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System-Level Performance Analysis of a Proton Exchange Membrane Fuel Cell System

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ABSTRACT

This report presents a performance analysis of a proton exchange membrane fuel cell (PEMFC) system, using GCtool software, from a system-level perspective. By systematic formulation, most of the operating parameters are derived through fuel cell equations and from empirical data. The most critical parameters are the working pressure and temperature of the fuel cell as well as the pressure gap across the cell membrane. When given a 100kW PEMFC stack with 45% efficiency and 80% fuel utility, the working pressure and its difference are selected at 4 atm and 0.1 atm via the system-level performance analyses. The selection of the working temperature of the PEMFC should take both thermal stability and humidity management into consideration. A PEMFC system with certain auxiliaries can achieve an estimated efficiency of more than 49%. It was found that the efficiency of the PEMFC system can be promoted with an increase in the working temperature.

***Key Words*: proton exchange membrane fuel cell (PEMFC), system-level performance, GCtool**

質子交換膜燃料電池系統的系統層次性能分析

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摘　要

本論文係從系統層次的觀點，運用 GCtool 軟體來進行質子交換膜燃料電池系統的生能分析，經由系統化的公式推導，燃料電池多數的操作參數可以由燃料電池方程式及經驗值獲得，其中最重要的參數爲燃料電池的工作壓力、溫度和質子交換膜兩面的壓力差。以一個 100 kW、轉換效率 45%、燃料使用率 80% 的質子交換膜燃料電池堆爲例，經由系統層次的性能分析，其最佳的操作壓力及電極兩端的壓力差分別爲 4 大氣壓力和 0.1 大氣壓力。質子交換膜燃料系統包含輔助設備的全系統轉換效能可達 49%，同時隨著操作溫度的增加，全系統的轉換效率可以再提昇，工作溫度的選擇需考量熱穩定和濕度管理。

關鍵詞：質子交換膜燃料電池，系統層次性能，GCtool

I. INTRODUCTION

With increasing concerns about global warming and environmental pollution, the incentives to develop power generation systems with high efficiency and with low emission are of great importance. Fuel cell systems (FCSs), which have the advantages of low emissions and high efficiency of energy conversion, are publicly intended for stationary and mobile power production. FCSs complement the internal combustion engines (ICEs) in order to reduce the ubiquitous dependence on fossil fuels, and thus have important and significant implication in both environmental implication and energy security. Particularly, proton exchange membrane fuel cell (PEMFC), also known as polymer electrolyte membrane fuel cell, can operate at relatively low temperature and allow for a fast start-up. With the advantage of high current density, fast start-up, and compactness, PEMFC is currently considered to be the most promising solutions for providing environmentally friendly power energy for hybrid and electrical vehicles [8]. In fact, a large number of open literatures have focused on the steady-state and dynamic performance analysis of a PEMFC cell or stack level from analytical and experimental point of view. They have drawn a lot of attention to the improvement by investigating the important working parameters of fuel cell (FC) itself such as operating pressure and temperature of FC, flow rate and humidity of inlets under different steady-state operating conditions [3, 5, 7, 10-14]. Recently, PEMFC systems are being actively developed with combined heat and power (CHP) systems which include some auxiliary subsystems such as compressor, gas-turbine, and condenser, etc. The operating parameters of a PEMFC system can be well controlled at desired operating conditions by supplementary units. This makes the operating variables of PEMFC controllable during the utilization. Therefore, the overall performance analysis of a PEMFC system from a system-level standpoint is becoming more and more important.

The challenge for a designer of energy system is to organize the various components in a system configuration that optimizes the efficiency of fuel cell, utilizes heat to the best extent, and minimizes the heat loss to the external environment. It is well known that it will be costly and time-consuming to perform experiments of systematic studies to obtain an optimal set of system parameters. It is better to conduct system simulations and analyses to reduce the number of experiments when many parameters are investigated. The GCtool (General Computational Toolkit) software package, which is developed by Argonne National Laboratories [6], allows for several defined inputs to conduct the comprehensive system design and analysis for fuel cell and power generation systems. There were some works [1, 4, 17] mainly using GCTool for investigating the comprehensive performance of a PEMFC-based FCS which consists of a fuel processor, PEMFC stack, and other supplementary instruments for different configurations and operating conditions. In fact, Larminie and Dicks [8] have well derived some operating parameters of a PEMFC system in the form of equations. For example, the amounts of hydrogen and oxygen usage are uniquely dependent on both output power and operating voltage of PEMFC stack, and then the air supply is related to the oxygen usage and air stoichiometry in practical applications. With the desired output power of PEMFC, the supply of fuel and air is transparently determined. In other words, some operating parameters can be formulated by taking systematic and practical considerations into consideration. These motivate us to develop a systematic procedure for the performance analyses of a PEMFC system from a system-level point of view.

