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Dynamic modeling and simulation test of a 60 kW PEMFC generation system*

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Abstract: In this paper, a 60 kW proton exchange membrane fuel cell (PEMFC) generation system is modeled in order to design the system parameters and investigate the static and dynamic characteristics for control purposes. To achieve an overall system model, the system is divided into five modules: the PEMFC stack (anode and cathode flows, membrane hydration, and stack voltage and power), cathode air supply (air compressor, supply manifold, cooler, and humidifier), anode fuel supply (hydrogen valve and humidifier), cathode exhaust exit (exit manifold and water return), and power conditioning (DC/DC and DC/AC) modules. Using a combination of empirical and physical modeling techniques, the model is developed to set the operation conditions of current, temperature, and cathode and anode gas flows and pressures, which have major impacts on system performance. The current model is based on a 60 kW PEMFC power plant designed for residential applications and takes account of the electrochemical and thermal aspects of chemical reactions within the stack as well as flows of reactants across the system. The simulation tests show that the system model can represent the static and dynamic characteristics of a 60 kW PEMFC generation system, which is mathematically simple for system parameters and control designs.

Key words: Proton exchange membrane fuel cell (PEMFC), Generation system, Dynamic simulation model, Reactant flow
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1 Introduction

The fuel cell generation system is composed of a proton exchange membrane fuel cell (PEMFC) stack and some auxiliary equipment. It exhibits the close nonlinear dynamic and coupling characteristics, including the stack chemical reaction, fuel and air flow, variable load, and water and heat management. The generation system must have steady and reliable operation and high efficiency in all working conditions. The performance design and coordination control are extremely important. Currently, fuel cell performance is limited due to the high cost and immature technology used in the early stages of commercialization. Modeling and simulation techniques are thus important in providing guidance for system research.

The fuel cell system has nonlinear multi-variable and dynamic coupling characteristics that are hard to model and control. Several modeling approaches with different aims have been used to describe the system. Pukrushpan *et al.* (2002) presented a control-oriented fuel cell system dynamic model in which the oxygen excess ratio was controlled. Rodatz *et al.* (2003) presented a dynamic

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model of the air supply and a variable pressure control strategy. Caux *et al.* (2005) considered anode and cathode compartments to control air and hydrogen flow rates as well as pressure. For the stack voltage and current control of a low PEMFC system, Yang *et al.* (2008) built a dynamic system model in which the stack was expressed as a multivariable configuration of two inputs and two outputs. An air pump and a hydrogen valve were included. Chrenko *et al.* (2008; 2009) developed an overall system model to investigate transient and nominal operations and rejuvenation process operation modes. They used an energetic macroscopic representation methodology to derive the maximum control structure of the air supply. An artificial intelligence algorithm has also been used for fuel cell system model development and control design (Hatti and Tioursi, 2009).

The objective of this paper was to develop a dynamic model of a 60 kW PEMFC generation system representing the static and dynamic characteristics of the overall system. Our investigation was based on a 60 kW PEMFC generation system designed for residential applications and takes account of the electrochemical and thermal aspects of chemical reactions within the stack and the flows of reactants across the system. The system model developed will be used for system parameter and control design in future studies.

2 Generation system overview

The structure of the 60 kW PEMFC generation system studied is shown in Fig. 1. The PEMFC stack is comprised of 300 series-connected cells and the cell active area is 600 cm^2. Nafion membrane is used with a thickness of 0.0175 cm. Hydrogen is stored in a high-pressure container and reduced to 0.6 MPa by a pressure relief valve. A second valve adjusts the flow rate of hydrogen, which is supplied to the stack anode for the oxidation reaction after humidification.

Air is supplied by the compressor to the manifold inlet, through filtering, cooling, humidifying, and then to the stack cathode for the reduction reaction.

The exhaust air leaving the cathode is discharged after water separation and decompression by the return manifold. The water recovered is stored in a hot water tank and pumped to the humidifier. The stack power is conditioned to match the user demand.

