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Irreversibility and Electrochemical Modeling of GT-SOFC Hybrid System and Parametric Analysis on Performance of Fuel Cell

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***Abstract*—**Since the heart of the hybrid system is the fuel cell and it has vital impact on efficiency and performance of cycle, in this study, the major modeling of electrochemical reaction within the fuel cell is analyzed. Also, solid oxide fuel cell is integrated with the gas turbine and thermodynamic analysis on different elements of hybrid system is applied. Next, in predefined operational points of hybrid cycle, the simulation results are obtained. Then, different source of irreversibility in fuel cell is modeled and influence of different major parameters on different irreversibility is computed and applied. Then, the effect of important parameters such as thickness and surface of electrolyte fuel cell are simulated in fuel cell and its dependency to these parameters is explained. At the end of the paper, different impact of parameters on fuel cell with a gas turbine and current density and voltage of fuel cell are simulated.

***Keywords*—**Electrochemical analysis, Gas turbine, Hybrid system, Irreversibility analysis.

I. Introduction

According to forecasts by the international energy agency, in the future the main power generation will be based on gas turbines. Therefore, access to production technology with high efficiency, lower emissions and low maintenance costs of electric power generation is an essential requirement. Using gas turbines in a new cycle is a way to satisfy this important and also it is safe and environmentally friendly. So finding effective power generation systems that have a stake in reducing pollutants is vital [1].

The efficiency of conventional power systems is estimated to be less than 39%, which means that the other 60% of energy is lost from the system. The overall efficiency of conventional systems that produce electricity and heat are independent. The main components of the fuel cell include a fuel processor, fuel cell power modules, DC to AC power and heat conversion [2]-[4].

Depending on the operating temperature of the fuel cell, differing levels of heat is created for heating the input products or the application of synergies for heating. The use of this waste heat can effectively improve system efficiency and cost savings plan or account [5]. Variations in the design of hybrid systems using a variety of fuel cells, causing them to be selected according to the application. Also, due to the lower temperature oxidation of carbon oxide and nitrogen oxide fuel output per kW is much higher than traditional gas turbines. It also should be noted that the fuel cell efficiency increases at half time that it is unlike the traditional components such as turbines and compressors [6]. Some of the profound features that related to this system is the length of their working life to 40,000 hours, which is almost has important role to justifying the economic cost [7].

Reference [8] projected a high temperature operation SOFC-GT combined system, combined with an auto thermal reformer for power generation. Also, [9] confirmed that alternative hydrogen carriers such as ethanol are very striking fuels for SOFC-GT systems. Reference [10] tried to improve ethanol-fed SOFC-based systems in terms of energy and exergy.

Thermodynamic analysis for a solid oxide fuel cell with direct internal reforming fueled by ethanol has been achieved [11]. Performance of ethanol-fuelled solid oxide fuel cells was also explored in terms of conductors used [12]. In [13], SOFC system is combined with an ethanol steam reforming unit and it is modeled with special attention to the kinetics of the ethanol equations [14], [15]. However, all the above works are built on theoretical models for the calculation of fuel cell performance. Low and intermediate temperature SOFCs have established extensive attention recently due to the improved stability, reliability and reduced cost. Besides, SOFCs' operation at lower temperatures could: (a) assist the use of inexpensive metal mechanisms as inter-connects, (b) develop the stability and strength of all the components and (c) deal the potential of more rapid start-up and shutdown procedure [16]-[18].

Taking into care that novel materials have recently been established for intermediate temperature solid oxide fuel cells, in the present investigation a mathematical model has been established. The model simulates—from energy and exergy point of view—the process of a middle temperature solid oxide fuel cell integrated with a predictable gas turbine (IT-SOFC-GT) [19].

It is the first time to our information that experimental results for a middle temperature fuel cell performance taken from the open works are used. Another aspect of this work is the energetic comparison of a single IT-SOFC system with an IT-SOFC-GT system in order to explore operating conditions where a hybrid system overcomes in terms of effectiveness [20], [21].

