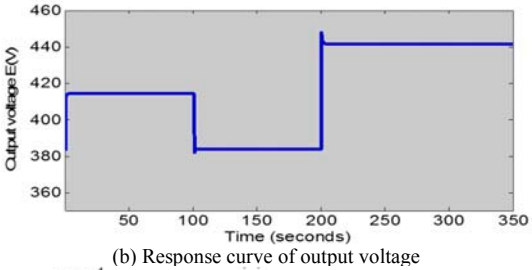
Observe curves in Fig. 10. With the air input decreasing $0.6mol/s$, the output voltage of stack decreases; the stack temperature rises. While the output voltage transition process is relatively faster than temperature. The influence trend of reducing air input on stack is same with influence trend of reducing hydrogen input. The difference is that the number of oxygen molecules involved in the reaction is 1/2 of hydrogen. And the influence of oxygen pressure on output voltage is square root in the Nernst equation. Thus, its reduction effect on the output voltage is smaller than hydrogen pressure.

C. The Influence of Load Current Changes on System

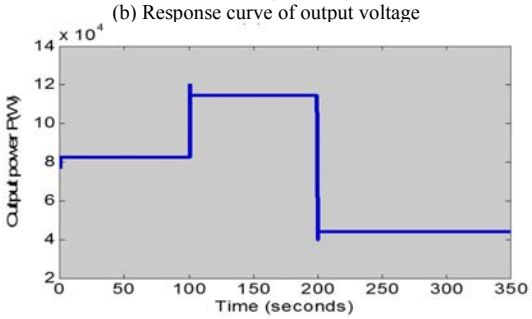
In this case the input parameters of the system are hydrogen input of $0.746mol/s$, air input of $3.10mol/s$ and stack load current of $200A$. The system is running until the output voltage, power and stack temperature stability. The load current has a step up disturbance at 100s, i.e. the current steps up from 200 A to 300 A. Then after the system running stable, load current has a step down disturbance at 200s, i.e. the current step down from 300A to 100 A. The hydrogen input and air input keep unchanged. We can observe the changes of output parameters. The simulation results are shown in Fig. 11.



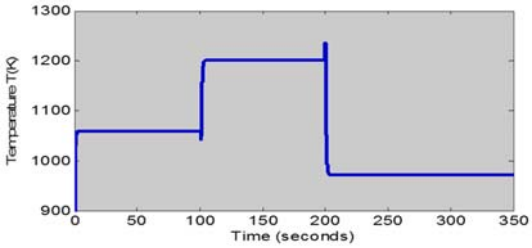
(a)Curve of load current



(b) Response curve of output voltage



(c) Response curve of output power



(d) Response curve of stack temperature

Figure. 11 Response curve of load current step input

Observe curves in Fig. 12. With the load current increasing 100 A, the output voltage of stack decreases; the output power and temperature of stack rise. While, with the load current decreasing 200 A, the output voltage of stack rises and the output power and temperature of stack decreases. The load current steps up, so the hydrogen and air quantity participated in the reaction of SOFC stack increase. And the heat generated in reaction increase, so the temperature of stack rise. After the reaction stable, the temperature of stack keeps at a high level. At the same time, with the current increasing, the chemical reaction degree increases. Hydrogen and air partial pressure reduces in the stack and the vapor partial pressure increases, resulting in the Nernst voltage decreases. At this time, the impedance increases, but its effect is small. The impedance is caused by activation loss, concentration polarization loss and ohm loss .So the output voltage finally decreases and stabilizes at a low level. But the up amplitude of the current is larger than the down amplitude of voltage, so the final output power of stack rises. Similarly, with the load current decreasing, the temperature and output power of stack decrease; the output voltage of stack rises.

V. CONCLUSION

SOFC operates under sealed high temperature conditions and the operation data is difficult to measure. Thus, performance analysis and simulation can only be based on the mechanism model. This paper first develops electrochemical model, temperature model and other models on MATLAB/Simulink platform. Then the influences of various input parameters on output voltage, power and temperature are analyzed based on the simulation of model.

This paper gives the influences of main input parameters on the system and the detailed simulation analysis. The variation of hydrogen input, air input and load current have influences on the output parameters of stack. In the allowable range of parameters, the output voltage and power of stack can increase with increasing of hydrogen input and air input, and the temperature can be decreased. And maintain hydrogen input and air input constant. The output voltage decreases with the increasing of load current, and the output power and stack temperature can be increased. While the output voltage increases with the decreasing of load current, and the output power and temperature of stack can be decreased. According to the above simulation conclusion, when load current changes, we can adjust the hydrogen input

and air input of stack to make the output power meets the user's needs.

ACKNOWLEDGMENTS

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