

SIMULATION OF A HYBRID SOLID OXIDE FUEL CELL–GAS TURBINE SYSTEM

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ABSTRACT

In this paper a methane-fed internal reforming solid oxide fuel cell (IRSOFC) –gas turbine (GT) power generation system is presented. The system consists of one fuel compressor and one air compressor, two heat exchangers for preheating fuel and air streams, an IRSOFC stack, a combustor and a gas turbine. All these system components are modeled for predicting the overall performance of the hybrid SOFC-GT system. Further, a parametric study is performed to evaluate the effect of various parameters such as fuel flow rate (FFR), current density and compressor pressure ratio (CPR) on system performance. Results showed that the IRSOFC voltage, stack temperature and the power density increase with FFR. The cell voltage decreases with increasing current density and the SOFC power density initially increases with current density but decreases beyond a limiting value of 0.3 A/cm². With the increase in CPR, the SOFC operating pressure increases but the SOFC stack temperature remains unchanged, therefore the cell voltage and power is not much affected by increase in CPR. The power produced by the GT however increases with increasing CPR, FFR and current density. The compressor work requirement also increases with CPR which however remains invariant with FFR and current density. The overall system efficiency of the system also increases with increasing FFR at fixed current density and with increase in CPR the efficiency initially increases and remains nearly constant thereafter. The overall efficiency of the hybrid system was found to be more than 50% for most of the cases at higher CPR and FFR considered in the present analysis. A comparison of the plant with and without the SOFC showed improvement in case of system efficiency of the hybrid cycle.

Keywords: Solid oxide fuel cell, Gas turbine, Hybrid system, Efficiency.

1. INTRODUCTION

Fuel cells have attracted considerable interest during the recent years. Fuel cell power generation system is an emerging technology with great promise and is expected to be one of the most efficient energy conversion system in the future with flexible fuel utilization and very low pollutant emissions. There are various types of fuel cells that are currently undergoing active development. Among the different types, the high temperature solid oxide fuel cells (SOFCs) have better potential to achieve higher efficiency for electricity production in a hydrogen fuel economy. This makes them particularly attractive for fuel efficient stationary power generation. Higher operating temperatures of SOFC allow direct internal processing of fuels reducing the system complexity involved with low-temperature power plants that require hydrogen generation in an additional process step [1]. SOFCs are suitable for small cogeneration unit as well. They can be integrated with a gas turbine to form large pressurized hybrid systems. Predicted results obtained from simulation study performed on integrated SOFC and GT plant indicates higher overall system efficiency with such plant [2-4].

However performance of such plants may vary depending upon the operating conditions, plant configuration and model formulations.

In the present study a model is developed for simulating the performance of simple methane fed hybrid SOFC-GT plant. The model predicts the system performance on the basis of first law of thermodynamics. Energy balance is done for each component of the system separately to obtain the inlet and outlet conditions of temperature, pressure and compositions. The performance of the overall system as a whole is assessed considering interaction between the various system components.

A MATLAB code is developed and used for the system simulation. The main program is linked with individual subroutines written for modeling various system components where mass and energy balance equations are solved simultaneously. The effect of various parameters, such as compressor pressure ratio, fuel flow rate, current density is studied on the cycle performance.

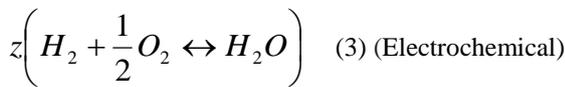
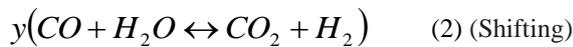
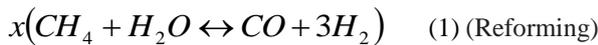
2. DESCRIPTION OF SYSTEM LAYOUT

The system layout of the integrated GT–SOFC layout is schematically shown in Fig. 1.

