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Evaluating the Impact of Afterburner and Reformer on the Power Generation and Efficiency of SOFC

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Keywords: Solid Oxide Fuel Cell (SOFC); Thermodynamic; Afterburner; Reformer; System analysis;

ABSTRACT

This study establishes a system loop analysis model for SOFC systems incorporating thermal components through thermodynamic theory. The model can be used to evaluate the overall efficiency, power generation, and operating status of components in SOFC systems under different operating conditions. Additionally, using a commercial stack module, the study completes the analysis of afterburner temperature and the effects of using SR and ATR reformers on the temperature, power generation, and efficiency of the SOFC system. The optimal system performance was found to be a power generation of 7.62 kW, an efficiency of 64.3%, and a stack temperature of up to 803℃. Finally, system analysis reveals that using an ATR reformer effectively reduces the combustor temperature and indicates room for optimization of the steam-to-carbon ratio when using an ATR reformer. This result can guide future experiments for optimizing SOFC system design and parameter control.

INTRODUCTION

Due to the current global issue of energy shortages, the development of renewable energy has become increasingly important. Among these, hydrogen energy, wind power, and solar cells are particularly noteworthy. In solid oxide fuel cell (SOFC), air is introduced at the cathode, oxygen ions pass through the electrolyte layer to the anode to react with hydrogen, thereby generating electricity, with water as the byproduct. The advantages of SOFC include high fuel utilization rate, high efficiency, long-term stability, and versatility in fuel usage (Somekawa et al. 2017, Vrečko et al. 2018, Liso et al. 2011).

SOFC possesses the characteristic of versatile fuel utilization, commonly using hydrocarbon fuels (such as methane and ethanol) and hydrogen. However, since hydrocarbon fuels are usually less pure, they can reduce system efficiency. Directly supplying large amounts of hydrocarbon fuels to the stack can easily cause carbon deposition. Therefore, SOFC systems typically use a reformer to convert most of the hydrocarbon fuels into hydrogen before supplying it to the stack. Thus, the commercialization of SOFC systems may depend on the current capability to convert available fuels into H_2 and CO (Bae et al. 2010). Besides these advantages, SOFC systems generate high-temperature exhaust gases. Many studies have suggested combining SOFC systems with external combustion engine power generation systems to effectively utilize the high-temperature exhaust gases from SOFC. Moreover, optimizing the system can also be achieved by altering different system pressurization methods.

In addition to the stack, SOFC systems mainly consist of hot box components such as reformers, start-up burners, afterburners, heat exchangers, and gas heaters, as well as cold box control components such as electric control circuits and power output. The performance and thermal recovery efficiency of the hot box components significantly impact the overall system efficiency. Therefore, when designing the system loop, it is necessary to analyze the energy changes within each component using thermodynamic methods and establish standards for each component to reduce system development costs and leverage the high efficiency advantages of high-temperature systems.

For SOFC system, burner is the primary heating module, with the main purpose of burning residual fuel and providing the necessary heat for the SOFC power generation system's stack and reformer. Thus, the temperature and performance of the burner will affect the power generation efficiency of the SOFC system. However, recent evaluations of SOFC burners have

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been limited. Consequently, this project will assess the impact of burner temperature effects on system performance and efficiency through system analysis.

On the other hand, the reformer is the hydrogen production device for SOFC, which affects the system's performance. Currently, there are three main reforming methods commonly used: steam reforming (SR), partial oxidation reforming (POx), and autothermal reforming (ATR) (Somekawa et al. 2017, Vrečko et al. 2018, Vita et al. 2019).

SR is the most commonly used method. It has a very high hydrogen production rate, allowing SOFC to achieve higher output power. However, many studies have found that the steam reforming reaction requires a significant amount of endothermic reaction, necessitating operation in a high-temperature system and more rigorous thermal management. POx is an exothermic reaction. Its advantages include not requiring an external heat source and the ability to start quickly. However, due to its much lower hydrogen production rate compared to steam reforming, the output power of SOFC using POx is relatively lower (Liso et al. 2011).

ATR combines steam reforming and partial oxidation reforming reactions. Hydrocarbon fuel, steam, and air are fed into the reformer together, with the feed composition adjusted to maintain a slightly exothermic reaction. Compared to SR, ATR has a faster start-up time and does not require a large system structure. Compared to PO_x, ATR has a higher hydrogen production rate and can generate greater output power. The methane conversion rate of ATR is the highest among the three, making it a reformer that combines the advantages of SR and PO_x.

