

Performance Analysis and Control Structure Design for Proton Exchange Membrane Fuel Cell

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A proton exchange membrane fuel cell (PEMFC) is regarded as a highly efficient power generation device. The performance of PEMFC depends on various key operating parameters, such as pressure, flow rate and humidity of reactant gases, and cell temperature (60 - 100 °C). Generally, the cell temperature is known to have an importance on transportation within the PEMFC and its performance. The fuel cell temperature should be limited under a working temperature that does not affect the material properties of the components. Therefore, the aim of this study is to perform the control structure design of the PEMFC. The steady-state analysis is done to find the suitable operating conditions of the PEMFC. The effect of input parameters on cell voltage and cell temperature is analyzed to investigate the dynamic behavior of PEMFC that is important for control design. To obtain an efficient control system, the suitable controlled and manipulated variables of the PEMFC are determined via the control structure design approach. The selection of input-output pairings is based on the relative gain array (RGA) as a controllability index. The results show that the cell voltage and cell temperature depend on the inlet molar flow rates and temperatures of hydrogen and air, and operating current density. According to the RGA, the inlet molar flow rates of air and hydrogen are manipulated variables to regulate the cell temperature and partial pressure of hydrogen, respectively.

1. Introduction

Fuel cells have been received great attention due to the promising alternative to traditional energy conversion technology. Among the various fuel cell types, the polymer exchange membrane fuel cell (PEMFC) has attracted considerable interest because of its high energy efficiency, low emission of pollutants to the environment, quick start-up and low-temperature operation (60 - 100 °C). It is also a promising fuel cell type for automotive, residential and portable applications due to its high power density and rapid response to changes in power demand (Arpornwichanop et al., 2014).

Regarding the control design of the PEMFC, the dynamic behavior is critical and the control system is needed to provide that the flow rates and temperatures of fuel and air can be stabilized during normal operation at variable loads, as well as during system start-up and shut-down. Fuel and air fed into the fuel cell have to be controlled in order to keep the cell temperature, hydration of the membrane and the reactants in a good level to avoid membrane degradation and to maintain efficiency of the PEMFC system (Gruber et al., 2008). Moreover, the cell temperature involves the rate of the electrochemical reaction and the transport of protons in the membrane, leading to the enhanced PEMFC performance. However, the cell temperature can affect the material properties of components when it is too high.

In the past, various control strategies have been proposed for PEMFC, but less attention has been given to the control structures design. To obtain the efficient control of the PEMFC system, the control structure design including the selection of manipulated variables, controlled variables, control configuration, and controller type is necessary (Chatrattanawet et al., 2014).

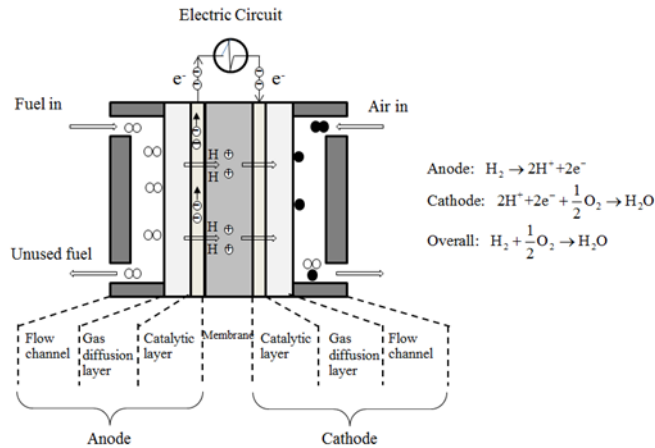


Figure 1: The structure of PEMFC.

The purpose of this study is to implement the control structure design to determine the good controlled and manipulated variables for PEMFC. The performance of PEMFC is first analyzed under steady-state and dynamic behaviors to find the optimal operating points. The analysis of the steady-state relative gain array (RGA) is used for pairing of the controlled and manipulated variables. The control structure is step-by-step designed using the method proposed by Skogestad (2004).