The system consists of the following components: (1) air compressor, (2) fuel compressor, (3) two recuperative heat exchangers, (4) IRSOFC stack, (5) combustor, (6) a GT. Compressed fuel and air are preheated in the respective recuperators utilizing the heat of GT exhaust gases before entering the fuel cell stack. Methane is fed as fuel to the anode of the fuel cell which is internally reformed in the anode to produce hydrogen rich gas for the fuel cell. It is assumed that initially the fuel is channeled to the combustor and the GT bypassing the SOFC and steam is produced by utilizing the heat of the GT exhaust gas in an external boiler. This steam is then mixed with the fuel before it enters the SOFC stack for the reforming to begin with. When the reforming reaction is fully activated, the electrochemical reaction would generate the steam required for the reforming reaction and the external boiler can be disconnected upon reaching the desired value of steam to carbon (S/C) ratio [5]. The S/C ratio is taken as 2.444 in the present simulation [3]. The heat generated during the electrochemical reaction is used partly for methane reforming and partly for heating the gaseous stream in the IRSOFC. The high temperature gaseous stream then enters the combustor where the residual gases (hydrogen, methane and carbon monoxide) are burnt with excess air. The products of combustion then pass through the GT that produces the mechanical work. Part of the mechanical work produced by the GT is used to drive the air and the fuel compressor and the remainder is the power available for electric power generation.

3.1 IRSOFC thermodynamic model

The IRSOFC model is necessary to study the complexities involved in an IRSOFC system for obtaining thermodynamic data for fuel cell operation and also to carry out the fuel cell performance analysis. The reactions mechanism for an IRSOFC stack is



Where, x, y and z indicate respective molar flow rate in the reactions. The equilibrium constants for the reforming and shifting reactions can be expressed as follows.

$$K_{pr} = \frac{(H_2^i + 3x + y - z)^3 (CO^i + x - y)}{(CH_4^i - x)(H_2O^i - x - y + z)(n_{tot}^i + 2x)} (p_{cell})^2 \quad (4)$$

$$K_{ps} = \frac{(H_2^i + 3x + y - z)(CO_2^i + y)}{(CO^i + x - y)(H_2O^i - x - y + z)} \quad (5)$$

H_2^i, CO^i, CH_4^i etc. are initial molar concentration of the respective gases. The hydrogen utilized in the fuel cell can be defined as follows:

$$z = U_f (H_2^i + 3x + y) \quad (6)$$

Where, U_f is the fuel utilization factor. The equilibrium constant as polynomial function of temperature [3, 6, and 7] is expressed as follows.

$$\log K_p = AT^4 + BT^3 + CT^2 + DT + E \quad (7)$$

The values of the constants in equation (7) for the reforming and the shifting reactions are known [3, 6, and 7] and the equilibrium constants (K_{pr}, K_{ps}) at any given temperature can be found out.

With known values of K_{pr}, K_{ps} and U_f and then replacing z in equations (4) and (5) we obtain two algebraic equations which are solved for x and y using Newton’s method and z is calculated using Equation (6).

The reforming and the shifting reactions are endothermic [2] and the heat required for these two reactions can be calculated using Equations (8) and (9) respectively [2].

$$Q_r = x(h_{CO} + 3h_{H_2} - h_{H_2O} - h_{CH_4}) \quad (8)$$

$$Q_s = y(h_{CO_2} + h_{H_2} - h_{CO} - h_{H_2O}) \quad (9)$$

$$Q_{rxn} = I(V_{ohm} + V_{act} + V_{conc}) + T\Delta S \quad (10)$$

where,

$$\Delta S = S_{H_2O}^0 - S_{H_2}^0 - \frac{1}{2}S_{O_2}^0 - \frac{R}{2} \ln\left(\frac{p_{H_2}^2 p_{O_2}}{p_{H_2O}^2}\right) \quad (11)$$

The molar specific enthalpy (h) and entropy (S) of the species is determined considering these to be function of temperature [3]. Q_{rxn} is the amount of heat generated during electrochemical reaction. It is assumed that the heat required for the reforming and the shifting reactions is supplied from Q_{rxn} . It also heats the gases in the anode and cathode stream to the stack temperature (T_s). The stack temperature is calculated in an iterative manner. Initially its value is guessed, then the following two terms are calculated.