The main contribution of this paper is to conduct the system-level performance analyses of a PEMFC system using GCtool software. The remainder of this paper is organized as follows. For easy presentation, the block diagram and some useful equations of a PEMFC system are addressed in Section II. In addition, the air, water, and thermal management for the PEMFC system are considered. Section III demonstrates the model and some simulation results for the PEMFC system using GCtool software package. An optimal working condition is found and some interesting issues are also discussed. Finally, brief conclusions are drawn in Section IV.

II. SYSTEM DESCRIPTION AND FORMULATION

With the remarkable benefits such as compactness, fast start-up, and high current density, PEMFC is a kind of purely hydrogen-fueled fuel cell which is suitable for powering vehicles for the future transportation. Hydrogen-fuelled fuel cell vehicles (H_2-FCVs) are actively being developed to meet the promise of greatly reduced environmental pollution and ever-increasing dependence on fossil energy. In general, PEMFC systems with auxiliaries can operate at ambient pressure for automotive propulsion and other power systems, whereas pressurized PEMFC systems significantly improves the improves power density and performance [2]. For H_2-FCVs applications, pure hydrogen is mainly stored in a pressurized cylinder. Even for an on-board fuel processing system (FPS) configuration, the purified reformate stream can be pressurized by a compressor. Therefore, the scope of this paper is focused on a pressurized hydrogen-fueled PEMFC system. Some working parameters of a PEMFC system are interactive each other and are closely related to the auxiliaries. For example, the mass flow rates of fuel and oxygen are dependent on the FC output power and voltage. The pressure of compressor is designed to provide a minimum pressure difference across the membrane. It would be better to develop a systematic procedure to evaluate the respective impacts of parameters and configuration from a system-level standpoint.

1. PEMFC System

For a system designer, the first stage is to analyze the possible chemical processing requirements and to arrange a system configuration disposing of all the process streams. Figure 1 shows a block diagram of hydrogen-fed PEMFC system. In general, most small PEMFCs (<1kW) are operated at atmospheric pressure. The larger PEMFCs are sometimes operating at higher pressures in order to increase the specific power and enhance fuel cell performance. As shown in Fig. 1, the pressurized hydrogen gas in a high-pressure container is directly fueled into a PEMFC stack and the ambient air is drawn and compressed by consuming some electrical power. Using a turbine-compressor, the energy of the PEMFC stack's exhaust gases is recovered and harnessed to increase the system efficiency.

2. Systematic Formulation

Larminie and Dicks derived some useful PEMFC equations. At the anode of a PEMFC, the hydrogen gas ionizes, release electrons and creates H^+ ions; at the cathode part, oxygen in the inlet air reacts with H^+ ions from the solid electrolyte and electrons form the electrode. The chemical reactions occurring in the process are described as follows.

Anode: $$2H_2 \rightarrow 4H^+ + 4e^- \quad (1)$$

Cathode: $$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O \quad (2)$$

Overall: $$2H_2 + O_2 \rightarrow 2H_2O \quad (3)$$

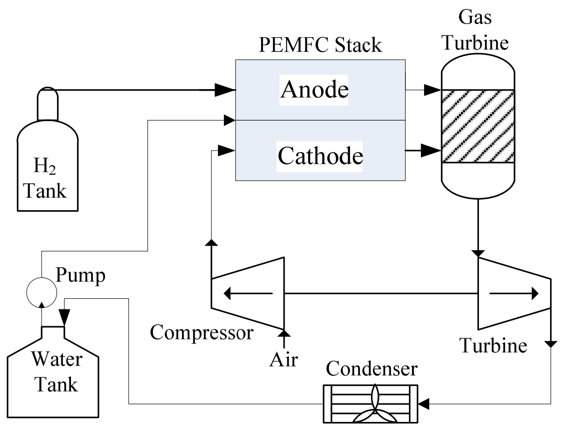

Fig. 1. Schematic diagram of PEMFC system

That is to say, two moles of hydrogen exactly reacts one mole of oxygen and literally produces 4F of charge for a single cell. For a PEMFC stack of *n* cells, the reacting mass flow rates of hydrogen and oxygen can be formulated as

$$\dot{m}_{H_2} = 1.05 \times 10^{-8} \times \frac{P_c}{V_c} (\text{kg/s}) \quad (4)$$

and

$$\dot{m}_{O_2} = 8.29 \times 10^{-8} \times \frac{P_c}{V_c} (\text{kg/s}) \quad (5)$$

where P_c and V_c are the electrical power and average voltage of PEMFC stack. For a practical application, the oxygen can be normally derived from ambient air. The mass flow rate of required air can be calculated by

$$\dot{m}_{\text{air}} = 3.57 \times 10^{-7} \times \frac{P_c}{V_c} (\text{kg/s}) \quad (6)$$