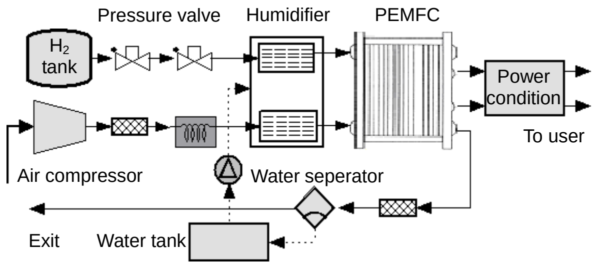

Fig. 1 60 kW PEMFC generation system

3 Generation system model

In a MATLAB/SIMULINK environment, all the modules of the 60 kW PEMFC generation system model, including the PEMFC stack, cathode air supply, anode fuel supply, cathode exhaust exit, and power conditioning, are connected to each other. Construction of the system model is mainly based on the reactants' dynamic flow, electrochemical reaction, and power transformation, i.e., the system operation parameters and power output variation. The model is based on the ideal gas equation, matter energy conservation, and physical chemistry laws. The system's heat management is described by Zhang *et al*. (2006). With relatively slow responses, the stack temperature can be viewed as a separate control system in heat management and assumed to be constant at 75 °C. The gases are all ideal.

3.1 PEMFC stack

The PEMFC stack model is the core of the system model and includes anode flow, cathode flow, membrane hydration, and stack voltage and power (Fig. 2). The module of stack voltage and power describes the main electrochemical reaction and output performance. A generalized power model of PEMFC stacks was developed previously using a combination of empirical and physical modeling techniques, and based on the generalized steady state electrochemical model (GSSEM) and studies of nafion membranes (Zhang *et al*., 2005). The PEMFC stack voltage V_{st} and power P_{st} are calculated as functions of the current, temperature, pressure, water content of the membrane, and some physical

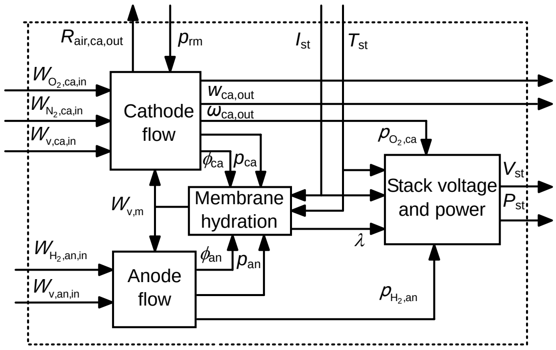

Fig. 2 PEMFC stack model in MATLAB/SIMULINK
$W_{O_2,ca,in}$, $W_{N_2,ca,in}$, and $W_{v,ca,in}$: oxygen, nitrogen, and vapor mass flow in the cathode, respectively; $p_{H_2,an}$: hydrogen partial pressure in the anode; $p_{O_2,ca}$: oxygen partial pressure in the cathode; p_{rm}: return manifold pressure; $\omega_{ca,out}$ and $R_{air,ca,out}$: humidity ratio and gas constant in cathode outlet, respectively

characteristics. The model is applicable to PEMFC stacks of various configurations and operating conditions and has been validated by some experimental results (Zhang *et al.*, 2005). The modules of anode and cathode flows aim to calculate internal stack pressures and humidity. The anode operates in a sub-saturated condition, i.e., $\phi_{an}<1$, to prevent anode flooding in a 60 kW designed system. Thus, it is assumed that the anode purge is zero (Pukrushpan *et al.*, 2002). The total anode pressure is the sum of hydrogen and vapor partial pressures:

$$p_{an} = p_{H_2,an} + p_{v,an} = \frac{m_{H_2,an} \times R_{H_2} \times T_{st}}{V_{an}} + \frac{m_{v,an} \times R_v \times T_{st}}{V_{an}}, \quad (1)$$