Moreover, using different reformers requires different loop designs due to the varying main control parameters, which can affect system efficiency. Therefore, selecting the appropriate operating parameters for the corresponding reformer is crucial for improving system efficiency. Currently, there is limited literature on systems with external ATR reformers. Thus, this paper proposes comparing the loop designs and operating parameters under the use of three different reformers to enhance system power and efficiency.

The purpose of this study is to understand the overall impact of thermal components under high-temperature operation on various system components and to reduce the costs of practical experiments through numerical analysis. Therefore, during the execution of this study, the system model will be established using the Thermolib module in Matlab/Simulink. The effects of different operating conditions of the combustion components on the system's operational state will be explored, including the burner, heat exchanger, and reformer. This study will compare the changes in performance and efficiency of the SOFC power generation system due to variations in thermal components and operating conditions.

Modeling Methodology

Modeling of the SOFC Stack

In establishing the SOFC simulation module, this study primarily uses the SOFC as the main structure of the power generation module. Oxygen or air is introduced at the cathode end of the cell as the oxidant, while hydrocarbon fuel, which can participate in the reaction, is introduced at the anode end as the fuel. If only hydrogen and oxygen are considered as the reactive gases in the SOFC system, the electrochemical reactions can be described by the following equations:

Cathode: $O_2 + 4e^- \rightarrow 2O^{-2}$ (1)

Anode: $H_2 + O^{-2} \rightarrow H_2O + 2e^-$ (2)

Overall reaction: $H_2 + 1/2O_2 \rightarrow H_2O$ (3)

To evaluate the performance of SOFC system, polarization curve of SOFC stack would be calculated in different operating temperature, therefore, calculating the performance of the SOFC, the reaction between SOFC cell could be evaluated by Gibbs free energy Equation, which is below in eq.4. (Aguiar et al. 2004, Takino et al. 2020)

$$\Delta G = \Delta G^{\circ} - RT \ln \frac{P_{H_2} P_{O_2}^{1/2}}{P_{H_2O}} \quad (4)$$

where, R is the constant of ideal gas, p_{H_2}, $p_{O_2}^{1/2}$ and p_{H_2O} are the partial pressure of reactant and product.

In order to calculate the voltage of SOFC, Nernst equation would be used and calculated with eq. 4.

$$E_r = -nF\Delta G \quad (5)$$

where, n is number of electronic, F is the constant of Faraday, E_r is the reversible of open circuit voltage.

Based up the above eq.5, the voltage of SOFC could be calculated be Nernst equation, however, the operating voltage would be influenced by irreversible losses. To evaluate the irreversible loss of SOFC, the eq. 5 should be considered by below:

$$E = E_r - (\eta_{act} + \eta_{ohm} + \eta_{con}) \quad (6)$$

where E_r is reversible voltage, η_{act} is activation overpotential, η_{ohm} is ohmic overpotential, η_{con} is concentration overpotential. The overpotential is calculated by Nernst equation, as follows:

$$\eta_{act} = \frac{2RT}{nF}\left[\sinh^{-1}\left(\frac{i}{2i_{0,a}}\right) + \sinh^{-1}\left(\frac{i}{2i_{0,c}}\right)\right] \quad (7)$$

$$\eta_{ohm} = i\left(\frac{\tau_{anode}}{\sigma_{anode}} + \frac{\tau_{cathode}}{\sigma_{cathode}} + \frac{\tau_{electrolyte}}{\sigma_{electrolyte}}\right) \quad (8)$$

$$\eta_{con} = \frac{RT}{2F}\ln\left(\frac{p_{H_2O,TPB}\ p_{H_2,in}}{p_{H_2O,in}\ p_{H_2,TPB}}\right) + \frac{RT}{2F}\ln\left(\frac{p_{O_2,in}}{p_{O_2,TPB}}\right) \quad (9)$$

where $i_{0,a}$ and $i_{0,c}$ are the exchange current density of anode and cathode, τ is the thickness of electrode, σ is the conductivity of electrode, p_{TPB} is the partial pressure of triple phase boundary.

Modeling of the SOFC heat exchangers

Each thermal component of the system will undergo heat exchange operations in the calculation process. Therefore, in addition to examining the flow

rates consumed by the stack, it is also necessary to investigate the heat exchange process of the components. Here, the heat exchanger will be used as an example to illustrate the relevant calculation process and theory of thermal components during the heat exchange process. The overall calculation theory will refer to the literature (Megren, 2012).