In practice, the air is often supplied at greater than the stoichiometric rate. The mass rate of inletting air can be determined by

$$\dot{m}_{\text{air}} = \lambda \times 3.57 \times 10^{-7} \times \frac{P_c}{V_c} (\text{kg/s}) \quad (7)$$

where λ is the air stoichiometry, typical twice as much. In general, the pressurized hydrogen gas comes from a high-pressure hydrogen container and the air must be compressed by a compressor. From the safety standpoint of PEMFC operation, the pressure difference between the anode and cathode sides must be less than 1 atm (atmospheric pressure) for fear of cell's structural destruction. In addition, the pressure of cathode side is 0.1 atm higher than one of anode side to keep appropriate humidification of a PEMFC stack and to make oxygen easily diffusing into the membrane. Therefore, the pressure in the anode and cathode sides can be assumes to be as

$$p_{\text{CA}} = p_{\text{AN}} + \varepsilon \quad (8)$$

where ε is the gas pressure between anode and cathode sides, $0.1 \le \varepsilon < 1$.

For a hydrogen-fuelled fuel cell, the fuel cell efficiency is given by

$$\eta = \mu_f \frac{V_c}{1.48} \times 100\% \quad (9)$$

where μ_f is the fuel utilization coefficient in a PEMFC stack. A good estimate for μ_f is 0.95. In general, PEMFCs have efficiency ratings from 40% to 50%. It is assumed in this study that the efficiency of a PEMFC is 45%. Therefore, the operating voltage of a PEMFC stack can be properly chosen by both fuel utilization and PEMFC efficiency. In addition, the inletting mass flow rates of hydrogen and oxygen can be calculated using both given electrical power and efficiency of a PEMFC stack. On the other hand, a simple equation has been found to give an excellent description for the operating voltage of a fuel cell at a current density. FC voltage is determined using a polarization curve based on the reversible cell voltage, activation losses, ohmic losses, and concentration losses. Given a current density i for a low-temperature FC, the cell voltage V_c is calculated [9]

$$V_c = E_{OC} - b\ln(i) - iR - m\exp(ni) \quad (10)$$

where E_{OC} is the reversible open circuit voltage (OCV) of a hydrogen fuel cell, b is the slope of the Tafel equation, R is the area-specific resistance (ASR), m and n are the constants in the mass-transport overvoltage equation. The example values of the coefficients for a Ballard Mark V fuel cell stack are given in Table 1. For easy formulation, I reformulate the current density using a function of cell voltage with a polynomial of degree 5 that is given by

$$i = -50438V_c^5 + 183460V_c^4 - 245080V_c^3 + 147120V_c^2 - 40030V_c + 4990.2 \quad (11)$$

Fig. 2 shows there is the good quality of curve fitting between Eqs. (10) and (11). After the operating voltage V_c being determined, the current density can be approximately calculated by Eq. (11).

Table 1. Values for coefficients of Ballard Mark V PEMFC

Constants	Values
E_{OC} (V)	1.05
A (V)	4.01×10^{-2}-$1.4\times10^{-4}T$
R (kΩcm^2)	4.77×10^{-4}-$3.22\times10^{-6}T$
m (V)	1.1×10^{-4}-$1.2\times10^{-6}T$
n (cm^{2}mA^{-1})	8×10^{-3}