where R_{H_2} and R_v are the gas constants of hydrogen and vapor, respectively. T_{st} is the stack temperature and V_{an} is the anode volume. $m_{H_2,an}$ and $m_{v,an}$ are the masses of hydrogen and vapor in the anode, and can be described based on the mass conservation law:

$$\frac{dm_{H_2,an}}{dt} = W_{H_2,an,in} - M_{H_2} \times \frac{nI_{st}}{2F}, \quad (2)$$

$$\frac{dm_{v,an}}{dt} = W_{v,an,in} - W_{v,m}, \quad (3)$$

where $W_{H_2,an,in}$ is the hydrogen mass of the intake flow, n is the cell number in the stack, M_{H_2} is the molar mass of hydrogen, I_{st} is the stack current, and F is the Faraday number. $W_{v,an,in}$ and $W_{v,m}$ are the water mass flows in the anode and across the membrane from anode to cathode, respectively. The gas humidity in the anode is

$$\phi_{an} = \frac{p_{v,an}}{p_{sat}(T_{st})}, \quad (4)$$

where p_{sat} is vapor saturation pressure, a function of temperature.

Similar to the anode, the cathode pressure p_{ca} is the sum of the oxygen, nitrogen, and vapor partial pressures. The relative humidity ϕ_{ca} is determined from the vapor partial pressure and the vapor saturation pressure. The oxygen in the air combines with the electrons in the external circuit and the protons flowing through the membrane, thus producing water. Based on the mass conservation law, three state equations of oxygen, nitrogen, and water in the cathode are

$$\frac{dm_{O_2,ca}}{dt} = W_{O_2,ca,in} - W_{O_2,ca,out} - M_{O_2} \times \frac{nI_{st}}{2F}, \quad (5)$$

$$\frac{dm_{N_2,ca}}{dt} = W_{N_2,ca,in} - W_{N_2,ca,out}, \quad (6)$$

$$\frac{dm_{v,ca}}{dt} = W_{v,ca,in} - W_{v,ca,out} + M_v \times \frac{nI_{st}}{2F} + W_{v,m}, \quad (7)$$

where M_{O_2} and M_v are the oxygen and vapor molar masses, respectively.

The total flow rate of the exhaust air from cathode $W_{ca,out}$ is determined using the simplified orifice equation. Then the flow rates of oxygen, nitrogen, and vapor at the cathode exit $W_{O_2,ca,out}$, $W_{N_2,ca,out}$, and $W_{v,ca,out}$ are all calculated.

The membrane hydration module is built for calculating water flow across the membrane (Ge *et al.*, 1999; Dutta *et al.*, 2001; Pukrushpan *et al.*, 2002), which occurs through three distinct phenomena: electro-osmotic drag, back-diffusion, and migration resulting from the pressure difference. Combining three water transports and approximating the water concentration gradient and pressure change in the membrane to be linear over the membrane thickness, the water flow rate across the membrane is calculated from

$$W_{\mathrm{v,m}} = M_{\mathrm{v}} \times A \times n \times \left(n_{\mathrm{d}} \frac{I_{\mathrm{st}}}{AF} - D_{\mathrm{w}} \frac{c_{\mathrm{w,ca}} - c_{\mathrm{w,an}}}{t_{\mathrm{m}}} - \frac{k_{\mathrm{p}}}{\mu} \lambda c_{\mathrm{f}} \frac{p_{\mathrm{ca}} - p_{\mathrm{an}}}{t_{\mathrm{m}}} \right), \tag{8}$$

where A is the cell active area, t_{m} is the membrane thickness, k_{p} is the hydraulic coefficient, μ is the water viscosity, c_{f} is the sulfonic density, λ is the water content in the membrane, n_{d} is the electro-osmotic drag coefficient, and D_{w} is the water diffusion coefficient. $c_{\mathrm{w,an}}$ and $c_{\mathrm{w,ca}}$ are the water concentrations at the anode and cathode surfaces respectively, which are all calculated empirically from the humidity.

