Analysis of a Solid Oxide Fuel Cell (SOFC) System Based on a Mass and Energy Flow Model

1 st Changjiang Liao[1,2]
College of Chemistry and Chemical Engineering
[1]*Southwest Petroleum University*
[2]*Chengdu MinShan Hydrenergy, Co.,Ltd.*
Chengdu, China
447612046@qq.com

2nd An'an Zhang
School of Electrical Engineering and information
Southwest Petroleum University
Chengdu, China
ananzhang@swpu.edu.cn

3rd Xinyu Liu
College of Chemistry and Chemical Engineering
Southwest Petroleum University
Chengdu, China
943336098@qq.com

4th Yong He
Chengdu MinShan Hydrenergy, Co.,Ltd.
Chengdu, China
heyonglalala@163.com

5th YuanXing Zhou
Chengdu MinShan Hydrenergy, Co.,Ltd.
Chengdu, China
zyx1231009@126.com

6th Xianzhang Lei
College of Chemistry and Chemical Engineering
Southwest Petroleum University
Chengdu, China
leixianzhang@hotmail.com

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***Abstract*—Solid oxide fuel cell (SOFC) power systems are known to be a promise alternative for power generation with high efficiency and fuel flexibility. The SOFC has been proved to be an excellent energy conversion device. In this paper, a mass and energy flow model is developed for a SOFC combined heat and power (CHP) system power generation system, which includes fuel/air supply system, SOFC stack, an afterburner and three heat exchangers. The model can analyze and measure how energy is transferred and transformed within each component of the system, as well as between different component of the system. This model provides a structured approach for understanding the complex processes of energy transfer and conversion and enables the optimum operating point to be obtained for different system output powers. Excessive air coefficient lambda (λ) is an important parameter in SOFC system that directly impacts fuel cell efficiency, fuel cell performance, and operating temperatures.**

Keywords—Solid oxide fuel cell, mass and energy flow model, energy transfer, conversion, system efficiency

I. INTRODUCTION

Solid Oxide Fuel Cell (SOFC) power generation systems offer several features and advantages that make them attractive for various applications. Firstly, SOFC systems possess high electrical efficiency, reaching up to 60%, as they can be directly converted from chemical energy to electrical energy without the intermediary energy conversion steps[1-4].

An added feature of SOFC systems is fuel flexibility, as they can use a wider variety of fuel such as hydrogen, natural gas, methane and propane. This multi-energy aspect of SOFC systems enable the simultaneous generation of electricity and heat, providing a more flexible and efficient power generation system.

In addition to fuel flexibility, SOFC systems have the advantage of being able to integrate with other energy systems, including gas turbines and steam turbines, to further improve their overall efficiency and reduce costs. The versatility of these systems makes them well-suited for various applications, ranging from power generation in residential and commercial settings to industrial applications[5-9]. Combination SOFC with a power generation cycle has led to the proposed use of the resulting hybrid system in new heating systems[10][11].

SOFC systems have the potential to become highly effective energy conversion technologies due to their ability to operate on a diverse range of fuels, provide higher power rates, and their user-friendly installation and operation. These qualities make SOFC systems an attractive option for achieving clean, efficient, and economically feasible energy conversion[12][13].

The temperature of each component in a SOFC system is important for system safety. The temperature of each component in the system affects the rate of electrochemical reactions, heat transfer, and gas flow. Since SOFC operate at high temperature, a decrease in the fuel cell temperature can cause a reduction in power output by slowing down the electrochemical reaction in the system. Conversely, if the temperature of any component is too high, it can pose a safety risk. For example, it can cause thermal runaway, where the system generates too much heat and starts to self-destruct.

II. ENERGY AND MASS FLOW SYSTEM DESCRIPTION

This paper focuses on the SOFC combined heat and power (SOFC-CHP) system, as illustrated in Fig. 1. The system comprises several components, which includes a fuel supply system, an air supply system, a SOFC stack, an afterburner, three heat exchangers, and two bypass valves. During operation, the system generates electricity and produces high temperature exhaust gases using the reaction of fuel and air in the SOFC stack.