2. Proton exchange membrane fuel cell

PEMFC can convert the chemical energy of a fuel and an oxidant into electrical energy. The PEMFC structure consists of seven components: anode flow channel, gas diffusion layer (GDL) of anode, anode catalytic layer, membrane, cathode catalytic layer, GDL of cathode, and cathode flow channel, as can be seen in Figure 1. The membrane electrode assembly (MEA) where the electrochemical reaction occurs is the critical interface between the membrane and the electrodes. At the anode side, the fuel or hydrogen is continuously supplied while the oxidizer or oxygen in air is supplied at the cathode side. Hydrogen flows through gas channel on the anode side and diffuses through diffusion layer to the catalytic layer where it is oxidized to form proton and electrons. Proton ions are transferred through the membrane to the catalytic layer of cathode while electrons pass through the current collector and external circuit to the cathode. At the cathode side, oxygen is reacted with protons ions and electrons to form water.

3. PEMFC model

The dynamic model of PEMFC includes the mass balances for describing gas variation, the energy balance, and the electrochemical model (Khan and Iqbal, 2004). Several assumptions are made as: (i) the fuel cell is described by a lumped model; (ii) all gases behave as the ideal gas; (iii) pure hydrogen is fed to the anode and air is supplied to the cathode; (iv) the outlet temperatures of hydrogen and oxygen are equal to the cell temperature and (v) the membrane is fully saturated with water.

3.1 Mass balances

The transient dynamics in the anode and cathode channels are studied. In the anode channel, it is simplified by assuming pure hydrogen (99.99%) flows into the channel. Then, hydrogen diffuses through the anode electrode into the anode active layer where it is consumed by the electrochemical reaction. Therefore, the dynamic change in the partial pressure of hydrogen (p_{H_2}) at the anode is as:

$$\frac{dp_{H_2}}{dt} = \frac{RT}{V_{an}} \left(\dot{m}_{H_2, in} - k_{an} (p_{H_2} - p_{atm}) - \frac{jA}{2F} \right) \quad (1)$$

The dynamic of the partial pressure of oxygen (p_{O_2}) at the cathode when oxygen in air flows into the channel can be described as:

$$\frac{dp_{O_2}}{dt} = \frac{RT}{V_{ca}} \left(\dot{m}_{O_2, in} - k_{ca} (p_{O_2} - p_{atm}) - \frac{jA}{4F} \right) \quad (2)$$

where $\dot{m}_{H_2,in}$ and $\dot{m}_{O_2,in}$ denote the inlet molar flow rates of hydrogen and oxygen (mol/s), respectively, T is the cell temperature (K), j is the current density (A/cm²), p_{atm} is the ambient pressure (atm), R is the gas constant (J/mol K), F is the Faraday constant (C/mol), A is the active area (cm²), k_{an} and k_{ca} are the flow constant for anode and cathode (mol/s atm), and V_{an} and V_{ca} are the anode and cathode volume (m³), respectively.

3.2 Thermal model

The heat produced from the electrochemical reaction causes the PEMFC temperature increase and can affect a membrane degradation. In this study, the temperature is defined as one of the state variables and a control strategy is developed to manage the transient thermal behavior of the PEMFC. The energy balance of the PEMFC can be written as:

$$C_i \frac{dT}{dt} = P_{tot} - \dot{Q}_{elec} + \dot{Q}_{in} - \dot{Q}_{out} - \dot{Q}_{loss} \quad (3)$$

The total energy (P_{tot}) is calculated by the product of the reaction heat (ΔH) and the molar flow rate of reacted hydrogen ($\dot{m}_{H_2,react}$). The electrical power output (\dot{Q}_{elec}) generated by the fuel cell can be expressed in Eq(5).

Heat loss (\dot{Q}_{loss}) at the stack surface is described in Eq(6) where T_{amb} is the ambient temperature and R_t is the thermal resistance of the cell stack.

$$P_{tot} = \dot{m}_{H_2,react} \Delta H = \frac{jA}{2F} \Delta H \quad (4)$$

$$\dot{Q}_{elec} = jVA \quad (5)$$

$$\dot{Q}_{loss} = \frac{(T - T_{amb})}{R_t} \quad (6)$$

The input heat flow rate (\dot{Q}_{in}) and the output heat flow rate (\dot{Q}_{out}) by the reactant can be described as:

$$\dot{Q}_{in} = (\dot{m}_{H_2,in} c_{p,H_2} + \dot{m}_{H_2O,an,in} c_{p,H_2O}^g)(T_{H_2,in} - T_0) + (\dot{m}_{O_2,in} c_{p,O_2} + \dot{m}_{N_2,in} c_{p,N_2} + \dot{m}_{H_2O,ca,in} c_{p,H_2O}^g)(T_{air,in} - T_0) \quad (7)$$