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In this paper, electrochemical analysis on solid fuel cell with combination of gas turbine is investigated. First electrochemical analysis on fuel cell is implemented and structure of hybrid system is shown. Next, the effect of electrolyte on performance and definition of operational range of fuel cell is explained. Then, different source of irreversibility on fuel cell is modeled and mathematical and thermodynamic relations for those are applied. Next, parametric analysis for performance of fuel cell is applied and simulation results for hybrid cycle are obtained.

II. Electrochemical Analysis of Fuel Cell and Parametric Analysis of Performance of Fuel Cell

In fuel cell, oxygen is combined with fuel that makes electricity. For designing fuel cell, the kinetic reaction in fuel cell should be considered as:

Anode: $H_2 + O^{-2} \rightarrow H_2O + 2e^-$
Cathode: $1/2O_2 + 2e^- \rightarrow O^{-2}$
Principal reaction: $H_2 + 1/2O_2 \rightarrow H_2O$

Totally for existing one disposable hydrogen mole, two mole of electron exists. For conversion of electricity, faraday constant is considered as equal as F=96,485 coulombs/mole of electrons. The purpose of this unit is delivery of power according to:

$$Power = Current \times Voltage \tag{1}$$

On the other hand, fuel cell attains power from the released enthalpy during the reaction of $H_2 + 1/2O_2 \rightarrow H_2O$. Also, only portion of this enthalpy is used for electricity and the rest of it liberated as reaction heat. This heat should be released by gas flow. So the efficiency of fuel cell is computed as division of delivered power to given reaction energy. In this section by using standard reaction equation, chemical modeling of fuel cell is done. As mentioned above, there is a function between the reaction rate and currency of fuel cell that if (r_i) is defined as a current on area of fuel cell, the below equation is gained.

$$\frac{J}{2F} = -r_{H_2} = r_{H_2O} = -2r_{O_2} \tag{2}$$

Where, J is current density that is defined as:

$$J_{cell} = \frac{(E_{ner} - E_{cell})}{\bar{R}_{int}} \tag{3}$$

Also, E_{cell} is the operation voltage of cell and Nernst voltage can be computed as:

$$E_{ner} = E^0 + \left(\frac{RT}{2F}\right)\ln\left(\frac{P_{H_2}P_{O_2}^{1/2}}{P_{H_2O}}\right) \tag{4}$$

$$-r_{H_2} = \frac{\left(E^0 + \frac{RT}{2F}\ln\left(\frac{P_{H_2}P_{O_2}^{1/2}}{P_{H_2O}}\right) - E_{cell}\right)}{\left(\frac{\delta}{\sigma}\right)2F} \tag{5}$$

Also, in literature [16], [17] the designed reaction equation is computed as volume unit.

$$CSTR: V = \frac{F_{A,o}X}{-r_A(X)} \tag{6}$$

$$PFR: V = F_{A,o}\int_0^X \frac{dX}{-r_A(X)} \tag{7}$$

Also due to the definition of reaction as an area of fuel, these equations are converted as:

$$CSTR: A_{cell} = \frac{F_{H_2,o}X}{-r_{H_2}(X)} \tag{8}$$

$$PFR: A_{cell} = F_{H_2,o}\int_0^X \frac{dX}{-r_{H_2}(X)} \tag{9}$$

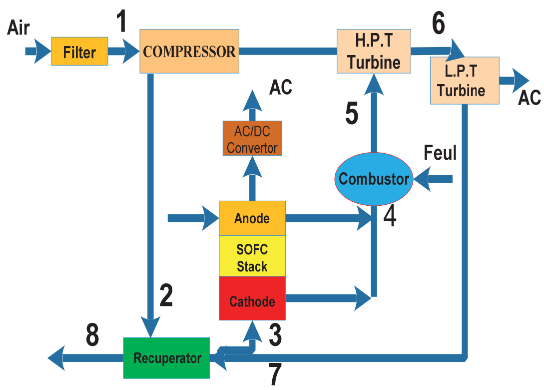

Fig. 1 Detailed schematic diagram of hybrid system

III. Electrode Role in Defining the Operational Range of Fuel Cell in Cycle

In recent years, fuel cell has been one of the most efficient energy sources. The fuel cell is an electrochemical device in which the reaction between hydrogen and oxygen is used to produce electricity and heat. The fuel cell is relatively calm and quiet, so is suitable for local power generation. Among the types of fuel cells, solid oxide type for high efficiency, low pollution, fuel consumption and more importantly the diversity of high temperature exhaust gas, is the best choice for use in gas turbines. This type of fuel cell power plants in combination with natural gas can produce an electrical efficiency of up to 70 to 80 percent. For this reason, in recent years, this technology has been very important. On the other hand, generally specify the electrolyte is very important in the temperature range of the fuel cell. Thus, shown in Table I, the fuel cell electrode and temperature are categorized as in table.

TABLE I
FUEL CELL CLASSIFICATION

Different types	PEMFC	AFC	MCFC	SOFC
abbreviation	Membrane proton exchanger Fuel Cell	Alkaline Fuel Cell	Molten Carbonate Fuel Cell	Solid Oxide Fuel Cell
electrolyte	Membrane Ion exchanger polymer	Potassium Hydroxide	Nickel and Nickel Oxide	Metal
catalyst	Platinum	Platinum	Electrode material	Electrode material
electrode	Carbon	Transition metals	Nickel and nickel oxide	Metal
temperature	40-80 c	65-220 c	605 c	600-1000c
efficiency	45	50	50	50
power	1-1000	10-100	100-10000	1000-100000
application	mobile	mobile	stationary	stationary

SOFC has high working temperature in the range of 600-1000°C, thus; it is suitable for combination with gas turbines. Today almost 96% of global production of hydrogen from fossil fuels is based on the use most of the methane as natural gas. In this section air is imported to the cathode and participates in electrochemical reaction.

IV. Modeling of Irreversibility of Fuel Cell

The true potential of the fuel cell due to the number of irreversibly will be removed from the real mode. These losses often occur because of the varied and original due to their importance in this field and modeling.

A. Activation Losses

The losses are related to the calm reaction on the surface of the voltage electrodes. On the other hand, production due to a chemical reaction that transfers electrons in the electrode was lost. In fuel cells with low and medium levels of temperature, excessive voltage for activation is one of the most important reasons of irreversible and particularly is reduce the voltage at the cathode electrode. On the other hand, in normal condition with more pressure and temperature, SOFC can reduce the voltage for activation. If the voltage drops in both the cathode electrode and just take in cathode, this share of voltage drop can be related to current density that is defined as:

$$\Delta V_{act} = A\ln\left(J + J_n / J_o\right) \tag{10}$$

J_n=current density for fuel cell, A=0.002.J_0=converted current density

Transition mass is defined as a portion of mass that is transformed from anode to cathode from electrolyte, and it has no effect on the production of electrochemical reaction. In the section of cathode, it reacts with oxygen directly and makes heat generation. On the other hand, electrolyte always is transformed some ion currency and makes to voltage drop. In researches, both of these losses are considered as a one loss that take place inside the fuel cell.

B. Ohmic Losses

Ohmic losses are electrolyte resistance through electrodes and also resistance of ion flow in electrolyte that has a simple modeling function. SOFC has Ohmic losses because of structure function of SOFC configuration. Total of these losses is formulated as:

$$\Delta V_{ohm} = Jr \tag{11}$$

Where is the thickness of fuel cell and also the dependency of this resistance according to temperature is exponential.

C. Transition of Mass losses

The circulation of air and lack of this source can be lead to decrease of oxygen of fuel cell and this variation makes of diminishing of current. Also the decrease in pressure of hydrogen or oxygen can lead to further drop of current density in fuel. For modeling these phenomena, M and N parameters is used for fitting of data that is shown in:

$$\Delta V_{trans} = M_{\exp}\left(N_J\right) \tag{12}$$

D. Overall Voltage Drop Equation

Total losses of voltage can be modeled in one equation as:

$$V = E_{oc} - Jr - A\ln\left(J\right) + M_{\exp}\left(N_J\right) \tag{13}$$

The constant parameters in above equation for fuel cell are written in Table II.