3.2 Cathode air supply

The cathode air supply model includes an air compressor, supply manifold, cooler, and humidifier. In the compressor module, the exit air temperature $T_{\mathrm{cp,out}}$ and the required power P_{cp} are both calculated using thermodynamic equations (Fig. 3). The air mass flow rate W_{cp} is selected as a variable directly for the simple system model and control. The supply manifold module represents the lumped volume associated with pipes and connections from the compressor to the stack cathode, including the air cooler and humidifier, where air varies in pressure, temperature, and flow. A nozzle flow equation is used to calculate the manifold outlet flow $W_{\mathrm{sm,out}}$ for a small pressure difference between the manifold and the stack cathode:

$$W_{\mathrm{sm,out}} = k_{\mathrm{sm,out}} (p_{\mathrm{sm}} - p_{\mathrm{ca}}), \tag{9}$$

where p_{sm} is the manifold pressure and $k_{\mathrm{sm,out}}$ is the nozzle constant.

Air cooler and humidifier modules describe the air flow state according to thermodynamics and mass conservation principles.

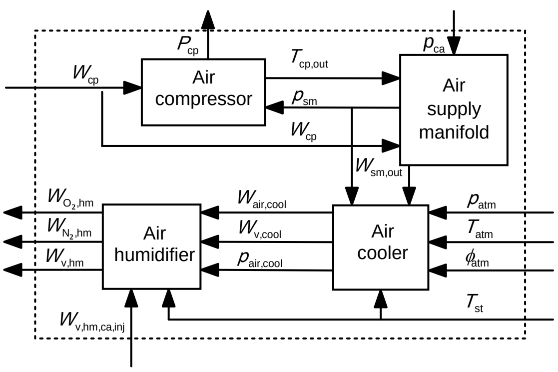

Fig. 3 Cathode air supply model in MATLAB/SIMULINK

$W_{\mathrm{O_2,hm}}$, $W_{\mathrm{N_2,hm}}$, and $W_{\mathrm{v,hm}}$: oxygen, nitrogen, and vapor mass flows out of humidifier; $W_{\mathrm{air,cool}}$ and $W_{\mathrm{v,cool}}$: air and vapor flows into humidifier; $p_{\mathrm{air,cool}}$: air pressure out of cooler; p_{atm}, T_{atm}, and ϕ_{atm}: pressure, temperature, and humidity in atmosphere; $W_{\mathrm{v,hm,ca,inj}}$: vapor mass flow injected into humidifier

3.3 Anode fuel supply

The anode fuel supply model includes the hydrogen valve and humidifier. The pressure drop across the hydrogen valve is reduced to the proportion of the flow rate $W_{\mathrm{H_2,valve}}$ square. The hydrogen humidifier module is the same as that for the cathode air supply. There is no purge on the anode side (Fig. 4).

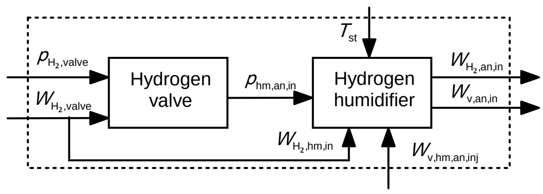

Fig. 4 Anode fuel supply model in MATLAB/SIMULINK

$W_{\mathrm{H_2,valve}}$: hydrogen mass flow through the second valve; $p_{\mathrm{H_2,valve}}$: hydrogen pressure after the first valve; $p_{\mathrm{hm,an,in}}$: hydrogen pressure after the second valve; $W_{\mathrm{H_2,hm,in}}$: hydrogen mass flow in humidifier

3.4 Cathode exhaust exit

The cathode exhaust exit model includes the exit manifold and water return (Fig. 5). The exit manifold model represents pipes and connections as for the air supply manifold, but its outlet flow is calculated based on the non-linear relationship for a large pressure difference between the stack working in the pressurization condition and the manifold exit. Air-water separation is the main process occurring in the cathode exhaust. It is assumed that 90% of water can be separated by the ideal process. The water used in a 60 kW PEMFC generation system can be determined by comparing the water recovered from the exhaust with that needed for reactant humidification.

