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Process Flow Model of Combined High Temperature Fuel Cell Operated with Mixture of Methane and Carbon Dioxide

Farshid Zabihian[*] [†], AlanS. Fung [†]
Department of Mechanical and Industrial Engineering
Ryerson University
350 Victoria Street, Toronto, Ontario, Canada
Email: farshid.zabihian@ryerson.ca, alanfung@ryerson.ca

* Address all correspondence to his author.
† ASME Member.

ABSTRACT

This paper investigates the impacts of carbon dioxide concentration in the inlet fuel on the performance of a hybrid tubular solid oxide fuel cell (SOFC) and gas turbine (GT) cycle with two configurations: system with and without anode exhaust recirculation. The reference case is introduced when the system is fueled by pure methane. Then, the performance of the hybrid SOFC-GT system is investigated when methane is partially replaced by CO_2 from concentration of 0% to 90% with an increment of 5% at each step. The steady-state macro level model of the SOFC-GT hybrid system was developed in Aspen Plus® using built in and user-defined modules. The performance of the system was monitored by estimating and recording performance parameters, such as SOFC and system thermal efficiency; net and specific work of SOFC, GT, and cycle as a whole; air to fuel ratio; and mass and molar flow rate and temperature of various streams. The results demonstrate that the CO_2 fraction in the inlet fuel has remarkable influences on the system's operating parameters, such as efficiency and specific work.

INTRODUCTION

Nowadays most power generation in the world is based on fossil fuel power plants. The nonrenewable nature of fossil fuels, their finite resources, and instability in their market as well as their environmental impacts are major drawbacks of the fossil fuel-based power generation [1]. On the other hand, it is predicted that the global power demand will increase dramatically in near future [2]. Renewable energy resources are ultimate solution for these problems. However, fossil fuel consumption is essential for global economical growth, at least in short- and mid-term. Therefore, it is important to increase the fossil fuel power generation efficiency and decrease its environmental impacts. These objectives can be achieved by combination of various methods, such as more efficient power generation, fossil fuel use with CO_2 capture and storage, biofuels, fuel cells, etc [3]. Fuel cells are promising technology for electricity generation that can fulfill these targets. Their operation is based on the direct conversion of fuel chemical energy to electrical energy (and possibly useful thermal energy) via electrochemical reactions.

Fuel cell attributes can be enumerated as follows: direct energy conversion (no combustion), potential for high efficiency, lower pollution, scalability, no moving parts in the energy converter, quiet operation, fuel flexibility, easier carbon capture, possibility for water production, and possibility for integrating to hybrid and cogeneration systems. Some of these characteristics are unique for fuel cells. For instance, their high efficiency, low emissions and costs, and other attributes are nearly unaffected by the size of the plant, which makes them scalable to all sizes, which in turn helps them to match load and increase their reliability [4].

However, fuel cells require some major improvements before they can compete conventional power generation technologies. The most important challenge is to reduce cost by developing new construction methods and materials, mass production and the economy of scale, which requires some mass markets. Also depending on the application, suitable durability, endurance, reliability, longevity, specific power, and power density need to be achieved.

There are many potential applications for fuel cells, such as stationary and distributed power generation, transportation applications, portable applications, auxiliary power units (APUs) for vehicles, electricity storage by regenerative (reversible) fuel cells, space applications, and military applications. Among various types of fuel cells, high temperature fuel cells, especially solid oxide fuel cells (SOFC), are suited for stationary power generation. This high temperature (between 600˚C-1000˚C) allows for the integration of SOFC with gas turbines (GT) or other bottoming cycles to form hybrid cycles. A hybrid cycle can be any combination of a SOFC coupled with a gas turbine, steam turbine, combined cycle power plant, coal integrated gasification combined cycle (IGCC), as well as combined heat and power production (CHP) [5]. A comprehensive literature survey of models of hybrid SOFC systems can be found in [6].