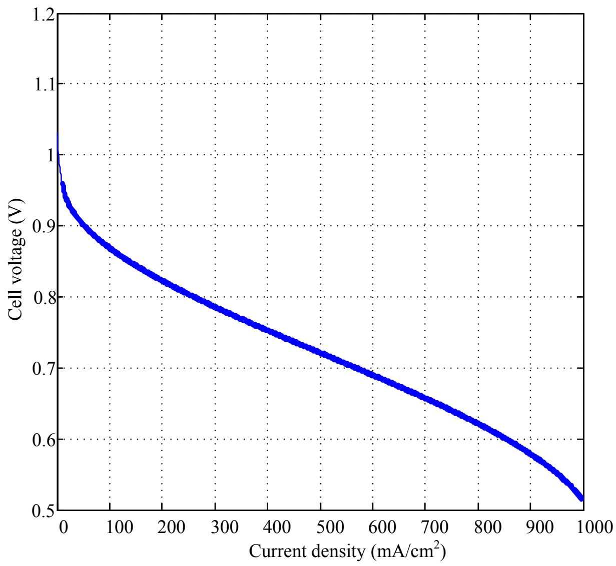

Fig. 2. Fuel cell voltage versus current density for a Ballard Mark V PEMFC

III. GCTOOL MODELING AND SIMULATION ANALYSIS

1. GCtool Modeling

Figure 3 shows the resulting modeling for a PEMFC system configuration using GCtool. Pure hydrogen (H2_Fuel) is directly fed into the anode of a PEMFC stack (PEMFC) as fuel. The ambient air (Air) is compressed by a two-stage compressor (Compressor) and is fueled into the cathode of the PEMFC stack. In addition, cooling air (Compressor_Air) is drawn by a circulating fan (Cpmpressor_Fan) through intercoolers. The pressurized hydrogen and compressed air flow through the anode and cathode of PEMFC stack. Both un-reacted air and product water from the cathode are split (Cathode_Splitter) and are mixed with the gas turbine (GT_Mixer) and the water-recovered condenser (Condenser_Mixer), respectively. The un-reacted hydrogen from the anode is mixed with the exhaust air in the GT_Mixer and is harnessed with a gas turbine (Gas_Turbine) to generate an electrical power for other accessories. A splitter (GT_Splitter) is used to separate the steam and residual air. The exhaust is discharged in ambient air. The steam is recycled and mixed in the Condenser_Mixer. The condenser (Condenser) condenses the proceeding vapor into water and mixes it with the cooling water of the PEMFC stack in the mixer (Water_Mixer). A fan (Condneser_Fan) circulates ambient air (Condenser_Air) to remove the waste heat in the Condenser. The PEMFC stack is water-cooled which originates from the water tank (Water_Tank). The water is pump by a water pump (Water_Pump) through the cooling channel of a PEMFC stack.

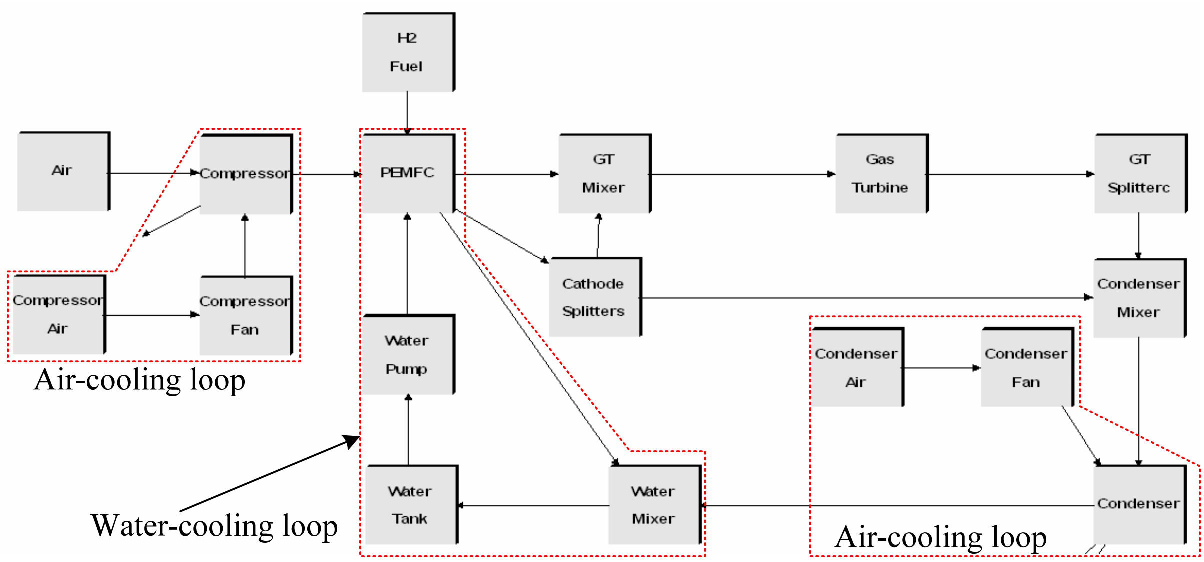

Fig. 3. Output diagram of PEMFC system using GCtool

Notice that there are three cooling systems which are circumscribed in dotted lines as shown in Fig. 3. The air-cooling system for air compressor uses a fan to circulate ambient air to the compressor to better its heat transfer. The other air-cooling system for the condenser uses a fan to circulate ambient air to condense exhaust vapor into liquid and mixed it with the cooling water of the PEMFC stack. PEMFC can be cooled by air or water. In essence, air cooling is simpler then water cooling but the former's cooling effect is less than one of latter based on the same size of cooling channel. In general, PEMFC above 5kW is water-cooled. The water-cooling system for the PEMFC stack originates from the water tank and uses a water pump to circulate water in the stack's cooling channels. The waste heat can be recovered using a heat exchanger and this makes the system efficiency more attractive. However, this will make the system more complex and costly.