3.5 Power conditioning

The power conditioning model includes DC/DC and DC/AC (Fig. 6). The net power output of the system P_{net} is that generated by the stack, P_{st}, minus the parasitic load consumed, consisting mainly of the power consumed by the compressor, P_{cp}. Wide fluctuations in stack voltage would make inverter control difficult, so the low direct voltage of the stack V_{st} is boosted to V_{dc} by DC/DC, and then inverted to alternating current voltage V_{ac} and power P_{out} for user load by DC/AC.

4 Generation system simulation test

The 60 kW PEMFC generation system model and simulation test interface is shown in Fig. 7. The system current I_{st} is instantaneously drawn from the load representing the user demand. The system current I_{st}, the air flow rate at the compressor exit W_{cp}, the water injection for air humidification $W_{v,hm,ca,inj}$, the hydrogen flow rate through the second pressure relief valve $W_{H_2,valve}$, and the water injection for hydrogen humidification $W_{v,hm,an,inj}$ are all input variables of the system model, that is, the adjustable variables in the system operation. Thus, regardless of whether the model is capable of describing the dynamic characteristics of the 60 kW PEMFC generation system, these variables are adjusted deliberately and the system simulation is tested.

Since the system model is complex in its structure and performance, and there are a lot of adjustable variables and monitoring parameters, the dynamics of the anode and cathode sides of the system model were tested separately to provide more detailed results.

Assuming the cathode side is steady, the simulation test on the anode side was conducted with

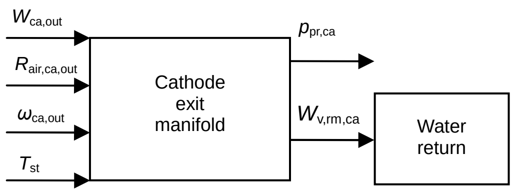

Fig. 5 Cathode exhaust exit model in MATLAB/SIMULINK

$W_{v,rm,ca}$: vapor mass flow that can be returned; $p_{pr,ca}$: pressure of the cathode return manifold

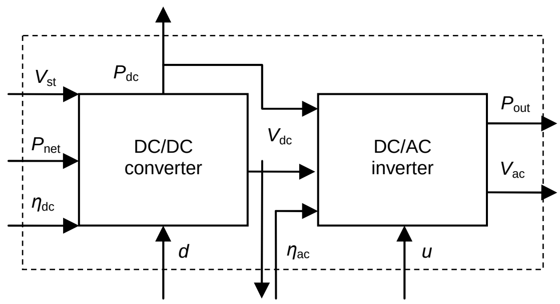

Fig. 6 Power conditioning model in MATLAB/SIMULINK

P_{dc}: power of DC/DC; η_{dc} and η_{ac}: conversion efficiencies of DC/DC and DC/AC; d: duty ratio; u: modulation factor