$$\dot{Q}_{out} = (\dot{m}_{H_2,out} c_{p,H_2} + \dot{m}_{H_2O,an,out} c_{p,H_2O}^g + \dot{m}_{O_2,out} c_{p,O_2} + \dot{m}_{N_2,out} c_{p,N_2} + \dot{m}_{H_2O,ca,out} c_{p,H_2O}^g + \dot{m}_{H_2O,ca,out}^{gen} c_{p,H_2O}^{liq})(T - T_0) \quad (8)$$

where c_{p,H_2} , c_{p,O_2} , c_{p,N_2} , and c_{p,H_2O} denote the specific heat of hydrogen, oxygen, nitrogen, and water, g and liq denote gas and liquid states, respectively, and $T_{H_2,in}$ and $T_{air,in}$ are the inlet temperatures of hydrogen and air, respectively.

The input molar flow rate of vapor is expressed as follow:

$$\dot{m}_{H_2O,an,in} = \left[\frac{\varphi_{an} P_{sat}(T_{an,in})}{P_{an} - \varphi_{an} P_{sat}(T_{an,in})} \right] \dot{m}_{H_2,in}, \quad \dot{m}_{H_2O,ca,in} = \left[\frac{\varphi_{ca} P_{sat}(T_{ca,in})}{P_{ca} - \varphi_{ca} P_{sat}(T_{ca,in})} \right] \dot{m}_{air,in} \quad (9)$$

The water generation rate and the output molar flow rate of vapor can be described by Eqs(10) and (11).

$$\dot{m}_{H_2O,ca,out}^{gen} = \frac{jA}{2F} \quad (10)$$

$$\dot{m}_{H_2O,an,out} = \dot{m}_{H_2O,an,in} - \left[\frac{\varphi_{an} P_{sat}(T)}{P_{an} - \varphi_{an} P_{sat}(T)} \right] \dot{m}_{H_2,react}, \quad \dot{m}_{H_2O,ca,out} = \dot{m}_{H_2O,ca,in} - \left[\frac{\varphi_{ca} P_{sat}(T)}{P_{ca} - \varphi_{ca} P_{sat}(T)} \right] \dot{m}_{O_2,react} \quad (11)$$

3.3 Electrochemical model

The electrochemical model for PEMFC is shown in Table 1. The cell voltage (V_{cell}) decreases from its open-circuit voltage (E) that is the maximum voltage due to activation overpotentials (V_{act}), ohmic losses (V_{ohm}), and concentration overpotentials (V_{con}). The activation overpotentials are caused by the slowness of the reactions taking place on the surface of the electrodes. The ohmic losses arise from the resistance of membrane to the transfer of proton and the resistance of the electrode and collector plate to the transfer of electron. Moreover, the concentration overpotentials are the result of the mass transport of gases to the reaction.

Table 1: Electrochemical models for PEMFC

Parameters	Equations*
Output voltage	$V_{cell} = E - V_{act} - V_{ohm} - V_{con}$ (12)
Open circuit voltage	$E = 1.229 - 8.5 \times 10^{-4} (T - 298.15) + \frac{RT}{2F} \ln [p_{H_2} p_{O_2}^{0.5}]$ (13)
Activation overpotentials	$V_{act} = -[\xi_1 + \xi_2 T + \xi_3 T \ln c_{O_2} + \xi_4 T \ln(jA)]$ (14)
	$\xi_1 = -0.948$
	$\xi_2 = 0.00286 + 0.0002 \ln(A) + 4.3 \times 10^{-5} \ln c_{H_2}$
	$\xi_3 = 7.6 \times 10^{-5}$
	$\xi_4 = -1.93 \times 10^{-4}$
Ohmic losses	$V_{ohm} = jR_{int}$ (15)
	$R_{int} = \frac{181.6 l_{mem} \left[1 + 0.03 j + 0.062 \left(\frac{T}{303} \right)^2 j^{2.5} \right]}{A [\psi - 0.634 - 3j] \exp \left[4.18 \left(\frac{T - 303}{T} \right) \right]}$
Concentration overpotentials	$V_{con} = \frac{RT}{2F} \ln \left(1 - \frac{j}{j_{max}} \right)$ (16)

*It is noted that c_{O_2} and c_{H_2} are the concentrations of oxygen and hydrogen at the catalytic interface of the cathode and anode, respectively. l_{mem} is the membrane thickness and ψ denotes the function of membrane humidity and stoichiometric ratio (usually from 10 to 23).