In the introduction to heat exchange calculations, both a hot side and a cold side are required. The heat capacity rate formulas for the two sides are defined as follows:

$$\begin{cases} C_C = \sum q_C C_{P,C} \left[\frac{mole}{s} \times \frac{J}{mole \times K} = \frac{W}{K}\right] \\ C_h = \sum q_C C_{P,h} \end{cases} \quad (10)$$

Based on the above, the heat capacity rates of the hot side (C_h) and the cold side (C_c) can be defined. Here, Cr is defined as the ratio of the heat capacity rates of the two sides. The formula is as follows:

$$C_r = \frac{C_{min}}{C_{max}} \quad (11)$$

where C_{min} is the smaller value of C_c and C_h, and C_{max} is the larger value.

To calculate the heat exchange efficiency, the unit heat transfer rate, Number of Transfer Units (NTU), is defined as follows:

$$NTU = \frac{UA}{C_{min}} \quad (12)$$

where U is the overall heat transfer coefficient, A is the heat transfer area, and C_{min} is the minimum heat capacity rate.

The heat exchange efficiency, denoted as ε, is defined as follows:

$$\varepsilon = \frac{q}{q_{max}} \quad (13)$$

where q is the actual heat transfer rate and q_{max} is the maximum possible heat transfer rate.

The theoretical maximum heat transfer rate can be calculated from the heat exchange perspective as follows:

$$q_{max} = C_{min}(T_{h,1} - T_{c,1}) \quad (14)$$

The heat exchange efficiency is given by:

$$\varepsilon = \frac{C_h(T_{h,1} - T_{h,2})}{C_{min}(T_{h,1} - T_{c,1})} = \frac{C_c(T_{c,1} - T_{c,2})}{C_{min}(T_{h,1} - T_{c,1})} \quad (15)$$

Modeling of the Reformer

The related calculations of the reformer are carried out through the gas-catalyzed chemical reaction equations, and the catalytic capability is calculated based on its chemical activity. Additionally, the reformer module also functions as a heat exchanger, so the gas will follow the aforementioned heat exchange process and exchange heat with the pre-reformed gas to increase the temperature. Below is the reforming reaction equation used for methane fuel in this simulation process:

$$CH_4 + H_2O \rightarrow CO + 3H_2 \quad (16)$$

$$CO + H_2O \rightarrow CO2 + H_2 \quad (17)$$

Additionally, the numerical model used for the reformer in this study is the CH4-reformer module in Matlab/Thermolib. The relevant operating parameters are set based on the parameters used in references (Larminie and Dicks, 2003, Cengel et al. 2006). Besides investigating the SR reformer, this study also explores the ATR reformer. Therefore, in the calculation process of the reformer, it is necessary to include the conditions for partial oxidation reforming. The related chemical reaction equation is shown below:

$$CH_4 + 0.5O_2 \rightarrow CO + 2H_2 \quad (18)$$

ATR is a reforming method that combines steam reforming reactions and partial oxidation reforming reactions. In this process, steam, oxygen, and fuel are simultaneously fed into the reformer to undergo reactions. The reaction mechanism involves initially conducting an exothermic partial oxidation reforming of the fuel with oxygen, allowing the products to gain thermal energy. Subsequently, the products react endothermically with steam, thereby increasing the methane conversion rate. This method integrates the advantages of the previously mentioned reforming methods, such as high methane conversion rates and simpler loop design.

Modeling of the Burner

The related calculations for the burner are primarily based on chemical reaction equations. These calculations involve the exothermic chemical reactions of the fuel contained in the gas, which then achieve the effect of combustion heating through heat exchange between the gases. The chemical reaction equations for the fuel used are as follows:

$$H_2 + 0.5\ O_2 \rightarrow H_2O$$

$$HHV = 143000\ kJ/kg \quad (19)$$

$$CH_4 + 2O_2 \rightarrow 2H_2O + CO_2$$

$$HHV = 55687.5\ kJ/kg \quad (20)$$

$$CO + 0.5O2 \rightarrow CO_2$$

$$HHV = 1180\ kJ/kg \quad (21)$$

System loop and Operational Parameters of the SOFC Power Generation System

The aforementioned constitutes the thermodynamic calculation theory for the thermal component calculation model of the SOFC system in Matlab/Simulink in this study. Based on the above theories and the system loop design shown in Figure 1, this study has established the relevant thermodynamic calculation theories for the thermal components.