$$Q = Q_{rxn} - (Q_r + Q_s) \quad (12)$$

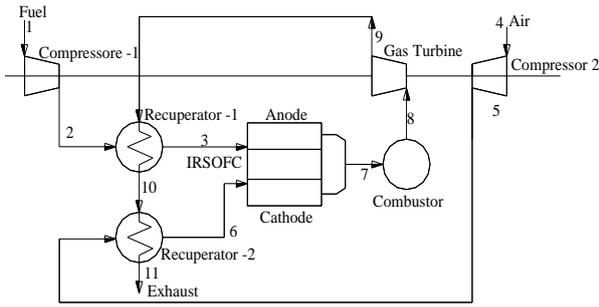


Fig.1. Layout of the hybrid IRSOFC-GT system

$$Q' = \left(\dot{n}_1 \int_{T_{an}}^{T_s} C_p dT \right)_r + \left(\dot{n}_2 \int_{T_{an}}^{T_s} C_p dT \right)_p + \left(\dot{n}_3 \int_{T_{ca}}^{T_s} C_p dT \right)_r + \left(\dot{n}_4 \int_{T_{ca}}^{T_s} C_p dT \right)_p \quad (13)$$

In Equation (13), T_{an} and T_{ca} are the anode and cathode inlet temperatures respectively. $\dot{n}_1, \dot{n}_2, \dot{n}_3$ and \dot{n}_4 are the corresponding molar flow rates of the reactant (r) and product (p) gases at the anode and cathode respectively. Specific heat, C_p for the gases are considered temperature dependent. Then iteration is continued until the convergence criterion is met. The convergence criterion is set as [2]:

$$Q_{error} = \left| \frac{Q' - Q}{Q} \right| \leq 0.5\% \quad (14)$$

3.2 Electrochemical model

The reversible open-circuit voltage of a single fuel cell can be calculated from the Nernst equation:

$$E = \frac{-\Delta G^0}{2F} + \frac{RT}{2F} \ln \frac{P_{H_2} P_{O_2}^{1/2}}{P_{H_2O}} \quad (15)$$

Where, F is the Faraday's constant, 'p's are the partial pressures of the reacting species; ΔG^0 is the change in Gibbs free energy and is a function of the SOFC operating temperature [8,9]. The losses that occur due to flow of electron and ions through the circuit include losses due to (i) ohmic resistance, V_{ohm} (ii) electrochemical reaction activation, V_{act} (iii) concentration depletion, V_{conc} . Hence the actual voltage of a fuel cell is less than the reversible open circuit voltage as given below.

$$V = E - (V_{ohm} + V_{act} + V_{conc}) \quad (16)$$

(1) Ohmic overpotential: Ohmic overpotential is calculated by the following equation [5]:

$$V_{ohm} = i \sum \rho_j \delta_j \quad (17)$$

with $\rho_j = A_j \exp\left(\frac{B_j}{T}\right)$, The values of the coefficients A_j and B_j of specific resistivity ρ and the thickness, δ of the SOFC components are given in Table 1 [2, 5]. This is valid for cathode supported SOFC (Ni-YSZ).

Table1: Constants and thickness of SOFC components

| | A(ohm- cm) | B(K) | Thickness(cm) |
|--------------|------------|-------|---------------|
| Anode | 0.00298 | -1392 | 0.015 |
| Cathode | 0.008114 | 600 | 0.2 |
| Electrolyte | 0.00294 | 10350 | 0.004 |
| Interconnect | 0.1256 | 4690 | 0.01 |

(2) Activation overpotential: The activation overpotential is the loss of energy consumed in speeding up the overall electrochemical reaction. The activation overvoltage is calculated using the following equations [6].