TABLE II
CONSTANT PARAMETERS OF SOFC IN MODELLING

E_{CO}(V)	1.01
R(KΩCM^2)	2×10^{-3}
A(V)	0.002
M(V)	1×10^{-4}
N(CM^{2}MA^{-1})	8×10^{-3}

E. Effect of Pressure and Temperature

During small operation times, the performance of SOFC due to the lack of free energy of system will be reduced. On the other hand, in high temperatures the resistance of SOFC decreases. In the literature, this function and dependency can be modeled as:

$$\Delta V_T\left(mv\right) = 0.008\left(T_2 - T_1\right) \tag{14}$$

SOFC as similar to other fuel cells has better performance in high pressure ranges. The effect of pressure to performance of fuel cell can be modeled as:

$$\Delta V_p\left(mv\right) = 59\ln\left(\frac{P_2}{P_1}\right) \tag{15}$$

The operational parameters of this simulation are shown in Table III.

TABLE III
OPERATIONAL PARAMETERS FOR FUEL CELL

Gas turbine	
Compressor efficiency	0.81
Turbine efficiency	0.84
Power turbine efficiency	0.89
Heat exchanger efficiency	0.8
Combustion efficiency	0.98
AC convertor efficiency	0.95
Solid oxide fuel cell	
Factor of air use	0.25
Factor of fuel use	0.85
Temperature of fuel cell	1273
Current density	0.3
Efficiency of AC/DC convertor	0.89
Area of fuel cell	834
Pressure losses	
Heat exchanger	4
Fuel cell	4
Combustion chamber	5
Environment conditions	
temperature	288
pressure	1

V. RESULTS OF SIMULATION FOR SOFC-GT

Performance of fuel cell is shown as polarization curve that relates voltage of fuel cell to current density. The polarization curve for this simulation is shown in Figs. 2-4.

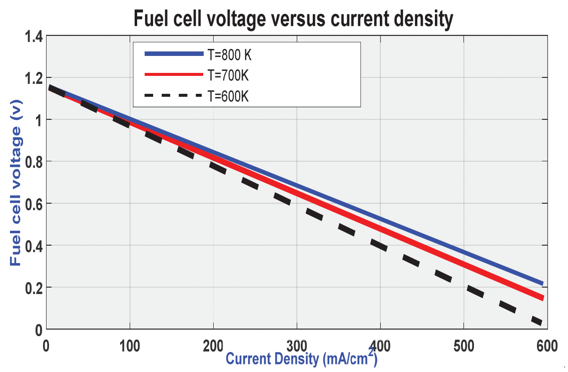

Fig. 2 Voltage of fuel cell according to the current density

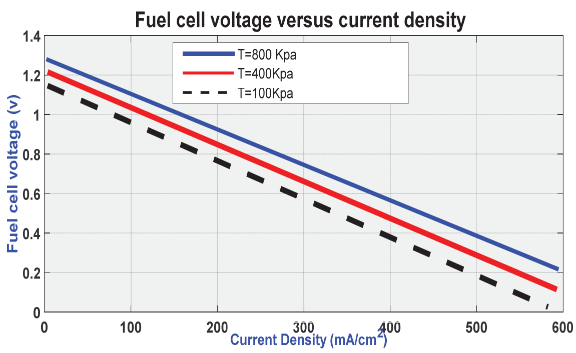

Fig. 3 Voltage of fuel cell in different temperatures according to the current density

In Fig. 3, the profound effect of SOFC voltage in different operational temperature is shown according to the ohmic losses. As obvious in these figures, by increasing current density voltage of fuel cell is decreased. This leads to irreversibility. According to the Nernst equation it is obvious that voltage of fuel cell is increased by operational pressure. So by increasing of pressure and optimizing of operational work of compressor, the performance can be increased. The shape of polarization curve is dependent to the activation and ohmic losses. As shown in simulation results, current density can increase the voltage of SOFC with increasing the temperature or decreasing the thickness of fuel cell. Also Fig. 5 illustrates concentration losses that have increased exponentially by adding the current density. In Fig. 6, activation losses that is most influenced by cathode is shown. On the other hand, it should be noted that the fuel cell, has a number of distinct air and fuel passages that flow can pass between them. For producing more power, the number of fuel cells must be increased. In Fig. 7, the effect of increasing the level of the fuel cell, in reaction of overall power production is shown. But as mentioned above, the increase in the absolute level of the cell response will generate more power.