4. PEMFC performance

4.1 Model validation

To confirm that the PEMFC model used in this study can reliably predict the performance of the PEMFC. The simulated polarization curve is compared with the experimental data (Mueller et al., 2007) under the range of current densities from 0 to 1 A/cm² as shown in Figure 2. It is observed that the simulated polarization curve shows a good agreement with the experimental polarization curve. The minor errors at the low and high current densities are caused by the estimated parameters, especially in the electrochemical model.

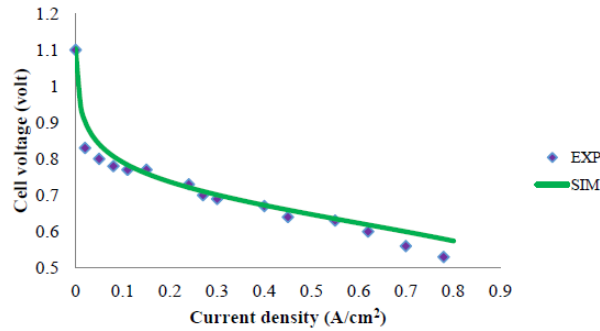


Figure 2: Comparison between the model prediction and experimental data from Mueller et al. (2007).

4.2 Steady state analysis and dynamic behavior

The performance analysis of the PEMFC at steady state conditions is performed and used to select its optimal operating conditions. Figure 3 shows the cell voltage, power density, and temperature as a function of the current density. It is revealed that the current density increases with decreasing cell voltage due to the concentration losses. The cell temperature increases at high current density because the electrochemical reactions are more pronounced. In this work, the steady-state operating points are selected at current density, $j = 0.51$ A/cm², cell voltage, $V = 0.59$ V, power density, $P = 0.30$ W/cm², and cell temperature, $T = 332$ K.

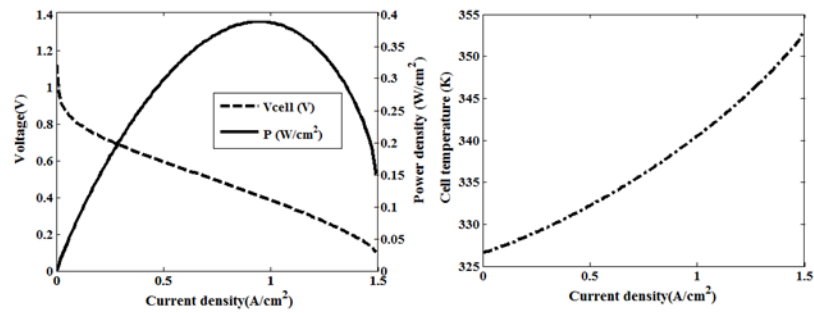


Figure 3: The cell voltage, power density, and the cell temperature as a function of the current density.

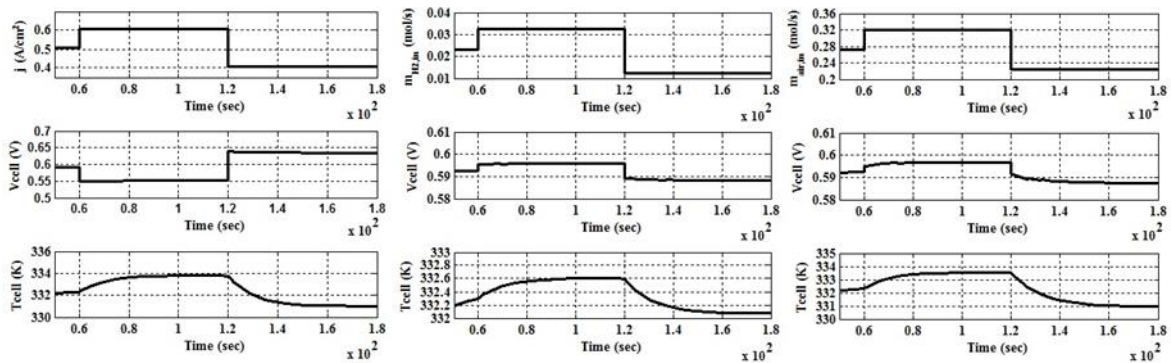


Figure 4: The responses of the cell voltage and cell temperature due to step changes of current density and flow rates of hydrogen and air