$$\frac{1}{R_{act,an}} = K_a \frac{2F}{RT} \left(\frac{P_{H_2}}{P_0} \right)^m \exp\left(-\frac{E_{act,an}}{RT}\right) \quad (18)$$

$$\frac{1}{R_{act,ca}} = K_c \frac{4F}{RT} \left(\frac{P_{O_2}}{P_0} \right)^m \exp\left(-\frac{E_{act,ca}}{RT}\right) \quad (19)$$

$$V_{act} = i(R_{act,an} + R_{act,ca}) \quad (20)$$

where, $K_a = 2.13 \times 10^4 \text{ Acm}^{-2}$,

$K_c = 1.49 \times 10^6 \text{ Acm}^{-2}$, $E_{act,an} = 110 \times 10^6 \text{ Jkmol}^{-1}$,

$E_{act,ca} = 160 \times 10^6 \text{ Jkmol}^{-1}$ and $m = 0.25$

(3) Concentration over potential: Concentrations of fuel and oxygen at the electrodes are different from their bulk concentrations in the main fuel and oxygen streams. These differences cause the concentration overvoltage which can be calculated by the following equation [5]:

$$V_{conc} = \frac{RT}{2F} \ln\left(1 - \frac{i}{i_L}\right) \quad (21)$$

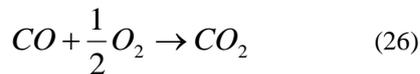
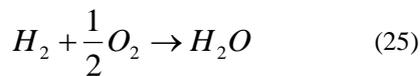
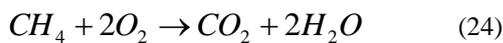
The total current produced (I) and the power produced by the SOFC can be calculated from the molar fuel flow rate of H_2 (\dot{z}) as follows.

$$I = 2F\dot{z} \quad (22)$$

$$P = VI \quad (23)$$

3.3 Combustor

Fuels for the combustor are residual hydrogen, carbon monoxide and methane. The oxidant is the depleted oxygen of the cathode outlet stream. The following are the combustion reactions considered.



The method of Calise *et al.* [5] is adopted for calculating the combustor outlet temperature.

3.4 Compressor and GT

The procedure of P.G. Bavarsad [7] is followed for calculating compressor outlet temperature and power consumption. The following are the equations used for the purpose.

$$\int_1^2 C_{p,a} \frac{dT}{T} = \frac{R_a}{\eta_{s,c}} \ln R_p \quad (27)$$

$$\dot{W}_c = \dot{n}_a \int_1^2 C_{p,a} dT \quad (28)$$

Same procedure is followed for the fuel compressor as well. For the GT, the equation used for calculating the turbine outlet temperature is given as,

$$\int_8^9 C_{p,g} \frac{dT}{T} = -R_g C_{p,g} \ln(TER) \quad (29)$$

TER is the turbine expansion ratio. High temperature turbine exhaust gases are used to preheat inlet air and fuel.

3.5 Recuperator

SOFC operating temperature should be high for better fuel cell operation [5].

Fuel and air therefore must be preheated before entering the fuel cell. This is accomplished in the two counter flow heat exchangers. Effectiveness-NTU is adopted for modeling the two recuperators in the present study. Effectiveness and overall heat transfer coefficient of the recuperators are given as input data. Inlet temperature and pressures are known a priori. The temperatures of air, fuel and the gases at the recuperator outlet are then calculated. The assumed parameters, efficiency and effectiveness of system components are shown in Table 2.

Table 2: Assumed values of parameters

| Parameter | Value |
|---|-------|
| Compressor isentropic efficiency | 90% |
| GT isentropic efficiency | 90% |
| Compressor mechanical efficiency | 95% |
| GT mechanical efficiency | 95% |
| Combustor efficiency | 98% |
| Generator efficiency | 98% |
| Recuperator effectiveness | 0.9 |
| Recuperator overall heat transfer coefficient | 0.5 |
| Fuel utilization factor | 0.85 |
| Limiting current density (A/cm ²) | 0.35 |
| Recuperator pressure drop | 4% |
| Fuel cell pressure drop | 4% |
| Combustor pressure drop | 5% |

4. RESULTS AND DISCUSSION

A parametric study is done by changing SOFC current density, FFR and CPR (one parameter at a time while keeping the other fixed) for investigating their effect on system performance. The air flow rate is kept constant at 170 kmol/h. The effect of CPR on compressor work required is shown in Fig. 2 and Fig. 3. Compressor work increases with pressure ratio, but varies very little with current density and FFR.