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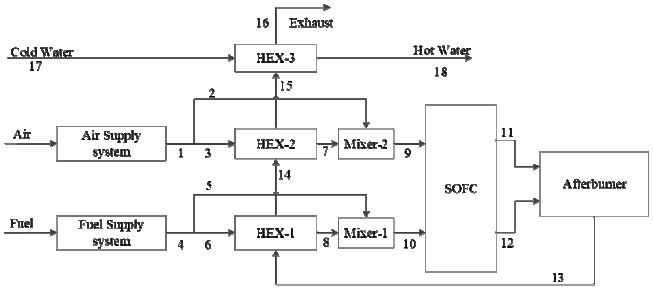


Fig. 1. Schematic diagram of SOFC

The system can be described in terms of gas flow, the first being the flow of gas and the second being the gas bypass included in the system. The system includes two gas bypasses, which include an air preheat bypass and a fuel preheat bypass. By utilizing a three-stage heat exchange, the heat transfer efficiency of the system is enhanced, and it enables the system to perform cogeneration.

The analysis in this paper is carried out with a focus on thermodynamic equilibrium and a constant state of operation. For a simplicity, in the presented analysis of the SOFC-CHP system, we have made several assumptions.

- Air contains 79% N_2 and 21% O_2.
- Ideal gas behavior is assumed for all gases.
- Heat loss to the surroundings is negligible.
- SOFC operates at constant temperature and pressure.
- The process is in steady state.

III. Energy and Mass Flow Modeling

A. SOFC mathematical modeling

The amount of heat generated in SOFC stack can be calculated by considering the various sources of heat generation and heat loss within the system.

The main sources of heat generation in an SOFC stack are:

The fuel oxidation at the anode and the oxygen reduction at the cathode both release heat.

Theoretical voltage and the actual voltage generated by electrochemical reactions in SOFC. This voltage difference is dissipated as heat.

Ohmic losses: The flow of current through the cell components results in resistance, which generates heat due to the Joule heating effect.

The chemical reactions of the stack are formulated as below:

Anode $H_2 \rightarrow 2H^+ + 2e$ (1)

Cathode $0.5O_2 + 2e \rightarrow O^{2-}$ (2)

Overall $H_2 + 0.5O_2 \rightarrow H_2O + \Delta H_r^o$ (3)

The electrode potential difference, E_{OCV} is the open-circuit voltage and is calculated by Nernst equation[14]:

$$E_{OCV} = E_0 + \frac{RT}{2F} ln \frac{p_{H_2} p_{O_2}^{0.5}}{p_{H_2O}} \quad (4)$$

where E_0 is the standard cell potential, p_{H2}, p_{O2} and p_{H2O} are the partial pressures of hydrogen, oxygen and steam, T is the fuel cell temperature, and F represents the Faraday constant and R represents the ideal gas constant, respectively.

In this paper, the SOFC stack is modeled to be a single, uniform entity, with the components presumed to have the same temperature at any point in time. This is predicated on the assumption that the materials utilized in the fuel cell stack have high enough thermal conductivity to rapidly balance out any temperature differentials between the various components. By applying an energy balance analysis to the complete SOFC stack, the dynamic temperature (T_s) of SOFC stack can be determined.

$$m_s \cdot c_{p,s} \frac{dT_s}{dt} = \sum_i N_i^{in} h_i(T_i^{in}) - \sum_i N_i^{out} h_i(T_i^{out}) - N_{H_2}^r \Delta H_r^o - V_s I \quad (5)$$

where m_s represent the mass of SOFC stack, $c_{p,s}$ represent the average specific heat of SOFC stack, ΔH_r^o refers to the specific heat of electrochemical reaction described in (3), and V_s is the output voltage of the stack, which can be expressed by the following formula:

$$V_s = E_{OCV} - \eta_{ohm} - \eta_{act} - \eta_{con} \quad (6)$$

where η_{ohm}, η_{act} and η_{con} represent the ohmic, activation and concentration polarizations.