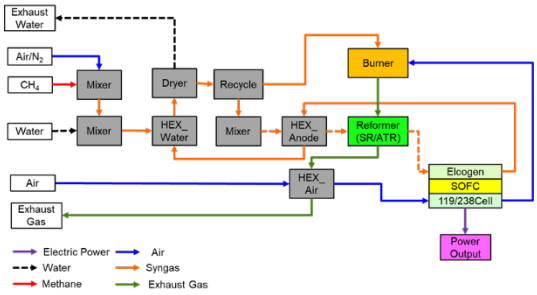

Figure. 1 Schematic diagram of the SOFC system

As shown in Figure 1, the thermal components used in this study include the burner, heat exchanger, reformer, and SOFC module. The reformer consists of a SR and an ATR. Therefore, this section will theoretically explain how to establish the thermal component calculation model in Matlab/Simulink. This study establishes the SOFC system model based on the aforementioned thermodynamic calculation theories of the thermal components and the P&ID of SOFC system shown in Figure 1. The schematic diagram of the system model with Matlab/Simulink is shown in Figure 2.

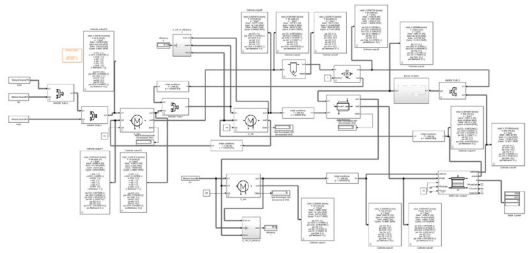

Figure. 2 System loop of the SOFC system with AGR in Matlab/Simulink

Additionally, to investigate the operational performance of the system and the impact of the combustion components on system efficiency, this study establishes the system based on thermodynamic theories and designs the system control parameters by referencing the flow control conditions for SOFC stack provided by Elcogen (Noponen et al., 2015). The preliminary parameter design is shown in Table 1.

Based on Table 1, during the process of establishing the system numerical model, it is necessary not only to understand the inlet and outlet flow rates of the stack but also to evaluate the heat exchange capabilities of each component and analyze the chemical reactions of the reformer and burner. Besides using the thermodynamic theories introduced earlier, this study also evaluates the heat exchange efficiency of currently available heat exchangers on the market. Therefore, the heat exchange efficiency for both the cathode and anode heat exchangers is set at 80% as the primary design target.

Moreover, since this study aims to evaluate the performance and efficiency of the burner at various operating temperatures, the system parameter design must consider the air utilization rate in addition to fixing the fuel utilization rate. Thus, during the operational simulation process, it is necessary to control the burner temperature through air regulation while ensuring that the air utilization rate of the stack complies with Elcogen's commercial specifications. The goal is to ensure that the results of the operational analysis closely approximate actual operating conditions, thereby allowing this study to be practically applied in system design and control logic development in the future.

Table. 1 Operating Parameters of the SOFC System (Noponen et al., 2015)

Operating Parameters	Value
Number of Cells	119/238
Operating Temperature (°C)	700-800
Flow rate of Air(nlpm)	Fixed for Stack Temperature
Flow rate of CH_4(nlpm)	Fixed for Stack Temperature
Ratio of S/C	3
Ratio of O/C in ATR	0.1
Steam Utilization (%)	70-80
Oxygen Utilization (%)	12-30
Efficiency of Exchanger (%)	80

Results and discussion

Influence of the doping effect of on the Proton Mobility Capability for Hydrogen

Through the aforementioned sections, it is evident that the main goal of this study is to establish an operational analysis model for a SOFC system and to explore the optimization of system parameters and design through the analysis model. This study will focus on designing a 5 kW SOFC power generation system. To achieve this goal, this study initially establishes the model for the SOFC system and verifies the performance of the core power generation module. The theoretical basis for the model

establishment has been explained in the previous sections. This chapter will begin to explain the system performance verification, as well as the related optimization parameter analysis and design results.

To ensure that the SOFC system model established in this study aligns more closely with the actual operating conditions of a power generation system, the core power generation components used in this study are primarily based on the literature. The system loop design and operational simulation analysis are conducted based on Figure 1. Before performing the system analysis, it is necessary to define the performance of the core SOFC stack. This involves referencing the performance described in the literature (Noponen et al., 2015) and using equation (6) to derive the cell performance. Finally, the cell polarization curve is calculated using Matlab, with the overall results shown in Figure 3.