2. Simulation Analysis

The optimal operating parameters of a PEMFC stack based on a steady-state model have been widely and actively studied for the attention of its performance. The most critical parameters are the working pressure and temperature of cell level, and the humidity of inlet air as well. The air humidity for a PEMFC stack can be well controlled in the range of 80-100%. It is assumed that the air fed the fuel cell is humidified to a relative humidity of 90% at the operating temperature of a PEMFC stack. By the way of systematic formulation in Section II, the cell voltage is uniquely determined by both PEMFC efficiency and fuel utility. Given a 100 kW PEMFC stack, the efficiency of PEMFC is assumed to be 45% and the utility of hydrogen fuel is 0.9. At a rated power point, the PEMFC can operate at the average cell voltage of 0.7V and the nominal temperature of 75°C. The cell voltage of PEMFC is calculated using Eq. (8) and the value is 0.701V. The current density is then obtained as 564.44mA/cm^2. Having an operating voltage of PEMFC stack, the mass flow rates of pure hydrogen and ambient air inletting into the PEMFC are only dependent on the power output of PEMFC stack. In a full-load condition, the mass flow rates of hydrogen and inlet air are calculated by Eqs. (4) and (7). With the air stoichiometry of 2, the mass flow rates of inlet fuels are $\dot{m}_{\mathrm{H_2}} = 1.426 \times 10^{-3}$ kg/s and $\dot{m}_{\mathrm{air}} = 1.039 \times 10^{-1}$ kg/s, respectively. The tunable parameters are the pressure and temperature of a PEMFC stack, as well as the pressure gap between the anode and cathode volumes. The software tool GCtool is used to analyze system-level performance of a PEMFC system with some auxiliaries.

As mentioned above, the inlet pressure of hydrogen in the anode of a PEMFC stack is determined by that of hydrogen container. The pressure of air in the cathode of a PEMFC stack is controlled by a compressor to provide a little pressure difference (0.1 atm) to make oxygen easily diffusing into the membrane and maintain approximate humidity in the membrane. In addition, the working temperature of a PEMFC stack is a key factor for its performance. Therefore, it is important to find the optimal operating pressure and the pressure difference across the membrane for different working temperatures.

A. Working pressure and temperature

Appleby and Foulkes [2] pointed out that PEMFC operating at high pressure significantly improves the reaction rate and thus FC efficiency and power density. Among well-done literatures about a PEMFC performance for different working pressure, Kaytakoğlu and Akyalçın [7] have ever conducted the experiment for the performance analysis a PEMFC system working at the pressure 5 bar (about 4.9 atm) and the temperature of 75°C. Other researches were performed under the pressure of 4 atm. However, a compressor and an electric drive motor are needed to be powered to compress to a desired level. They will consume some power and decline the overall efficiency form system-level point of view. In this paper, the working pressures are varied from 2 atm up to 6 atm with intervals of about 0.5 atm and the working temperatures are varied in the range of 70-90°C with an interval of 5°C. The working pressure is directly imposed on the hydrogen pressure. The pressure gap being 0.1 atm, the pressure being 0.1 atm higher than the working pressure is imposed on the cathode by a compressor. Figs. 4-8 show the power production of the PEMFC stack and gas turbine, the power consumption of the compressor, as well as net power production and system-level efficiency for the PEMFC system. Complying with other researches, the output power of both PEMFC stack and gas turbine are proportionally increasing with the increase of working pressure and temperature. In the PEMFC system, the compressor, the fans in the compressor and condenser, and water pump, etc, are power-consuming auxiliary devices. Being a main power-consuming component, the power consumption of compressor is shown in Fig. 6, which shows the power consumption is uniquely proportional to the working pressure. The net produced power and system efficiency of PEMFC system is also shown in Figs. 7-8. From a practical view of application, the increase of working pressure and temperature can not make sure the increase of system efficiency. The reason is that the power is consumed by the compressor is higher than the total power produced by both PEMFC stack and gas turbine at high pressure. The optimal working pressure can be selected at 4 atm. Although the system efficiency is promoted with the increase of working temperature, the temperature selection should take both thermal stability and humidity management into considerations. It is assumed that the nominal temperature of PEMFC stack at a rated power output is selected at 75°C. As the optimal working pressure is selected at 4atm from the system-level standpoint, the overall efficiency of the PEMFC system achieves over 49% as shown in Fig. 8