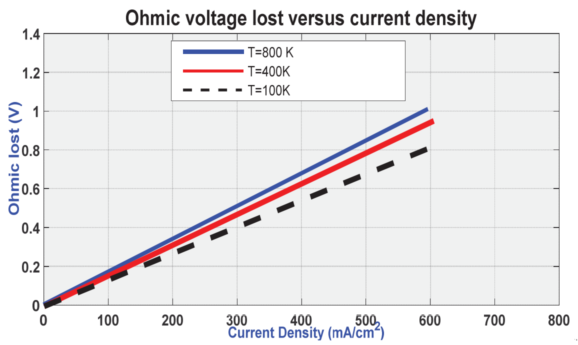

Fig. 4 The effect of ohmic voltage on current density at different temperatures

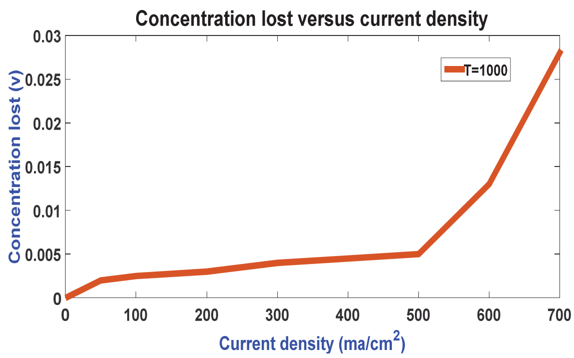

Fig. 5 Comparison of concentration losses according to the current density

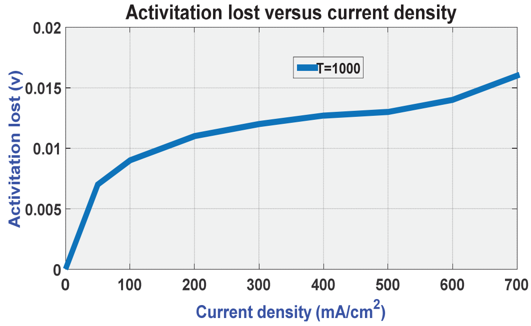

Fig. 6 Comparison of activation losses versus of current density

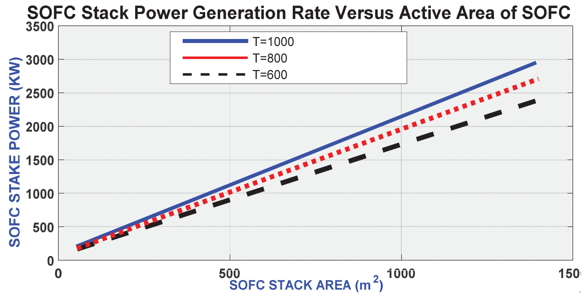

Fig. 7 Comparison of power of fuel cell to increasing of area of fuel cell

The functionality of area of fuel cell in respect to the rate of converted hydrogen in fuel cell is simulated in Fig. 8.