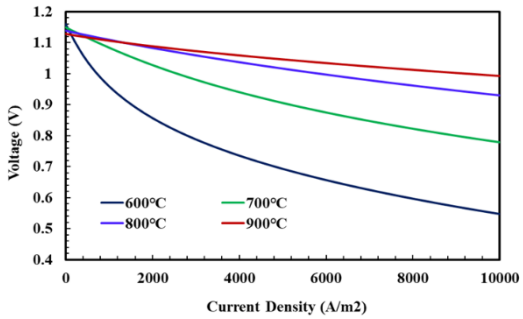

Figure. 3 Polarization curves of the solid oxide fuel cell at different operating temperatures

As shown in Figure 3, the SOFC system used in this study belongs to the SOFC stack, with an operating temperature range of 600-900℃. Additionally, as the operating temperature increases, the performance of the power generation components also improves. This indicates that the operating temperature is an important parameter for the system's power generation capacity.

To investigate the impact of the burner on the core power generation component temperature, system power output, and system efficiency in the SOFC system, this study compares three different burner temperatures. The study observes the changes in the core power generation temperature and its effect on system efficiency. The overall results are shown in Table 2.

As shown in Table 2, when the burner temperature reaches 1075.76℃, the stack temperature could reaches 803.01℃. At this point, the system power output reaches 7.62 kW (with two stacks totaling 238 cells), and the system efficiency can reach 64.3%. To investigate the effect of burner temperature variations, this study controls the burner temperature through air flow rate adjustments and observes the changes in system operating conditions when the burner temperature increases or decreases by 20℃.

From Table 2, it can be seen that when the burner temperature decreases by 20℃, the core power generation component (stack temperature) also decreases by approximately 19℃, illustrating the burner's influence on the core power generation component. At this point, the system power output drops to 7.58 kW, and the efficiency is 64%. Conversely, when the temperature increases by 20℃, the stack temperature rises by 11℃, resulting in a system power output of 7.66 kW and an efficiency of 64.6%.

Table. 2 Effects of Burner Temperature on Stack Temperature, Power, and Efficiency for system

Temperature Of Burner / State of System	1075.76℃	1055.31℃	1095.50℃
Stack Temperature (℃)	803.01	786.09	814.35
Temperature of Anode for Stack (℃)	672.10	662.38	681.05
Temperature of Cathode for Stack (℃)	691.10	673.70	695.10
Power (kW)	7.62	7.58	7.66
Efficiency (%)	64.3	64.0	64.6

By comparing the three different burner temperatures and based on the system loop design shown in Figure 1, it is evident that the burner temperature causes significant changes in the reformer and cathode heat exchanger temperatures, which in turn affect the stack temperature. This leads to changes in the final power output and system efficiency.

Through the aforementioned analysis, it is clear that the burner temperature has a significant impact on the stack temperature. However, the effect of stack temperature on system power and efficiency, besides operating temperature, also requires consideration of the stack material and temperature characteristics. The stack used in this study is an anode-supported cell stack developed by literature, which is characterized by high performance and can be applied not only at high temperatures but also in the mid-temperature range. Therefore, in addition to exploring the temperature effects of the burner on the 5-kW SOFC system, this study also compares the performance of the system using 119-cell stacks operating at 700℃ with steam reforming (SR) and autothermal reforming (ATR). The results are shown in Tables 3 to 6.

According to Table 3, when using the SR reformer and operating the system at 700℃, the system power output can reach 3.59 kW with an efficiency of 60.6%. However, based on Table 4, it is

found that when using the ATR as the reformer, the burner temperature can effectively decrease to 843℃, and the system power output is 3.58 kW with an efficiency of 60.4%. This indicates that using different types of reformers results in significant differences in the endothermic and exothermic reactions affecting the burner temperature. Additionally, from the comparison of reformer components in Tables 5 and 6, it is evident that when the external input conditions are the same, the water-to-carbon ratio in the ATR reformer can be reduced. The reason is that during the ATR process, air with an oxygen-to-carbon ratio of 0.1 is introduced for autothermal reforming, which reduces the amount of steam required for the second stage of steam reforming.