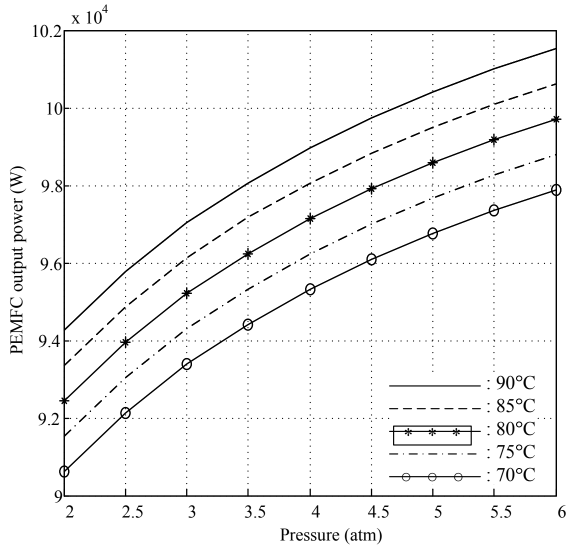

Fig. 4. Output power of PEMFC stack for different working pressure and temperatures

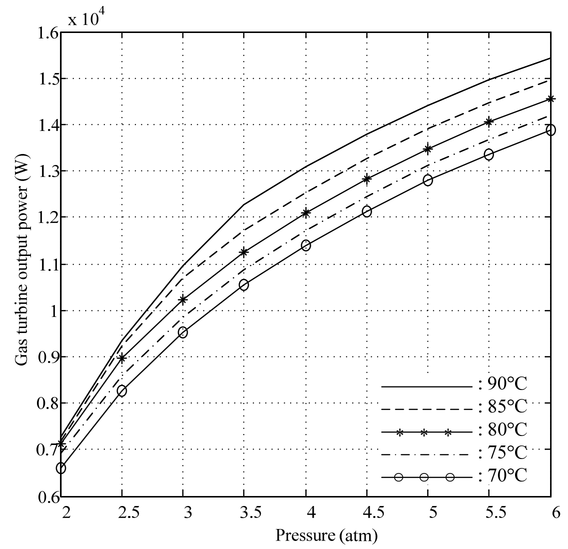

Fig. 5. Output power of gas turbine for different working pressure and temperatures

B. Pressure difference and working temperature

Among the open literatures, it seems that there is no study about the performance posed by the pressure difference across the PEMFC membrane. According to the working characters of PEMFC, the pressure of cathode must be 0.1 atmospheric pressure higher then that of anode. This makes oxygen in the air easily diffusing into the membrane and maintains a certain humidification in the membrane. However, high pressure difference makes it possible that the membrane of a PEMFC stack has a structural breakdown. In addition, it consumes some added power of compressor and electric motor

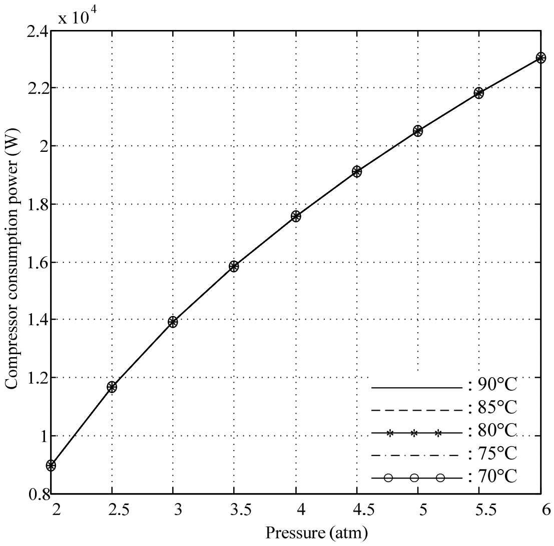

Fig. 6. Power consumption of compressor for different working pressure and temperatures