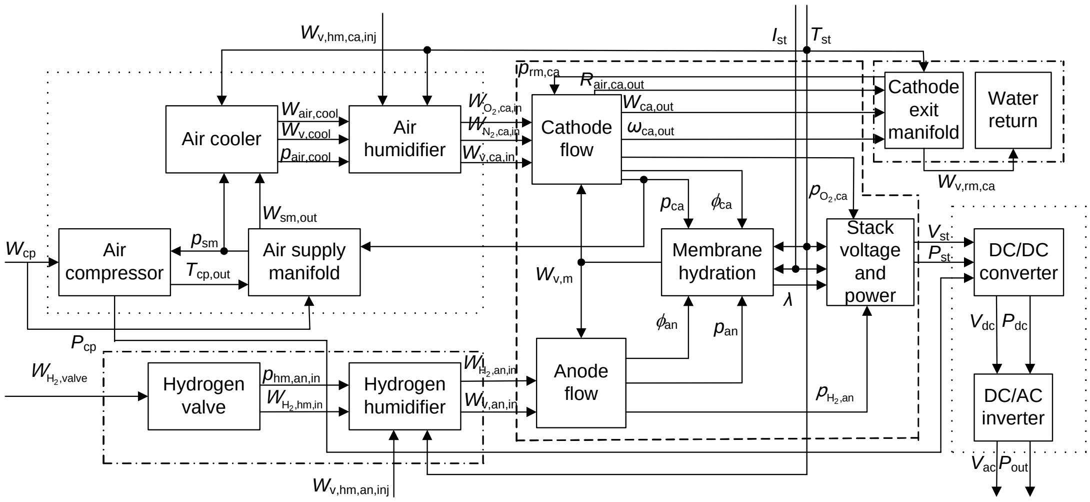

Fig. 7 60 kW PEMFC generation system model in MATLAB/SIMULINK

variable inputs $W_{H_2,valve}$, $W_{v,hm,an,inj}$, and I_{st}. Simulation results are shown in Fig. 8.

1. At t=6 and 12 s, the anode pressure p_{an}, humidity ϕ_{an} and stack voltage V_{st} all drop off dramatically due to a step increase of I_{st}, while the stack power P_{st} increases dramatically. In contrast, at t=18 s, p_{an} and V_{st} increase suddenly with the sharp decline in I_{st}, ϕ_{an} is maintained at a saturation state, and P_{st} drops off. These situations are mainly due to more hydrogen being consumed in the electrochemical reaction as I_{st} increases and more water flow to the cathode across the membrane. The hydrogen and water then both decrease in the stack anode, leading to decreases in both p_{an} and ϕ_{an}. When I_{st} decreases, the opposite process occurs. The relationships between V_{st}, P_{st}, and I_{st} conform to the stack output polarization characteristics.

2. The dynamic response in the hydrogen supply is shown in Fig. 8. $W_{H_2,valve}$ increases suddenly at t=8 and 14 s, and then p_{an} increases. This is because the hydrogen mass increases in the anode and the hydrogen partial pressure increases. At t=20 s, $W_{H_2,valve}$ decreases suddenly, and then the hydrogen mass and partial pressure in the anode both decrease. The increase in p_{an} clearly slows down.

3. According to the principle of PEMFC, the water mass in the anode is affected by the water injection into the hydrogen. The partial pressure of the water changes. The anode humidity, pressure, and stack output all change eventually. At t=10 and 16 s, there are sudden increases in p_{an}, ϕ_{an}, V_{st}, and P_{st} with the increase in $W_{v,hm,an,inj}$ (Fig. 8). But at t=22 s, there is no obvious dynamic variation with the sudden decrease in $W_{v,hm,an,inj}$. This situation is due to long term water super saturation in the anode.

The simulation results above show that the model describes well the dynamic characteristics and the effects of variables on the stack output performance in the anode side.

Next, the simulation test of the cathode side was conducted with variable inputs I_{st}, W_{cp}, and $W_{v,hm,ca,inj}$, assuming the system anode side was steady. The simulation results are shown in Fig. 9.