Furthermore, through the system operation analysis from Tables 3 to 6, it is observed that the stack can still achieve a system efficiency of 60% at a stack temperature of around 700℃, with a fuel utilization rate of approximately 60.9%. This operating condition is beneficial for the lifespan of the stack module, the labor required for the system BOP (Balance of Plant), and waste heat recovery. However, the stack is more sensitive to temperature differences in thermal components and the system's heating rate compared to the power generation modules previously referred to as electrolytes. Therefore, when using different types of stacks, it is necessary to explore the changes in performance and operating parameters, as well as to investigate the control of materials during dynamic heating to reduce damage to the stack during the system's heating and cooling processes.

Table. 3 Effects of Using SR Reformer on Temperature, Power, and Efficiency for System

Temperature Of Burner / State of System	891.0℃	870.5℃	911.5℃
Stack Temperature (℃)	702.62	687.70	715.45
Temperature of Anode for Stack (℃)	644.56	637.09	652.15
Temperature of Cathode for Stack (℃)	600.18	581.79	610.07
Power (kW)	3.592	3.505	3.624
Efficiency (%)	60.6	59.15	61.2

Table. 4 Effects of Using ATR Reformer on Temperature, Power, and Efficiency for System

Temperature Of Burner / State of System	843.12℃	822℃	864.34℃
Stack Temperature (℃)	698.60	683.5	710.3
Temperature of Anode for Stack (℃)	642.24	633.63	651.2
Temperature of Cathode for Stack (℃)	591.62	572.5	595.63
Power (kW)	3.577	3.478	3.61
Efficiency (%)	60.4	59.15	61.0

Table. 5 The concentration profiles of fuel when using SR reformer in different Temperature

Temperature of Reformer / Concentration	644.6℃	637.09℃	652.15℃
H_2	0.545	0.540	0.549
CO	0.074	0.071	0.077
CO_2	0.081	0.082	0.079
CH_4	0.018	0.021	0.015
H_2O	0.283	0.287	0.280

Table. 6 The concentration profiles of fuel when using ATR reformer in different Temperature

Temperature of Reformer / Concentration	642.24℃	633.63℃	652.15℃
H_2	0.493	0.489	0.497
CO	0.066	0.063	0.069
CO_2	0.082	0.083	0.080
CH_4	0.013	0.015	0.010
H_2O	0.285	0.289	0.283

Conclusion

This study conducts an operational analysis of a SOFC system and an optimization of operational parameter analysis and design using Matlab/Simulink. In addition to theoretical analysis to establish the model, the study also establishes monitoring modules for flow, temperature, and power to investigate the impact of burner temperature on system power and efficiency. The overall related conclusions are as follows:

1. Through thermodynamic theory, the study

completes the system loop design and thermodynamic calculation model for a SOFC system, including thermal components. This model can be used to evaluate the overall efficiency, power output, and operating state of the SOFC system under different operating conditions.

2. To investigate the impact of operational parameters on the system, the study establishes different monitoring modules for external flow, temperature, and power control. The purpose is to separately control each flow, temperature, and power parameter, thereby conducting an optimized parameter analysis and design for the system.
3. By using two stack modules, the study completes the operational analysis of the SOFC system. By comparing the impact of the burner on the system, the study completes the optimized parameter analysis and design. The system power output can reach 7.62 kW, with a system efficiency of 64.3% and a core power generation component temperature of 803℃.
4. Finally, based on the characteristics of the SOFC stack, the study explores the impact of using different reformers on system power efficiency and power output. It is found that using an ATR reformer can effectively lower the burner temperature. Additionally, when using an ATR reformer, there is room for optimization in the water-to-carbon ratio. This result can provide a direction for system parameter control and optimization when using different commercially available stack modules in the future.

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後燃器組件與重組器對於 SOFC 發電功率與效率分析

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摘 要

本研究透過熱力學理論，建立SOFC系統包含熱組件之系統迴路分析模型，而該模型可以用於評估SOFC系統於不同操作狀態下之系統整體效率、發電功率以及組件的運轉狀態。此外，透過使用商用型之電堆模組，本研究完成後燃器溫度與使用SR以及ATR兩種不同重組器對於SOFC發電系統溫度、發電功率與效率分析，並且發現其最佳系統性能為系統發電功率7.62kW，效率64.3%，Stack溫度

可達803℃。最終，透過系統分析可以發現使用ATR重組器時，可以有效降地燃燒器之溫度，並且發現當使用ATR重組器時，其水碳比有下修優化之空間，此結果可以提供未來進行實驗的過程中，作為SOFC系統設計與參數控制優化之方向。