The η_{ohm} is the ohmic loss because of internal resistance of SOFC.

$$\eta_{ohm} = iAR_{ohm} \quad (7)$$

The η_{act} represents the activation loss for the voltage decrease required to overcome the activation energy of hydrogen and oxygen ions during their reaction. It can usually be found by the Butler-Volmer equation[15][16].

$$\eta_{act} = \frac{RT}{F} sinh^{-1}\left(\frac{i}{2i_{0,an}}\right) + \frac{RT}{F} sinh^{-1}\left(\frac{i}{2i_{0,ca}}\right) \quad (8)$$

The η_{con} stands for the concentration polarization, which refers to the low concentration voltage loss of the reacting gas near the reaction interface due to poor diffusion, affecting the electrochemical reaction. The expressions for η_{con} is given below[17]:

$$\eta_{con} = \frac{RT}{2F} ln\left(1 - \frac{i}{i_L}\right) \quad (9)$$

where i denotes the current density, i_L represents the limiting current in the fuel cell, which corresponds to the maximum current density achievable when all the hydrogen present in the anode chamber undergoes complete reaction.

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$i_{0,an}$ and $i_{0,ca}$ in (8) are the anode and cathode exchange current densities, respectively, which can be described in the following exchange current densities are calculated using[18][19]:

$$i_{0,an}=\gamma_{an}\left(\frac{p_{H_2}}{p_{amb}}\right)\left(\frac{p_{H_2O}}{p_{amb}}\right)^{m} exp\left(-\frac{E_{act,an}}{RT}\right) \quad (10)$$

$$i_{0,ca}=\gamma_{ca}\left(\frac{p_{O_2}}{p_{amb}}\right)^{0.25} exp\left(-\frac{E_{act,ca}}{RT}\right) \quad (11)$$

where $E_{act,ca}$ and $E_{act,an}$ are the cathode activation energy and the anode activation energy, p_{amb} is the reference pressure (usually atmospheric pressure), γ_{an} and γ_{ca} are anode diffusion coefficient and cathode diffusion coefficient.

B. Fuel/Air Supply system

The fuel/air supply system is a vital component in providing various types of fuel/air to satisfy the specific requirements of the SOFC. It is essential to consider the fuel flow rate and composition fluctuations and to establish the mass flow rates of different fuel components (e.g. hydrogen, methane, etc.) for subsequent thermodynamic calculations. Accurately calculating fuel and air mass flow rates is extremely important for the fuel and air supply systems, as it can enhance thermal management and improve fuel utilization.

Assuming that the SOFC stack consists of N cells, equations (12) and (13) are used to calculate the fuel molar flow rates N_{Fuel} and the air molar flow rates N_{air}.

$$N_{Fuel}=N\frac{I}{2F} \quad (12)$$

$$N_{air}=\lambda\cdot FU\cdot N\frac{I}{2F\cdot 0.21} \quad (13)$$

where I is the current of SOFC, λ is excessive air coefficient, FU is fuel utilization, N is the total number of fuel cell pieces.

C. Heat exchanger mathematical modeling

The heat exchangers in the SOFC system play a crucial role in recovering and utilizing the heat from the SOFC stack and the afterburner. The exhaust gas generated in the afterburner is used to increase the temperature of fuel, air, and water via three distinct heat exchangers. The fuel is pre-heated through the initial heat exchanger, whereas the second heat exchanger preheats the air. Lastly, the exhaust flows through a third heat exchanger to produce hot water.

Respectively, the heat capacity rates of the cold and hot gases are provided as follows:

$$C_{Cold}=\sum_{S_1} N_{in,s_1}^{cold} C_{P,s_1}^{cold}\left(T_{in}^{cold}\right) \quad (14)$$

$$C_{hot}=\sum_{S2} N_{in,s_2}^{hot} C_{P,s_2}^{hot}\left(T_{in}^{hot}\right) \quad (15)$$

$$S_1=\{N_2, O_2\}$$

$$S_2=\{CH_4, CO_2, H_2, H_2O, N_2, O_2\}$$

where N_{in,s_1}^{cold} and N_{in,s_2}^{hot} are the molar flow rates of different species and $C_{P,s_1}^{cold}\left(T_{in}^{cold}\right)$ and $C_{P,s_2}^{hot}\left(T_{in}^{hot}\right)$ are the specific heat capacities at the temperature of the cold-side gas and hot-side gas, respectively.