In addition, the high operating temperature of SOFCs allows for the internal reforming of natural gas, syngas from coal and biomass, and biogas within the cells, which provides fuel flexibility for SOFCs. Various fuels have been adopted for hybrid SOFC systems modeling in open literature. In most modeling works, natural gas or methane was considered as fuel [7-16]; however, there have been models that used hydrogen [17, 18], syngas from coal [19-21], various biofuels [22], and even jet fuel [23].

To avoid problems associated with conventional fuels, the application of alternative fuels, such as biomass and syngas, has been greatly studied. However, before the commercialization of the utilization of these fuels can be achieved, some problems such as variation of fuel composition should be addressed. Typically, depending on feed material to the system, the fuel production process, and process control parameters, alternative fuels are composed of methane, hydrogen, carbon dioxide, water, nitrogen, carbon monoxide, and minor amounts of other components with different percentage of each species [24]. Therefore, in order to have a proper utilization of these fuels in hybrid SOFC cycles, it is essential to investigate the impacts of fuel composition variation on the performance of the overall system.

There have been very limited numbers of modeling works that investigate the effects of fuel composition on the hybrid SOFC system performance. For instance, Sucipta et al. [24] evaluated the effects of biomass fuel chemical composition, namely, H_2, CO, CO_2, H_2O, and N_2 on the hybrid system performance. They also studied [25] efficiency and temperature distributions when natural gas were mixed or completely replaced by biofuel. Similarly, Van Herle et al. [22] performed the energy balance analysis on an existing biogas production unit, equipped with a 1 kW SOFC demonstrational stack as a small CHP system.

Further studies are required in this field to investigate all aspects of the issue for different configurations and assumptions. This paper focuses on how CO_2 concentration in inlet fuel can affect the performance of the hybrid SOFC-GT system. Table 1 shows the concentration of methane and carbon dioxide in some fuel sources. As this table points out, concentration of carbon dioxide can vary from around 2% to almost 40%. This range for methane is from around 1% to more than 97%.

Table 1: VARIATION OF METHANE AND CARBON DIOXIDE FRACTION IN SOME FUELS

Fuel type	CH_4 (%)	H_2 (%)
Natural gas [12]	97.4	1.6
Farm biogas [22]	63.0	36.0
Sewage biogas [19, 24]	61.5-62.6	34.8-38.3
Syngas (dry coal feed) [26]	1.4	1.6
Syngas (dry biomass) [26]	4.7	12.9
Biofuel [27]	13.0	15.0
Gasified biomass, H_2O-blown [28]	10.0	20.0
Gasified biomass, Air-blown [28]	5.0	10.0

As this table indicates the concentration of methane and carbon dioxide can vary widely, which means their effects can be profound. In the following sections, the hybrid system configuration for this study and developed model characteristics will be explained.

CYCLE AND MODEL DESCRIPTION

For this work a steady-state model of the SOFC-GT hybrid cycle was developed in Aspen Plus®. Aspen Plus® is a tool for realistic steady-state simulation of thermodynamic cycles by connecting built-in (in this case, gas turbine, fuel reformer, combustor, material stream mixer and splitter, and heat exchanger) and user-defined components (in this case SOFC) with material, work, and heat streams. Macro level approach was used for this work because for hybrid SOFC system, simulation emphasis was placed on the interaction of the fuel cell and the rest of the system and how the fuel cell can affect the overall performance of the system.

The model included the activation, concentration and ohmic losses within the SOFC with following inputs: current density, fuel and air composition, flow rates, temperature, pressure, and fuel utilization factor. The model outputs were the composition of the exhaust, work produced, heat available for reformer, etc. The mathematical model, modeling steps, and modeling assumptions for the developed model of the hybrid SOFC-GT cycle have been already documented elsewhere [16, 29]. The required model constants were determined considering the data from the Siemens Westinghouse SOFC [30]. Also, the model was validated by comparing the simulated output voltage of the SOFC versus current density for different temperatures and pressures with the experimental data from the Siemens Westinghouse tubular SOFC [30].Generally, there was an acceptable qualitative agreement between the simulation results and experimental data [16, 29].

