

# Thermodynamic Modeling and Analysis of the Ratio of Heat to Power Based on a Conceptual CHP System

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**Abstract:** The CHP system not only produces electrical energy, but also produces thermal energy. An extensive analysis of the CHP market reveals that one of the most important engineering characteristics is flexibility. A variable heat-to-power ratio has compelling advantages over a fixed one and enables a power plant to achieve reliability and flexibility, which are very important characteristics for a CHP system. In this paper, a conceptual SOFC/GT CHP system is presented. The parameters' effect on the variable heat-to-power ratio is investigated. As SOFC reactors are still under development, a flexible simulation tool based on mass and energy balances coupled with appropriate expressions for the reaction kinetics, thermodynamic constants and material properties, is presented for adaptation to different cell geometries and operating conditions. Simulation results show that the SOFC/GT CHP system's advantage over the engine is that a low stack running temperature can achieve a low heat-to-power ratio.

**Key words:** Heat to Power ratio, SOFC, Gas turbine, Simulation

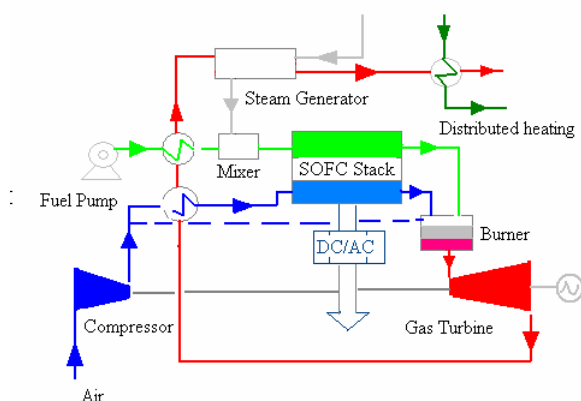
## 1. INTRODUCTION

Solid oxide fuel cells (SOFCs) are electrochemical reactors currently under development for applications in the field of energy conversion<sup>[1]</sup>. As the fuels are concerned, pure hydrogen and methane are generally being studied with internal and external steam reforming. Among the reactor geometries, planar<sup>[2]</sup> and tubular<sup>[3][4][5]</sup> shape have been proposed with a number of variation such as planar cells with integrated air pre-heater<sup>[6]</sup>. Even though it is difficult to quote an average SOFC performance, the experimental data reported in the

literature being distributed over a wide range demonstrated that, with an operating temperature in the range 900-1000 °C, with pressure of 1 bar and hydrogen as fuel, the energy efficiency of the cell alone is at least 50%. Another power sources suited to small energy demand is the small gas turbine (GT) which is currently being introduced into the distributed electrical power generation market, and many companies are involved in the R&D project of micro-turbines<sup>[7][8]</sup>. With a compressor pressure ratio of about 4, a turbine inlet temperature of 880-900 °C, and a recuperator effectiveness of 0.85-0.88, the estimated thermal efficiency is about 30%<sup>[9]</sup>. Factoring in other aspects, including the generator and the power required for the fuel compressor, the overall efficiency of the micro-turbine that stands alone is about 27%. To advance significantly beyond this level will require an increase in turbine inlet temperature, which will necessitate the use of ceramics in the hot-end components<sup>[10]</sup>. SOFCs integrated with GT of small size are attracting wide interest<sup>[11][12]</sup> as these systems are able to simultaneously solve some of the key problems of small GT and of SOFC, such as low efficiency and NO<sub>x</sub> emission, high cost. Integrated SOFC/GT are investigated by many developers and at early stage of testing at the moment<sup>[9]</sup>.

CHP system based on SOFC/GT not only produces electricity energy, but also produces thermal energy. An extensive analysis of the CHP market includes that one of the most important engineering characteristics is the flexibility<sup>[13][14][15][16]</sup>. The heat-to-power ratio is defined as the rate of useful thermal energy production to that of electrical energy production. A variable heat to power ratio has

compelling advantage over a fixed one<sup>[17][18]</sup>. Firstly, the more closely a CHP unit can match the instantaneous demand for the heat and power, the more efficient it will be. Secondly, a variable heat to power ratio that leads to higher fuel efficiency also results in low emissions. Finally, and most importantly, a variable heat to power ratio enables a power plant to achieve reliability and flexibility that are of the most important characteristics for CHP system.



**Fig. 1 Scheme of the conceptual CHP system based on SOFC/GT**

In this paper, a conceptual CHP system based on SOFC/GT is presented and analyzed for the variable heat to power ratio. All the models are presented and discussed in detail in this paper, the details of the configuration of the SOFC module and GT group and overall plant are discussed and presented together with the modeling equations in the next section of the paper. And this paper briefly outlines design options for achieve the goal of a variable heat to power ratio.