The theoretical maximum heat transfer can be calculated as:

$$q_{max}=C_{min}(T_{in}^{hot}-T_{in}^{cold}) \quad (16)$$

C_{min} is the minimum of C_{Cold} and C_{hot}.

The actual amount of heat transfer is calculated as follows:

$$q=\varepsilon\cdot q_{max} \quad (17)$$

For a counter flow type heat exchanger, the heating exchanger efficiency ε is:

$$\varepsilon=\frac{1-e^{[-NTU(1-C_r)]}}{1-C_re^{[-NTU(1-C_r)]}} \quad (18)$$

where $C_r=\frac{c_{max}}{c_{min}}$ and NTU is called the number of transfer units given as:

$$NTU=\frac{UA}{c_{min}} \quad (19)$$

where A is the heat transfer surface area and U is total heat transfer coefficient and.

The temperatures of the cold and hot gases at the heat exchanger outlet are given as:

$$T_{out}^{cold}=T_{in}^{cold}+\frac{q}{C_{cold}} \quad (20)$$

$$T_{out}^{hot}=T_{in}^{cold}-\frac{q}{C_{hot}} \quad (21)$$

D. Afterburner mathematical modeling

The afterburner combusts unreacted fuel and oxidant exhaust from SOFC, reducing emissions and increasing efficiency. The afterburner fully burns the fuel from the stack, as illustrated in Fig. 2. The thermal energy generated by the afterburner can be utilized for preheating the air and fuel that enters the system. It is critical to the effective combustion of unreacted fuel and oxidant and must be carefully designed and optimized to ensure optimal performance and efficiency.

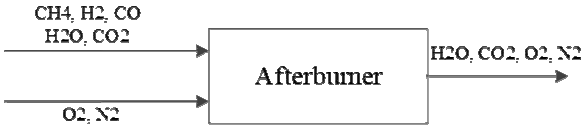


Fig. 2. Inlet and outlet gas composition of afterburner

Under excess air, it is assumed that CH_4, H_2 and CO are completely combusted in the burner.

$$CH_4+2O_2\rightarrow CO_2+2H_2O \quad (22)$$

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$$H_2+0.5O_2 \rightarrow 2H_2O \quad (23)$$

$$CO+0.5O_2 \rightarrow CO_2 \quad (24)$$

The mass balance of the gases at the inlet and outlet is given as:

$$N_{O_2}^{out}=N_{O_2}^{in}-2N_{CH_4}^{in}-0.5N_{H_2}^{in}-0.5N_{CO}^{in} \quad (25)$$

$$N_{H_2O}^{out}=N_{H_2O}^{in}+2N_{CH_4}^{in}+N_{H_2}^{in} \quad (26)$$

$$N_{CO_2}^{out}=N_{CO_2}^{in}+N_{CH_4}^{in}+N_{CO}^{in} \quad (27)$$

$$N_{N_2}^{out}=N_{N_2}^{in} \quad (28)$$

The energy conservation principle is utilized to describe the temperature dynamics.

$$m_{ab}\cdot c_{p,ab}\frac{dT_{ab}}{dt}=\sum_{s_3}N_{ab,s_3}^{in}h_{s_3}\left(T_{ab}^{in}\right)-\sum_{s_4}N_{ab,s_4}^{out}h_{s_4}\left(T_{ab}^{out}\right) \quad (29)$$

$$S_3=\{CH_4, CO, CO_2, H_2, H_2O, N_2, O_2\}$$

$$S_4=\{H_2O, CO_2, N_2, O_2\}$$

where m_{ab} represents the mass of the afterburner, $c_{p,ab}$ represents the specific heat capacity of the afterburner; N_{ab,s_3}^{in} and N_{ab,s_4}^{out} are the molar mass flow rates of different types of gases at the inlet and outlet, respectively, $h_{s_3}\left(T_{ab}^{in}\right)$ and $h_{s_4}\left(T_{ab}^{out}\right)$ are the enthalpies of different species of the gases at the inlet and outlet temperatures, respectively.