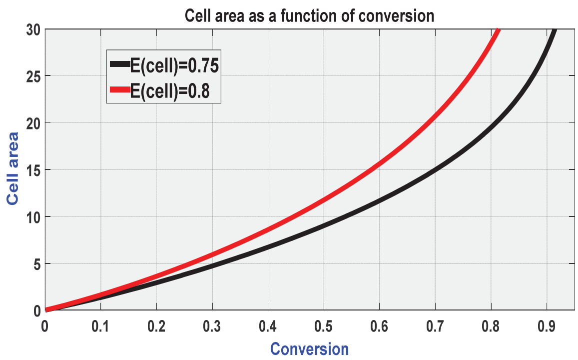

Fig. 8 Functionality of area of fuel cell to converted hydrogen

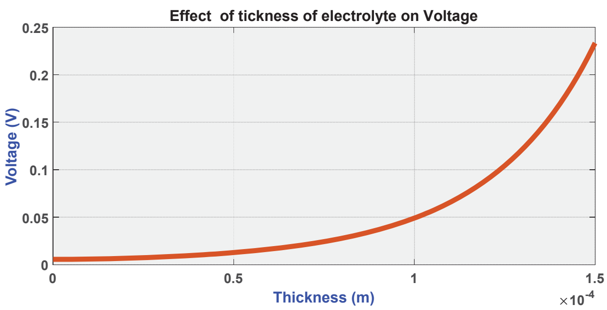

Fig. 9 The influence of thickness of electrolyte to fuel cell voltage

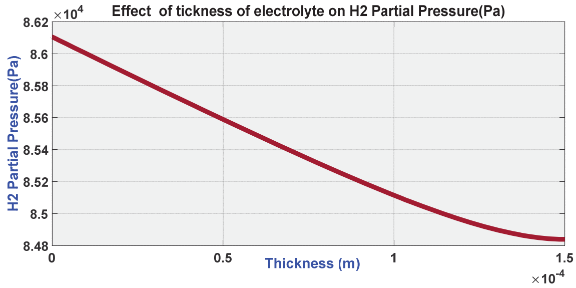

Fig. 10 The influence of thickness of electrolyte to partial pressure of hydrogen

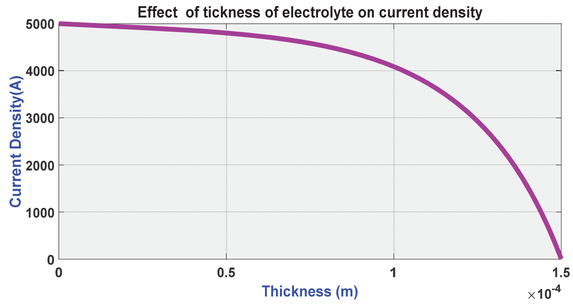

Fig. 11 The influence of thickness of electrolyte to current density

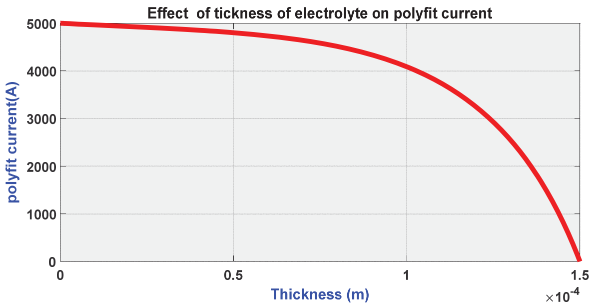

Fig. 12 The influence of thickness of electrolyte to polyfit current

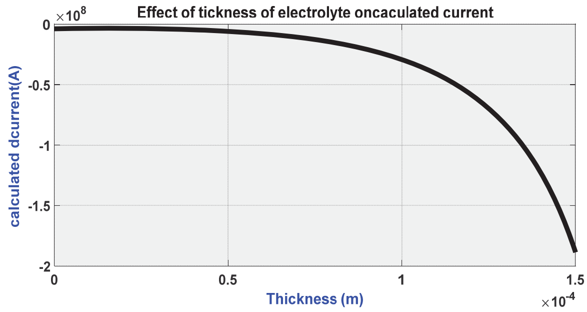

Fig. 13 The influence of thickness of electrolyte to losses current

At last the influence of thickness of fuel cell to voltage of fuel cell, partial pressure of hydrogen, current density, polyfit current and losses current is shown in Figs. 9-13.

VI. Conclusion

In this study, Exergy and entropy analysis for gas turbines with fuel cell, has been performed and a comparison is made between the results and those obtained in other references. In summary, the effect of significant parameters on performance of fuel cell is simulated and the choice of optimal ranges is done.

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