HYBRID CYCLE CONFIGURATION

Figure 1 illustrates the basic configuration of the hybrid SOFC-GT cycle investigated in this research. The equipment models encircled by the dashed line represent the SOFC stack and its internal components. In this system, the inlet fuel to the system is first compressed from standard temperature and pressure (STP) to system pressure at F-COMP and its temperature is increased at FHX by heat recovered from GT exhaust. Then, in order to provide required water for the fuel reforming reactions and preventing coking in the reformer and SOFC stack, the fuel is mixed with recycled part of the anode off-gas stream in a mixer (AN-MIXER). The mixture of fuel and anode exhaust recycled stream, containing enough steam for fuel reforming process, is then fed to the fuel reformer.

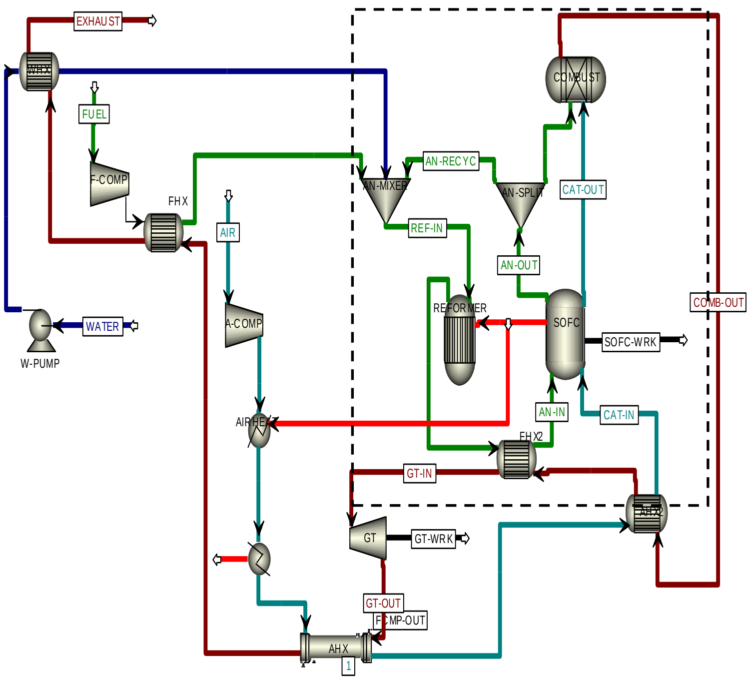

Figure 1: HYBRID SOFC-GT CYCLE CONFIGURATION IN THIS STUDY

The fuel reforming reactions are endothermic. On the other hand, there is excessive heat generated in the SOFC. In an actual SOFC stack, since the fuel reformer and SOFC stack are physically close, required heat for the reformer can be provided by the SOFC. In the simulation, the excessive heat released by the SOFC stack is first exchanged with the reformer and then with the incoming air (at AIR HE) and finally discharged to the environment. The reformer outlet is fed to the SOFC at AN-IN. However, if the outlet temperature is not high enough, it is heated to the SOFC operating temperature at FHX2 before being fed into the SOFC.

On the other hand, the inlet air, entering the system at STP, is compressed at A-COMP and heated at AIR HE and AHX by the excess heat extracted from the SOFC and the gas turbine exhaust, respectively. If the temperature at AHX outlet is lower than the SOFC operating temperature, the air is heated by the high energy COMB-OUT stream at AHX2 before being fed to the SOFC at CAT-IN.

Fuel mixture and air, entering SOFC at anode and cathode, respectively, participate in electrochemical and reforming reactions producing electrical work and releasing heat. The anode off-gas is split into two streams at AN-SPLT, part of this stream recycles to mix with the fuel. The user-defined steam to carbon ratio (SCR) determines anode recirculation flow rate to provide steam for the fuel reforming reactions. The rest of the anode exhaust stream (AN-OUT) is burnt with the cathode exhaust stream (CAT-OUT) at the GT combustor. The combustor outlet, after passing through AHX2 and FHX2, enters the gas turbine.