1. At t=2 s, I_{st} increases suddenly, followed by a gentle rise in cathode humidity ϕ_{ca}. ϕ_{ca} increases and decreases with the step increase of I_{st} at t=12 s and the decrease at t=22 s. All these situations are due to the increase and decrease of the water generated in the cathode and the flow across the membrane from anode to cathode when the electrochemical reaction rate increases and decreases. Observing the effect of I_{st} on the cathode pressure p_{ca}, at t=2 s, p_{ca} stops

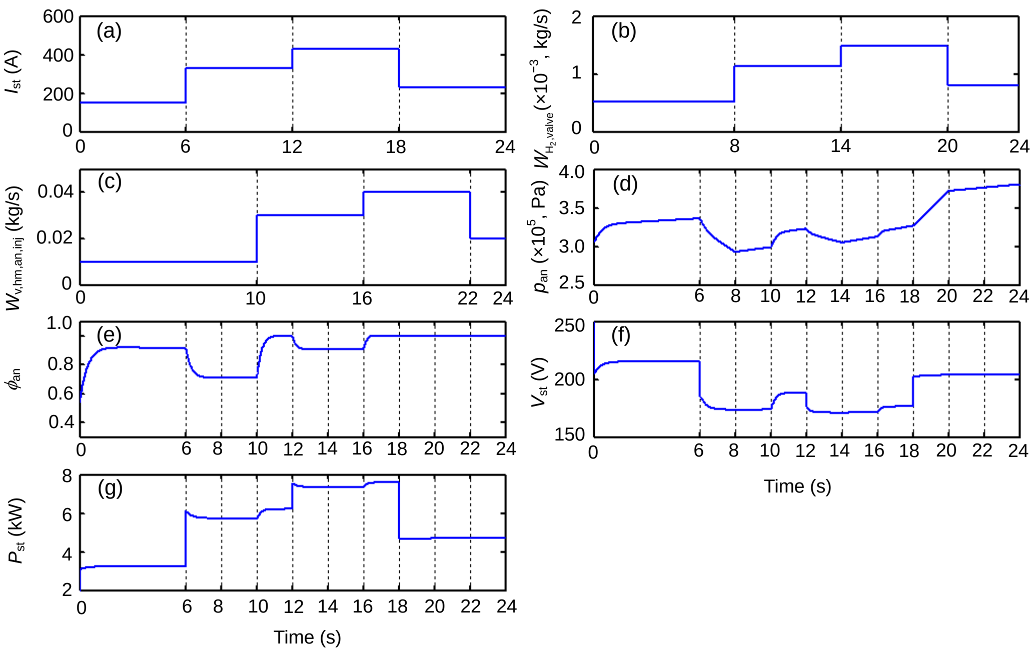

Fig. 8 Results of the anode side dynamic simulation test
(a) System current; (b) Hydrogen flow through the second valve; (c) Water injected into the hydrogen humidifier; (d) Anode pressure; (e) Anode humidity; (f) Stack output voltage; (g) Stack output power