E. Mixer mathematical modeling

Gas mixers are used to control the quality of the fuel or air that is supplied to the SOFC system. The mixer can be used to adjust the ratio of different gases, such as cold air and hot air, to ensure that the fuel meets the required specifications for the SOFC, as shown in Fig. 3.

The opening of the bypass valve of the mixture BP (bypass valve Opening Ratio) determines the percentage of the cold air accounted for the total air flow of the input SOFC.



Fig. 3. Inlet and outlet gas composition of mixers

The inlet molar flow rates($N_{air,cold}^{in}$ and $N_{Air,hot}^{in}$) and outlet molar mixed air flow rates N_{Air}^{out} are determined by a mass balance equation, which is provided below:

$$N_{Air}^{out}=BP\cdot N_{Air,cold}^{in}+(1-BP)N_{Air,hot}^{in} \quad (30)$$

where the *BP* is bypass valve opening ratio.

By rearranging the energy balance equation and solving for outlet temperature $T_{air,out}$, we can obtain the temperature of the mixed air. It's important to note that the below equation assumes perfect mixing, which may not always be the case in practice.

$$m_{air}\cdot c_{v,air}\frac{dT_{air,out}}{dt}=\sum N_{air,cold}^{in}h_{air}\left(T_{air,cold}^{in}\right)+\sum N_{air,hot}^{in}h_{air}\left(T_{air,hot}^{in}\right)-\sum N_{air}^{out}h_{air}\left(T_{air}^{out}\right) \quad (31)$$

where $c_{v,air}$ is the specific heat capacity at constant volume, $N_{air,cold}^{in}$ and $N_{air,hot}^{in}$ are the inlet molar flow rate of the cold air and hot air respectively, $N_{air,out}^{in}$ is the air mass flow rate after mixing.

IV. Model Validation and Result

As for this model, it is validated with data in Tab. 1.

TABLE I. Model Parameters

Component	Parameter	Value	Unit
Fuel	H_2、N_2	80% H_2 in N_2	[-]
	Inlet temperature	25	[°C]
Air	λ	2-5	[-]
	Inlet temperature	25	[°C]
SOFC	Power of SOFC	3	[kW]
	Fuel utilization	0.5-0.85	[-]
	Cell size	0.0127	[m^2]
	Number of cells	120	[-]
	Rated power output per cell	30	[W]
	Inlet temperature	973	[K]
Afterburner	Specific heat capacity of afterburner bed ($C_{p,ab}$)	773	[J/(kg·K)]
Heat Exchanger	Heat transfer coefficient	12	[W/(m·K)]
	Area	7.6	[m^2]

The goal of this model is to calculate and design an optimal air excess coefficient, opening of bypass valve 1 and opening of bypass valve 2 to maintain fuel and air temperatures between 650°C and 700°C at the SOFC inlet. This will be achieved through iterative calculation to determine the best operating point for different stack output powers.

Tab. 2 shows the temperature and molar flow rate at each node in the flow chart under the condition of 3 kW power output of the SOFC system (fuel utilization is 0.7).

TABLE II. Temperature and Mass Flow Rate of Different Nodes in SOFC Systems

Nodes	Component	Molar Flow Rate (mol/s)	Temperature(K)
1	O_2	0.06550	298
	N_2	0.24642	298
2	O_2	0.00983	298
	N_2	0.03696	298
3	O_2	0.05568	298
	N_2	0.20945	298
4	H_2	0.03173	298
	N_2	0.02115	298
5	H_2	0.00317	298
	N_2	0.00212	298