## 2. CONCEPTUAL CONFIGURATION OF SOFC/GT SYSTEM

A conceptual SOFC/GT system with internal reformer is examined in this study and is shown schematically in Fig. 1. The system consists of one SOFC stack, one combustor, one gas turbine, one compressor, one pump, three recuperators and one steam generator. The compressed fuel and air are preheated in their respective recuperators prior to enter the SOFC stack, and heated fuel mixes with steam from steam generator before channeling

through the anode. Natural gas is internally reformed in the anode compartment and hydrogen-rich products are produced. Electrical energy is produced together with heat generation during the process, in which electrochemical reaction occurs at the three-phase boundaries of the electrodes. The heat generated is partly dissipated to the surroundings, partly used to reform the natural gas, and partly used to heat up the feedstock gases<sup>[7]</sup>. The burner is used to combust the unutilized fuel and depleted air, and exceed air (dashed line in Fig. 1) is required to ensure the exit gas temperature under the allowable turbine inlet temperature. The combusted gas mixture flows through the GT and mechanical power is produced to compress air and produce electricity. The effluent gases from the GT pass through a series of two recuperators where preheating of air and fuel occurs. The steam generator is to generate steam for internal reforming and the last recuperator is used to produce distributed heating.

## 3. MODEL OF SOFC/GT SYSTEM

### 3.1 The Electrochemical Model

As SOFC reactors are still under development, a 'state of the art' fuel cell performance cannot be defined, and it would be very useful to have a flexible simulation tool, which could easily be adapted to different cell geometries and operating conditions, and this is possible with a model based on mass and energy balances coupled with appropriate expressions for the reaction kinetics, thermodynamic constants and material properties<sup>[9][10][16]</sup>.

For the simulation of the system, the following assumption were made<sup>[10]</sup>: 1) all components exterior wall are adiabatic; 2) uniformity of temperature within all the components of the SOFC group; 3) cathode flow composed of  $O_2$  and  $N_2$ , and anodic flow composed of  $CH_4$ ,  $CO$ ,  $CO_2$ ,  $H_2$ ,  $H_2O$ ; 4) internal reforming and shifting reactions at equilibrium; 5) stoichiometric fuel-air reaction throughout all the process.

To avoid the ambiguity of simplified models used under different operating conditions, the general Butler-Volmer equation is used to calculate the respective over-potential of the anode and cathode.

Ohmic over-potential, which contributes by the electrolyte, electrodes and inter-connector of the fuel cell, occurs because of the resistance to the flow of ions in the ionic conductors and the resistance to electrons through the electronic conductors. Since these resistances obey Ohm's law, the Ohmic over-potential can be simulated by the Ohm's law.

Concentration over-potential occurs when the diffusion of the reactants through the electrodes is slower than the electro-chemical reaction. However, at the high operating temperature of SOFCs, diffusion is usually a very efficient process, and thus this effect is usually negligible, unless under conditions of very high fuel or oxidant utilization, which are not taken into consideration here. Thus, concentration losses have been neglected in this work..

The mass balance equations of the SOFC stack account for the process of conversion of chemical energy to electrical energy. The energy balance equation includes the electrical power and the enthalpy changes of the chemical and electrochemical reactions.

### 3.2 Model of Heat Exchangers

For the heat exchangers, such as recuperator, the effectiveness-number of transfer units ( $\epsilon$ - $NTU$ ) method<sup>[16]</sup> is used to model the performance. In this study, counter-flow types of heat exchanger are selected as the pre-heater.

### 3.3 Model Gas Turbine and the Compressor

A polytropic positive displacement compressor model<sup>[10]</sup> was used and allowed the user to specify pressure, power or performance curves to determine the discharge conditions. For the gas turbine, an isentropic model was also used with the outlet pressure specified, as well as the isentropic and mechanical efficiency. Results from both models are net power and discharge conditions, such as outlet pressure and temperature.

### 3.4 Model of Combustion Chamber

A stoichiometric reactor was used to model the combustion in this study when the reaction kinetics are unknown or unimportant, and the stoichiometry and the degree of conversion are known for each

reaction. All reactions occurring in the reactor and their stoichiometry must be specified, together with the molar extent (product flow) or fractional conversions of key components.

### 3.5 Model of Electrical Components

The performance of the inverter that converts the DC to AC is simply included as an efficiency 95%. The same is true for the turbine generator efficiency, normally set to 98%.