The turbine inlet temperature (TIT) is a critical parameter in the GT operation. The TIT should not exceed a certain limit because of material thermal stress limitation. In the model, in order to achieve the user-defined TIT, the air to fuel ratio of the system is automatically adjusted. Finally, the GT exhaust is used to heat the inlet fuel in AHX and FHX.

The model can simulate two cycle configurations, with anode off-gas recirculation and with heat recovery steam generator to provide steam for the reforming reaction. By enabling or disabling the anode exhaust recirculation feature, both cycles can be studied. If the anode recycling is disabled, steam provided by the heat recovery steam generator (WHX) is mixed with the fuel to meet the required steam to carbon ratio of fuel reforming reactions. With anode exhaust recirculation disabled, the heat recovery steam generator covers the entire steam requirement of the reformer. Otherwise no steam is generated in the heat recovery steam generator.

RESULTS AND DISCUSSION

The model described in the previous section was used to investigate the effects of CO_2 in the fuel on the performance of the hybrid SOFC-GT cycle with two configurations: with and without anode recirculation. In this work, performance parameters, such as SOFC and system thermal efficiency; net and specific work of SOFC, GT, and entire cycle; air to fuel ratio; as well as air and fuel mass flow rate were investigated. In order to perform the analysis, the reference case is introduced, then, discussion for the cases where methane is partially replaced by CO_2 is presented.

Reference case

The hybrid SOFC-GT system fueled by pure methane is considered as the reference case. The data presented in this subsection for reference case can be observed from corresponding figures (Figures 2 to 10) at 0% CO_2 concentration.

In this case, the overall efficiency of the hybrid cycle for configurations with and without anode recirculation is 74.6% and 73.9%, respectively. The corresponding efficiencies for SOFC are 58.2% and 50.3%, respectively. On the other hand, since the molar flow rate of the fuel is fixed for all cases, the fuel mass flow rate for both configurations is 16 kg/h with the lower heating value (LHV) of 50 MJ/kg. However, the air mass flow rate and air to fuel ratio for the system with anode recirculation are lower than that in the other configuration (19.6 vs. 25.3 kg/h, and 19.6 vs. 25.3, respectively). The specific work for the SOFC and GT in the system with anode recirculation is 827 and 369 kJ/kg_{air}, respectively. These specific works for the system without anode recirculation are 551 and 394 kJ/kg_{air}, respectively.

To evaluate the effects of fuel composition on the cycle performance, sensitivity analysis were performed on the model, when the fuel is a mixture of CH_4 and CO_2 with different percentages. In this analysis, 5% of methane has been replaced by CO_2 at each step in the range of 0% to 90%.

Output power

Figure 2 shows the output power of the SOFC, GT, and system versus the concentration of CO_2 in the inlet fuel for two configurations, with and without anode recirculation.