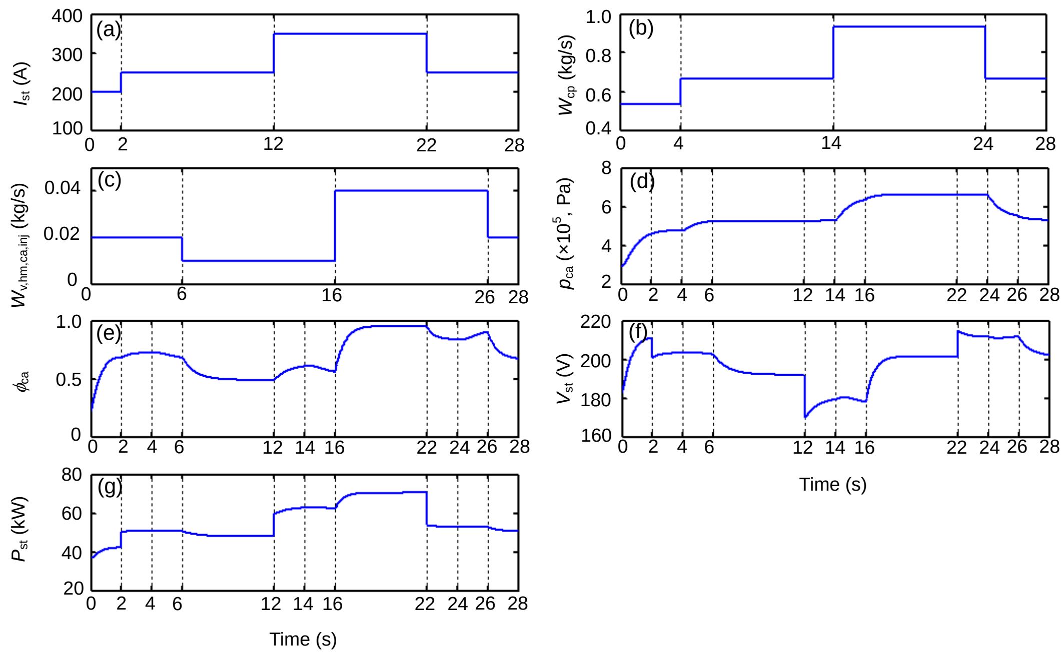

Fig. 9 Results of the cathode side system dynamic simulation test

(a) System current; (b) Air flow in compressor outlet; (c) Water injected into the air humidifier; (d) Cathode pressure; (e) Cathode humidity; (f) Stack output voltage; (g) Stack output power

increasing with the sudden increase of I_{st}, because more oxygen is consumed in the electrochemical reaction in the cathode, and then the oxygen partial pressure decreases. But at t=12 and 22 s, there is no clear change in p_{ca}. This can be explained as follows. The cathode pressure p_{ca} is the sum of the partial pressures of nitrogen, oxygen, and water. The electrochemical reaction rate increases with the current, which causes the oxygen partial pressure to decrease as more oxygen is consumed, and the water partial pressure to increase as more water is generated and flows from the anode to the cathode. The water partial pressure is also affected by the pressure difference between the anode and cathode. As a result, there is a total effect of I_{st} on p_{ca}, which is not simple as p_{ca} increases with I_{st} or decreases with I_{st}. The relationships between V_{st}, P_{st}, and I_{st} are observed especially at t=2, 12, and 22 s, which conform to the stack output polarization characteristics.

2. As shown in Fig. 9, p_{ca} increases or decreases suddenly at t=4, 14, and 24 s with the step increase or decrease in W_{cp}, due to the sudden increase or decrease in oxygen mass, or oxygen partial pressure, in the cathode flow. According to the principle of PEMFC, V_{st} should increase with p_{ca}, but there are no obvious changes in V_{st} and P_{st} at t=14 s. We can see that ϕ_{ca} then begins to decrease, which affects the response of V_{st}.

3. At t=6, 16, and 26 s, with the sudden decrease or increase in $W_{v,hm,ca,inj}$, there is a sudden decrease or increase in ϕ_{ca}. These changes are due to the decrease and the increase of the water mass, or water partial pressure in the cathode flow. The relationships between V_{st}, P_{st}, and ϕ_{ca} conform to the stack operation principle.

Based on these simulation results, the dynamic characteristics of the cathode side are more complex than those of the anode side. This is because of more equipment, a longer supply manifold, the presence of an exhaust exit, and the use of air, not oxygen, as the oxidant on the cathode side. The responses of the cathode pressure, humidity, and the stack voltage and power to all the adjustable parameters in the simulation test were in agreement with the system operating rules. The system model describes well the dynamic characteristics of the cathode side.

5 Conclusions

A 60 kW PEMFC generation system is currently at the stage of design and simulation research. System simulation tests show that the system model built in a MATLAB/SIMULINK environment can approximate the dynamic responses of the generation system. The simulation system is consistent with published data and operational experience of the system performance and characteristics, and can be used for system dynamic analyses and design. Moreover, the system simulation tests show that the dynamic behavior of a PEMFC generation system is very complex, so a comprehensive control design is very important for achieving ideal operation and high efficiency.

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