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6	H_2	0.02856	298
	N_2	0.01904	298
7	O_2	0.05568	1053
	N_2	0.20945	1053
8	H_2	0.02856	1093
	N_2	0.01904	1093
9	O_2	0.06550	952
	N_2	0.24642	952
10	H_2	0.03173	955
	N_2	0.02115	955
11	O_2	0.05440	1048
	N_2	0.24642	1048
12	H_2	0.00953	1048
	H_2O	0.02220	1048
	N_2	0.02115	1048
13	O_2	0.04964	1255
	N_2	0.04230	1255
	H_2O	0.03173	1255
14	O_2	0.04964	1209
	N_2	0.04230	1209
	H_2O	0.03173	1209
15	O_2	0.04964	488
	N_2	0.04230	488
	H_2O	0.03173	488
16	O_2	0.04964	333
	N_2	0.04230	333
	H_2O	0.03173	333
17	H_2O(cold)	0.00103	313
18	H_2O(hot)	0.00103	333

The temperatures at different nodes in the SOFC-CHP system are presented in Fig. 4, with fuel and air temperatures of 952K and 955K at the inlet of the reactor, respectively. All components of the system operate within a reasonable temperature range.

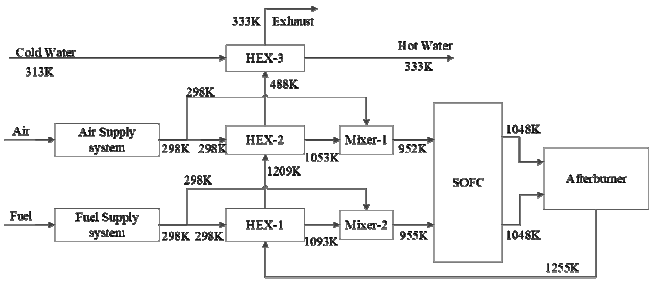


Fig. 4. Node temperatures in SOFC-CHP system(3kW)

The efficiency of the SOFC-CHP system is determined as the ratio of the total electrical and heat energy generated by the system to the chemical energy contained in the incoming fuel. It can be expressed mathematically as:

$$\eta_{CHP,sys} = \frac{P_{SOFC} + Q_{heat}}{m_{H_2} LHV_{H_2}} \tag{32}$$

where m_{H_2} represents the mass flow rate of the inlet fuel, LHV_{H_2} denotes the lower heating value of the H_2, P_{SOFC} is the net electricity that is generated by the system, and Q_{heat} is the heat recovered by heat exchanger 3.

The λ is a crucial parameter in SOFC-CHP system as it not only affects the performance but also the efficiency of the system, as demonstrated in Tab. 3.

When λ is less than 3, it means that there is insufficient air supplied to in the stack, which can cause the temperature inside the fuel cell to rise rapidly, leading to thermal stress and damage to the cell components. Therefore, it is important to maintain the proper air ratio within the system to prevent over-temperature and damage. Conversely, when λ is greater than 3, it can negatively impact system performance and efficiency.

TABLE III. EFFECT OF LAMBDA ON STACK TEMPERATURE AND SYSTEM EFFICIENCY

λ	Stack temperature (K)	System efficiency（%）
2	Forbidden	
2.5		
3		
3.5	1123	66.9
4	1104	64.3
4.5	1086	62.0
5	1071	59.6
5.5	1058	57.1

V. CONCLUSION

In this paper, a mass and energy flow model is established to calculate the mass flow and temperature of each node in the typical SOFC-CHP system. The mass and energy flow model provides a systematic way to understand and quantify the energy transfer and conversion processes that occur within each component and between different components of the system.

By analyzing the energy flow, we can identify the sources and sinks of energy within the system, as well as the inefficiencies and losses that occur during energy transfer and conversion. This model can also determine the optimal operating conditions for the SOFC system based on various factors. It can identify the most effective working point of the SOFC system under different working conditions.

The λ is an important parameter in SOFC systems that directly impacts system efficiency, stack performance, and operating temperatures. Optimizing the λ is essential for obtaining high-efficiency operation and long-life stable operation of the SOFC systems.

Overall, the mass and energy flow model is a powerful tool for analyzing the performance and efficiency of SOFC power generation systems. By quantifying the material and energy flow within the system, we can identify ways to optimize the system design, improve its efficiency, and reduce its environmental impact. The multi-energy capabilities of SOFC power generation make it a promising technology for the

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future, as it offers a flexible, efficient, and sustainable solution for meeting our energy needs.

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