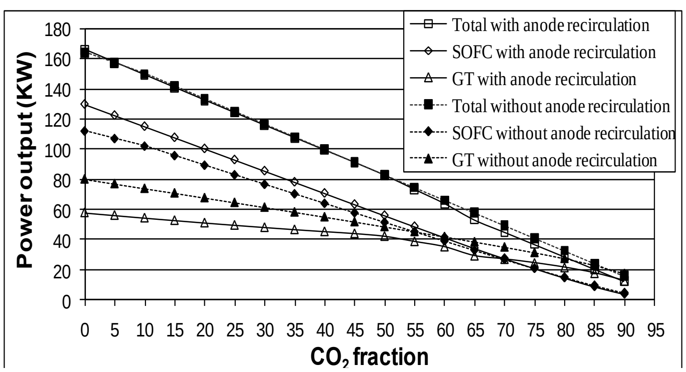

Figure 2: OUTPUT POWER OF GT, SOFC AND CYCLE FOR DIFFERENT CONFIGURATIONS VERSUS CO_2 CONCENTRATION

This figure shows that in all cases output power reduces with the increase in CO_2 concentration. This is because of variation in the inlet fuel energy content, as shown in Figure 3. The figure shows the variation of input fuel LHV, mass flow rate, and energy content versus CO_2 concentration in the inlet fuel for both configurations. These graphs are for both configurations because in the model the fuel molar flow rate is kept constant (1 kmole/hr). Thus, the fuel flow rate is an independent variable in the model and is equal for both configurations. Figure 3 illustrates that when CO_2 concentration increases, LHV of the fuel is decreased. The reason is that in this case methane (with 50 MJ/kg LHV) is replaced by CO_2 with no energy content. On the other hand, for constant molar fuel rate (1 kmole/hr), the fuel mass flow rate increases due to the higher atomic weight of CO_2 in comparison to CH_4 (16 for CH_4 vs. 44 for CO_2). Figure 3 points out that the rate of increase in the fuel mass flow rate is lower than the rate of reduction in the inlet fuel LHV. As a result, the input energy content of the fuel reduces as CH_4 concentration decreases, which in turn causes lower output power from the GT and SOFC (Figure 2). The rate of inlet fuel energy content reduction is 2.23 kJ/hr for 1% of CO_2, which causes output power reduction (in both configurations) with the rate of 1.7 kW per 1% of CO_2. Also, reduction in the efficiencies of the GT, SOFC and whole cycle causes further reduction in the output power, which will be shown later.

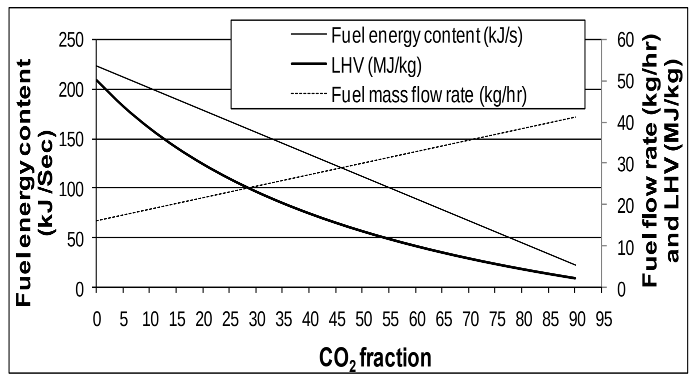

Figure 3: INPUT FUEL LHV, MASS FLOW RATE AND ENERGY CONTENT WITH RESPECT TO CO_2 CONCENTRATION

Figure 2 also indicates that the power output of GT in the configuration without anode recirculation is higher than that of the cycle with anode recirculation. This is because when the SOFC exhaust is partially recycled before entering the GT, the actual mass flow rate of GT reduces, which means less power is generated in the GT. Figure 4 shows the GT mass flow rate for both configurations and, as explained, the mass flow rate through GT in the configuration with anode recirculation is lower than that in the configuration without anode recirculation.

The comparison of the SOFC output power and GT output power (Figure 2) shows that for low concentrations of CO_2, the SOFC output power is higher than the GT output power. However, above 55% of CO_2 for the cycle without anode recirculation and 70% of CO_2 for the cycle with anode recirculation, the GT output power dominates the SOFC output power. This will be further explained later. In addition, in Figure 2, the output power for all cases is obviously close to zero when there is a very high concentration of CO_2.

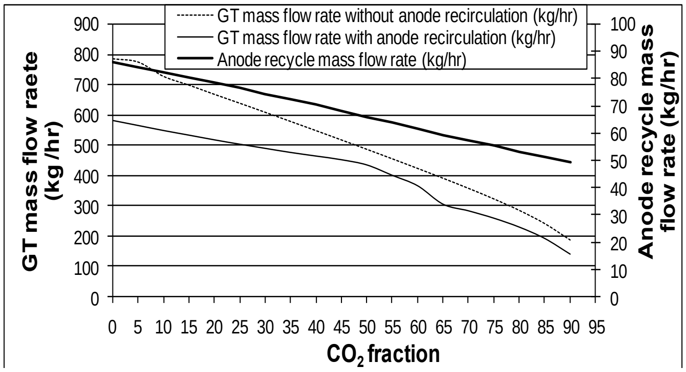

Figure 4: GT MASS FLOW RATE AND ANODE RECIRCULATION MASS FLOW RATE VERSUS CO_2 FRACTION IN THE INLET FUEL

Figure 4 also illustrates that the curves for the GT mass flow rate for two configurations converge with the increase of CO_2 concentration in the inlet fuel. The reason is that when the CH_4 concentration reduces, the flow rate of the fuel that requires reforming decreases, so the steam required for reforming reduces, which decreases anode recirculation mass flow rate (Figure 4, curve for the anode recirculation mass flow rate).