Next, the dynamic responses of the cell voltage and cell temperature are discussed. The dynamic responses are analyzed under a variation of various inputs, such as current density and flow rates of hydrogen and air. Figure 4 shows the effects of these inputs on the cell temperature and voltage. When the current density increases, the voltage rapidly decreases due to large concentration overpotentials, whereas the cell temperature increases because of an increase in the hydrogen consumption by the electrochemical reaction (exothermic reaction). The increased inlet flow rates of hydrogen and air can improve cell performance in terms of the cell voltage and temperature because they can increase the partial pressures of hydrogen, oxygen and membrane conductivity and excess water can be removed.

5. Control structure design

The stepwise procedure of Skogestad (2004) for selecting an active constraint and a self-optimizing variable is presented. Moreover, the relative gain array (RGA) considered as a controllability index for the selection of input-output pairings is also implemented.

5.1 Self-Optimizing control

The self-optimizing control is used to alter the controlled variables for PEMFC.

Step 1: Define the cost J and constraints. With a given load (current density), an economic cost function J is defined to minimize the cost of the hydrogen feed minus the power value, subject to the constraints on the cell temperature kept constant at 332 K.

Step 2: Identify the degree of freedom. At steady state, there are two operational degrees of freedom; the inlet flow rates of hydrogen and air. We have to optimize the system in detail, the fuel cell temperature constraint of $T = 332$ K is assumed to always be active.

Step 3: Identify importance disturbances. The main disturbances are the current density and the temperatures of hydrogen and air.

Step 4: Solve the optimization problems when the PEMFC is operated with/without disturbances.

Step 5: Identify candidate controlled variables. The cell temperature is active constraint. The following candidates for the controlled variable are considered three alternatives that are partial pressure of hydrogen (p_{H_2}), partial pressure of oxygen (p_{O_2}), and cell voltage (V).

Step 6: Evaluation of loss. The loss, $L(u,d) = J(u,d) - J_{opt}(d)$ is calculated with each of the candidate variables kept constant at their nominal optimal value. The results of the loss for alternative controlled variables show that the partial pressure of hydrogen is selected as self-optimizing variable because it results in a small economic loss.

Step 7: Evaluation and selection. This is the pairing issue which is discussed on "controllability analysis".

5.2 Controllability analysis

Relative gain array (RGA) is chosen as the controllability index for the selection of control pairing. Generally, the RGA formed in the gain matrix close to the unity matrix is preferred but control structures with high RGA elements should be avoided. A change in manipulated variables impacts all of the controlled variables; therefore, pairing of the controlled and manipulated variable is important for minimizing the interactions in PEMFC system. In this work, the cell temperature (y_1) and partial pressure of hydrogen (y_2) as the controlled variables are needed to be regulated by manipulating inlet flow rates of hydrogen (u_1) and air (u_2) as the manipulated variables. The result of the RGA is 1 for the diagonal pairings (u_1 - y_2 , u_2 - y_1). This implies that the partial pressure of hydrogen is controlled by using the inlet flow rate of hydrogen as manipulated variable. The cell temperature is controlled by using the inlet flow rate of air as manipulated variable.

6. Conclusions

In this work, the performance analysis and control structure design for PEMFC are performed. The steady state analysis is used to select the optimal operating point of the PEMFC. The dynamic responses of PEMFC in terms of the cell voltage and temperature are investigated with respect to a step change in current density and inlet molar flow rates of air and fuel. Moreover, the self-optimizing control is implemented to find good controlled variables and RGA as the controllability index is also used to pairing suitable input-output. The results show that the cell temperature and fuel cell voltage are dependent on the fuel and air inlet flow rates as well as current density. The cell temperature is selected as an active constraint that should be maintained at its setpoint. Furthermore, the partial pressure of hydrogen is selected as good controlled variable based on the self-optimizing concept. According to the RGA, the inlet molar flow rates of hydrogen and air are the manipulated variables to control the partial pressure of hydrogen and the cell temperature, respectively.

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