### 3.6 Simulation Strategy

In simulation, there are two important iteration loops. One is to calculate the stack temperature in the SOFC stack model, which is unknown at the beginning of the computation but is necessary for both reforming and electrochemical reaction calculation. The other is to determine the corrected speed and additional fuel/air flow rate for the SOFC/GT system, which requires heat, flow, and shaft speed. Since both the compressor and GT performance calculation requires a corrected mass flow rate, tedious iteration is unavoidable.

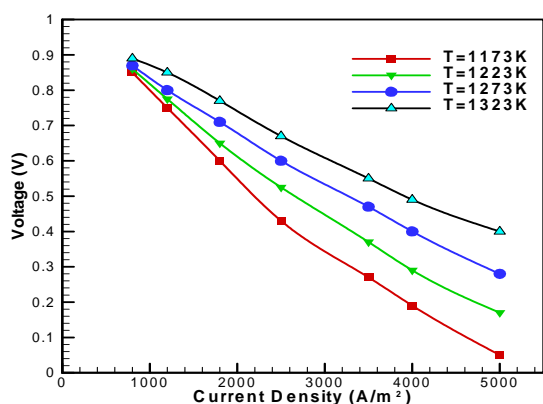
For the whole system model, since the recuperators need the heating fluid parameters (such as the exit gas temperature of the turbine), which are not known at the beginning of the simulation, a set of initial parameter has to be assumed in order to run the system model until convergence is met eventually<sup>[7]</sup>.

## 4. RESULTS AND DISCUSSION

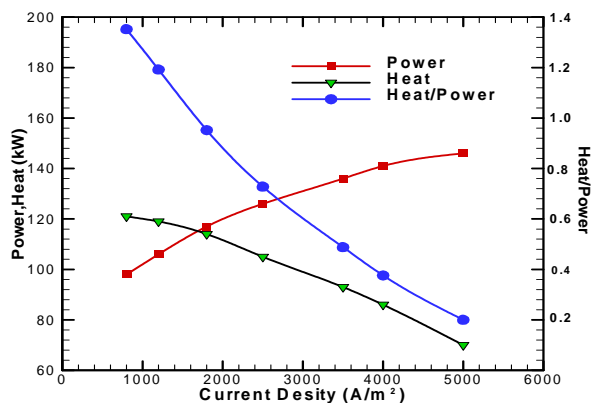
In our case study, the design point of the SOFC/GT system is the operating condition where the turbine flow rate, rotational speed, pressure, and turbine inlet temperature are compatible with the limitations of this technology and the size of the turbine under consideration. The typical operating parameter is: fuel (natural gas) and air entrance temperature is 25 °C, pressure is 1 bar and the compressor ratio of fuel pump and compressor is 10.5 and 3.8 respectively, the inlet temperature of the gas turbine is 900 °C.

In order to facilitate the understanding the results of the overall plant simulation, the performance characteristics of the SOFC stack alone

are present and discussed. In particular, the current-voltage curves obtained under different operating conditions for the SOFC stack are present. One of the most important parameters influencing the SOFC performance is the operating temperature of the fuel cell stack, for this purpose, and in order to vary according to the energy balance equation, but is was imposed as input datum, in order to determine its effects on the electrical performance. Those results are interesting also for a better understanding of the plant behavior. In all the runs, the pressure was 3.8 bar, and the inlet temperature of the gases were 450 and 650°C at the fuel and air sides, respectively.



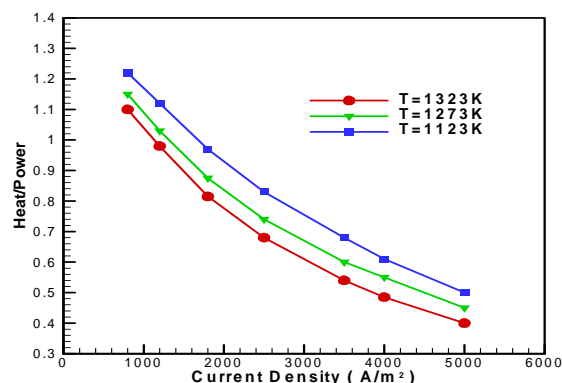
**Fig. 2 Effect of cell current density on the voltage at different running temperature**