Moreover, Figure 4 shows the GT mass flow rate in the cycle with anode recirculation experiences sudden shift after the CO_2 fraction of 55%. This GT mass flow rate reduction causes lower power output of GT, which in turn results in the lower SOFC-GT power output. This can be seen in Figure 2, where total power output in the configuration without anode recirculation is slightly higher than that in the other configuration, especially for the CO_2 concentration of more than 60%.

The comparison of the power output of SOFC in configuration with and without anode recirculation shows that the output power of the former is higher than that of the latter. The reason is that when anode exhaust is recycled, the overall net fuel utilization factor is higher even though the fuel utilization efficiency of the fuel cell is constant. This is because some of the unused fuel in the recycled anode exhaust is consumed in the fuel cell. Figure 5 illustrates the molar flow rate of H_2 and CO in the anode exhaust that enters the combustion chamber. The H_2 molar flow rate in the system with anode recirculation is lower than that in the system without anode recirculation. But CO molar flow in configuration with anode recirculation overtakes the other configuration at 55% of CO_2. However, overall, more fuel is consumed in SOFC in the cycle with anode recirculation, which requires higher net fuel utilization factor in SOFC.

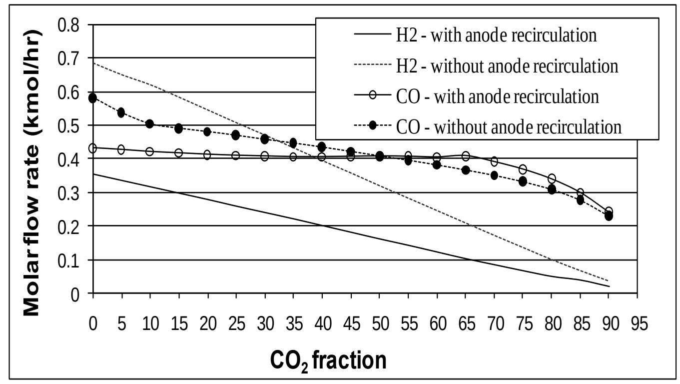

Figure 5: MOLAR FLOW RATE OF H_2 AND CO IN ANODE EXHAUST

Specific work

Figure 6 shows how the specific work of the GT, SOFC, and cycle as a whole for different configurations vary with respect to variation of CO_2 concentration in the inlet fuel. The specific work is defined as the output power divided by the inlet air mass flow rate and is used as an indication for the size of the system and its component. In this figure, the GT specific work is almost constant. However, SOFC and whole cycle specific work decrease with increase in the CO_2 concentration. Moreover, there is a shift at the 65% of CO_2 fraction in the cycle with anode recirculation.