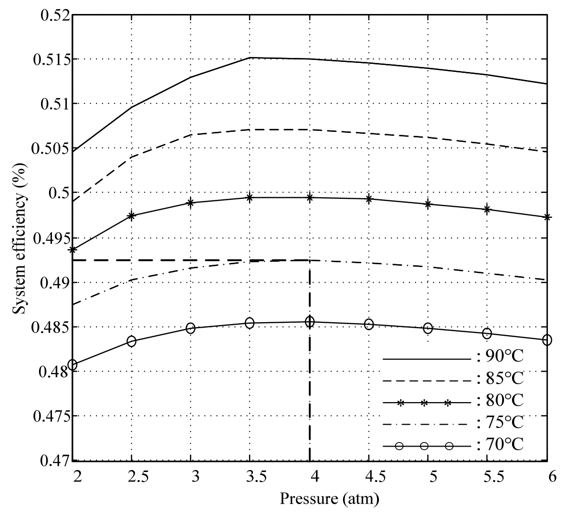

Fig. 8. Efficiency of PEMFC system for different working pressure and temperatures

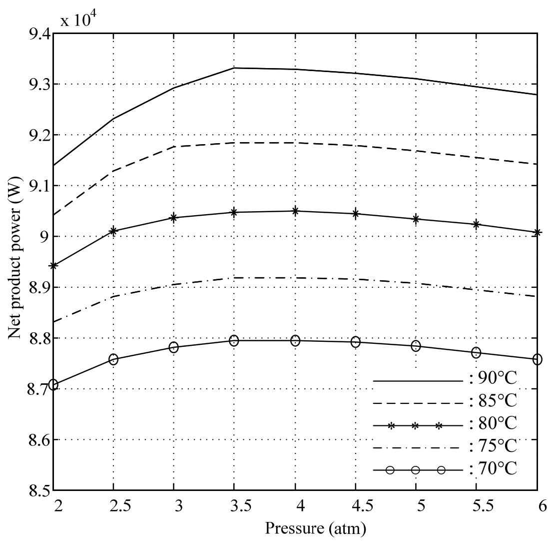

Fig. 7. Net power production of PEMFC system for different working pressure and temperatures

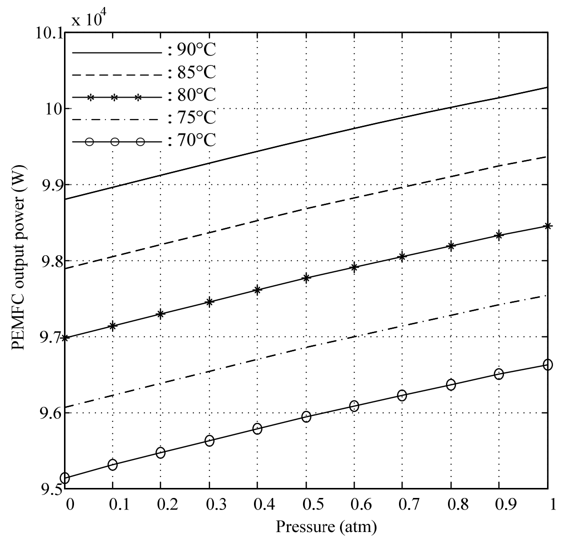

Fig. 9. Output power of PEMFC stack for pressure gap at different working temperatures

for the high pressure gap. This motivates us to analyze the effect of pressure gap on the PEMFC stack and auxiliary components from a system-level standpoint. The working pressure is set at 4 atm and the pressure gap is varied form 0 atm to 1 atm with intervals of 0.1 atm. Fig. 9 shows the output power of PEMFC stack proportionally increases with the increase of pressure gap. This means the increase of pressure gap across the membrane can promote the performance of PEMFC stack. Moreover, this reduces the remaining hydrogen fuel into the gas turbine and makes its output power as shown in Fig. 10 decrease with the increase of pressure gap. At the same time, the increase of pressure gap raises the power consumption of compressor as shown in Fig. 11. In Figs. 12-13, both net power production and system efficiency are proportionally reduced with the increase of pressure gap. Therefore, the pressure gap between anode and cathode is selected 0.1 atm with the consideration for both oxygen diffusion and humidification.

IV. CONCLUSIONS

The results of this paper indicate that the efficiency is dominantly influenced by the working temperature and pressure from a system-level point of view. The determination of working pressure may still take into account that the storage pressure of hydrogen container and/or the outlet pressure of