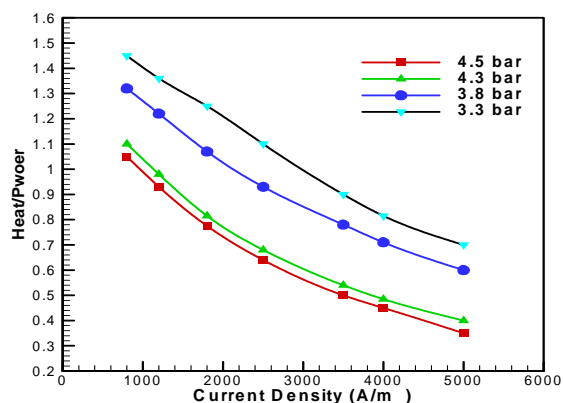
**Fig. 3 Effects of cell current density on the heat, power and heat to power ratio at the stack running temperature of 1123 K**

Fig.2 shows the current-voltage simulated characteristic curves at different stack operating temperature, from 800 to 950°C. By decreasing the temperature, the voltage decreases due the increase

both the activation and Ohmic resistance. In general, as the temperature rises, activation polarization decreases due to the higher reaction rate, Ohmic polarization decreased due to decrease in the resistance in the electrodes and the electrolyte, and the concentration polarization decreases due higher mass diffusion rates. Also, as temperature rises, low temperature fuel cells have a higher tolerance to carbon monoxide. On the other hand, as temperature rises, polarization may increase due to material constraints. These temperature changes are, for the most part, instantaneously reflected in the cell's polarization curve and hence its heat-to-power ratio. Therefore, a FCS can be operated in such a way that it changes its stack temperature to alter its heat-to-power ratio to respond to changes in electricity demand.



**Fig. 4 Effects of cell current density on the heat to power ratio at different stack running temperature**

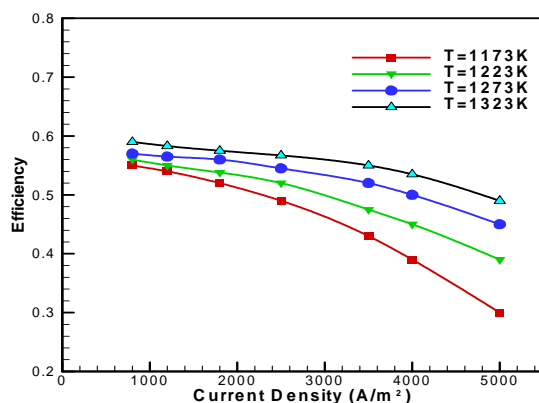


**Fig. 5 Effects of cell current density on heat to power ratio at different stack running pressure**

Fig.3 shows the relation between current density and power and thermal energy. With the current density rises, the power production increases and the

thermal energy available decreases. This is increasing power need more energy to reform the fuel. Fig. 4 shows that high stack running temperature causes the heat to power ratio decrease. The heat to power ratio advantage over an engine is that, at low temperature, unlike the engine, it can achieve low heat to power ratios. This relativity inimitable technical characteristic can be used as a competitive economic advantage.

Pressure has a similar effect as temperature (Fig. 5), an increase in pressure shifts the heat to power curve down, and vice verse. An increase in pressure increases the partial pressure of reactants and the rate of mass diffusion, and more thermal energy is needed to reform and more electricity is produced by gas turbine. As a result, the heat to power ratio is decreasing. The drawbacks to increase pressure include thicker piping, the need for a compressor with a higher rating and turndown ratio, and potential materials problems, such as reactant leakage through the electrolyte and seals. Also, the gains in fuel cell electrical efficiency from increasing the pressure are partly offset by the increase in parasitic power losses via the compressor.



**Fig. 6 Effects of the cell current density on efficiency at different stack running temperature**

The efficiency of the SOFC is an important parameter to be studied to understand the system behavior. Fig.6 shows the relation between efficiency and current density at different stack temperatures. The same tendency is observed by many researchers.

## 5. CONCLUSIONS

In this work, a conceptual CHP system based on SOFC/GT, which includes internal reforming SOFC stack, gas turbine, recuperator, mixer, etc., is presented. As SOFC reactors are still under development, a 'state of the art' fuel cell performance cannot be defined, and a flexible simulation tool, which based on mass and energy balances coupled with appropriate expressions for the reaction kinetics, thermodynamic constants and material properties are presented to be easily adapted to different cell geometries and operating conditions. Different from other research focus on increasing the electricity efficiency, the research is focus on the variable heat to power ratio. Simulation results show the SOFC/GT CHP system's advantage over the engine is that low stack temperature can achieve low heat to power ratio.

## ACKNOWLEDGMENTS

The Project was supported by Hunan Provincial Natural Science Foundation of China (05JJ30100) and by the Postdoctoral Science Foundation of Central South University 2005~2006

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