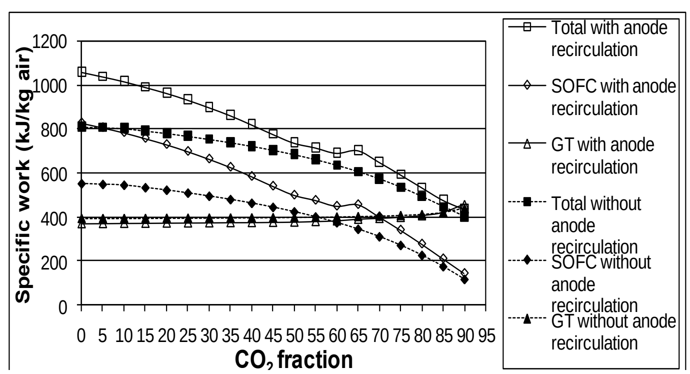

Figure 6: SPECIFIC WORK OF GT, SOFC, AND CYCLE AS A WHOLE VERSUS CO_2 CONCENTRATION IN THE INLET FUEL

Both the power output and air mass flow rate should be considered in order to investigate these graphs. Figure 7 shows the inlet air mass flow rate and air to fuel ratio for different configurations versus CO_2 concentration in the inlet fuel. Based on the system control strategy, when fuel energy content is reduced, the air to fuel ratio should be reduced accordingly in order to keep the TIT constant (Figure 3). That is why the inlet air mass flow rate and air to fuel ratio reduce with the increase in CO_2 concentration for both configurations.

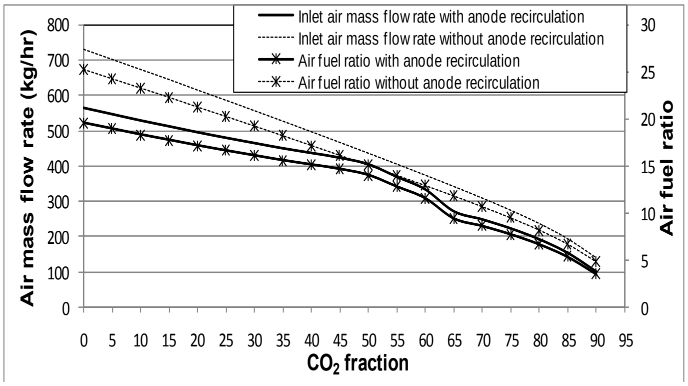

Figure 7: INLET AIR MASS FLOW RATE AND AIR TO FUEL RATIO VERSUS CO_2 CONCENTRATION

Both air to fuel ratio and inlet fresh air mass flow rate in Figure 7 are lower in the cycle with anode recirculation and the graphs converge. This is because of the higher net fuel utilization factor in the SOFC with the anode recirculation (Figure 5), which means there is less fuel to be burnt in the combustion chamber to keep the TIT constant.

Another important feature of Figure 7 is a shift in the graphs for configuration with anode recirculation. The main reason for this shift is the temperature reduction in the fuel reformer. When CO_2 concentration exceeds 45%, the reformer temperature gradually declines, as shown in Figure 8. Therefore, there is no heat to be recovered in the air heater (AIRHE). Instead, the reformate should be heated at the heat exchanger (FHX2) to increase its temperature to 1000˚C before entering the SOFC module. Thus, although the physical configuration of the cycle is unchanged, the real cycle configuration (those equipments that are actually involved in the process) has been altered. As a result of all these events, the inner working of the cycle has been changed, and that is why there is a shift in Figures 6 and 7, as well as figures presented earlier, for the cycle with anode recirculation.

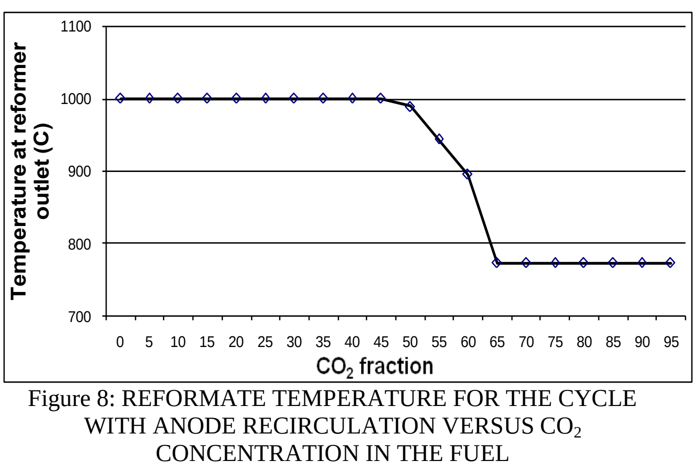

Figure 8: REFORMATE TEMPERATURE FOR THE CYCLE WITH ANODE RECIRCULATION VERSUS CO_2 CONCENTRATION IN THE FUEL

In Figure 6, the reason for the reduction in the specific work of SOFC module and SOFC-GT cycle is that the reduction rate of the output work of both configurations (Figure 2) is higher than the reduction rate of the air mass flow rate (Figure 7).