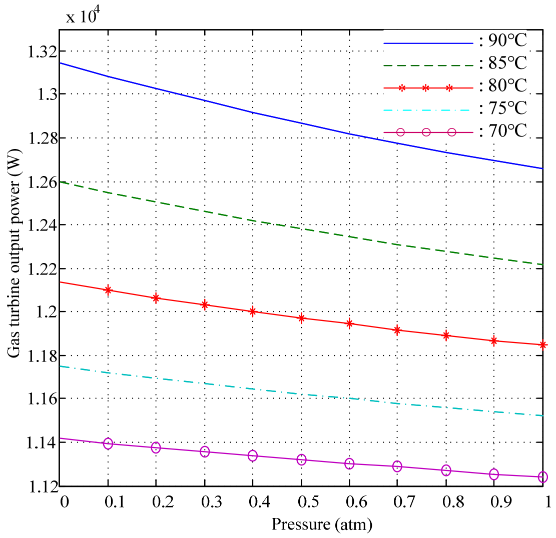

Fig. 10. Output power of gas turbine for pressure gap at different working temperatures

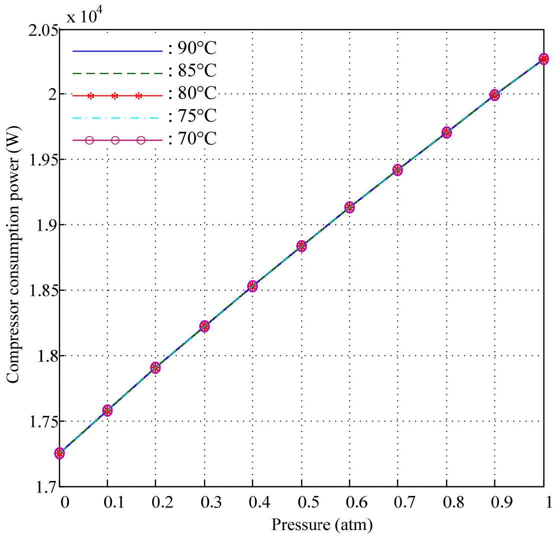

Fig. 11. Power consumption of compressor for pressure gap at different working temperatures

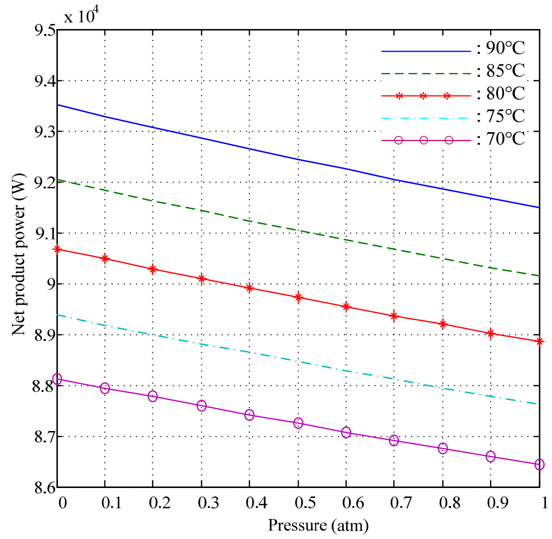

Fig. 12. Net power production of PEMFC system for pressure gap at different working temperatures

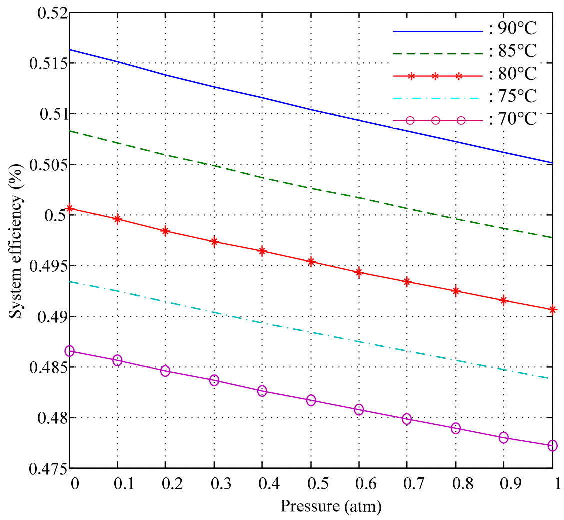

Fig. 13. Efficiency of PEMFC system for pressure gap at different working temperatures

proceeding FPS. The selection of temperature must take both thermal stability and humidity management into considerations. This paper reveals that the increase of working temperature simultaneously increases the output power of both PEMFC stack and gas turbine, and promotes the net output power and system efficiency of PEMFC system as well. Therefore, some high-temperature PEMFC systems with the advantage of reduced CO sensitivity, which is capable of operating at 150-200°C, is currently at a promising development. The optimal working pressure is supposed to decrease form both efficiency and safety of system-level standpoint. The pressure of PEMFC cathode is 0.1 atm higher than that of anode to avoid the detrimental degradation of oxygen starvation and to keep the appropriate humidity for the PEMFC membrane. The pressure control for a PEMFC system will be a very important interest from a system-level point of view.

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