Efficiency

Figure 9 shows the efficiency of the SOFC and GT modules and SOFC-GT cycle for different configurations versus CO_2 concentration in the inlet fuel. The variation in this figure should be investigated in conjunction with output power (Figure 2) and the energy content of the consumed fuel (Figure 3).

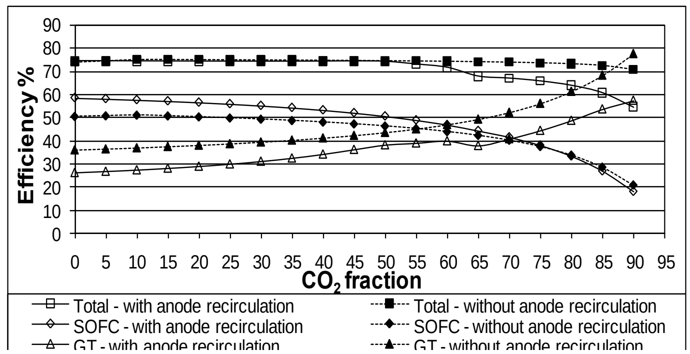

Figure 9: EFFICIENCY OF SOFC, GT, AND CYCLE VERSUS CO_2 CONCENTRATION IN THE INLET FUEL

Figure 9 illustrates that for both configurations, the SOFC efficiency decreases and GT efficiency increases. The SOFC-GT efficiency for the cycle without anode recirculation is almost constant, which means the reduction of SOFC output power is compensated by the increase in the GT efficiency. However, in the configuration with anode recirculation, the increase of GT power could not compensate the power decrease of SOFC module.

SOFC to GT output power ratio

Another important parameter in this hybrid system is the ratio of the work generated in the SOFC and GT, as shown in Figure 10. The figure indicates that less power is generated in SOFC and more power is generated in GT when the concentration of carbon dioxide increases in the inlet fuel.

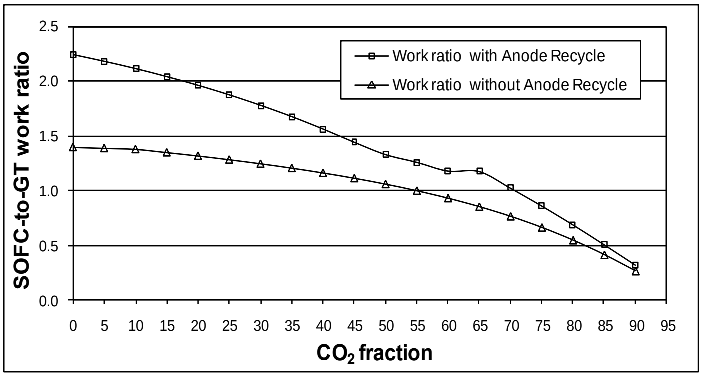

Figure 10: SOFC TO GT OUTPUT POWER RATIO FOR TWO CONFIGURATIONS VERSUS CO_2 CONCENTRATION IN THE FUEL

CONCLUSIONS

A macro level model of the SOFC system was developed considering the activation, concentration, and ohmic losses within cells. The SOFC model was implemented in a hybrid SOFC-GT cycle model using Aspen Plus® to simulate two configurations, system with and without anode recirculation. The simulation results were presented with respect to a reference case, when the system was fueled by pure methane. Then, the performance of the hybrid SOFC-GT system when methane was partially replaced by CO_2 from concentration of 0% to 90% with an increment of 5% at each step was investigated.

The results showed that all important parameters of the cycle, including the SOFC and system thermal efficiency, as well as the SOFC, GT, and cycle net and specific work decrease when methane was replaced by carbon dioxide. This study confirms the importance of fuel composition effects on the SOFC-GT system performance.

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NOMENCLATURE

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