The IRSOFC voltage and the electrical power output don't vary much with CPR; however both these parameters decrease with increase in current density as can be seen from Fig. 4 and Fig. 5. The IRSOFC power actually decreases with current density due to reduction in cell voltage and area at higher current density. At higher current density, the cell voltage decreases due to increase in cell over potential. At a fixed current density, IRSOFC voltage and power however increases with increase in FFR (Fig. 6 and Fig. 7). This is because the cell voltage and current increase at higher FFR. The power density of a fuel cell is the product of its voltage and current density which is plotted in Fig. 8. The power density increases with increasing current density up to a maximum, the position of which depends on the design and quality of assembly of the electrode employed [1].

The fuel cell area in the present simulation study is a model output which decreases with increasing current density, hence the power density increases with current density initially. Beyond the maximum, the drop in cell voltage is stronger than the increase in current density and hence a decrease in power occurs. Power density is more due to high SOFC power output at increased FFR as already explained.

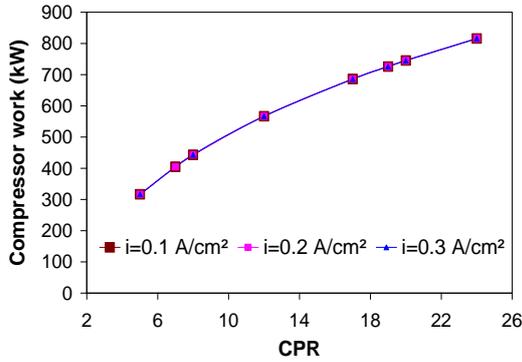


Fig.2. Compressor work vs. CPR at various current densities for FFR=17 kmol/h

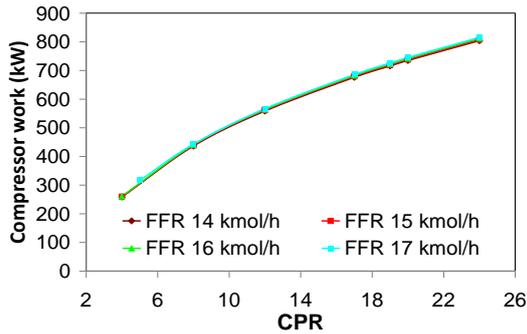


Fig.3. Compressor work vs. CPR at various FFRs for current density = 0.3 A/cm²

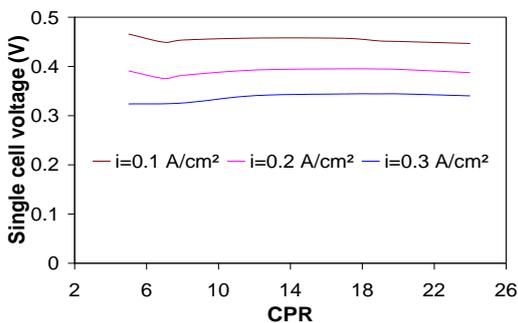


Fig.4. Cell voltage vs. CPR at various current densities for FFR=17 kmol/h

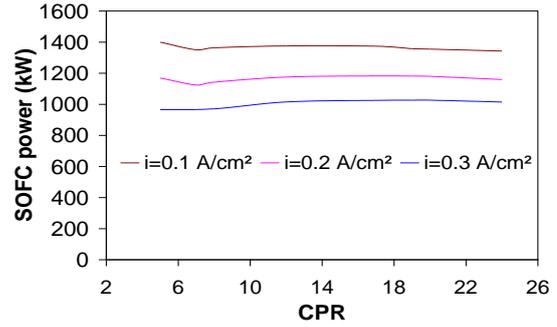


Fig.5. SOFC power vs. CPR at various current densities for FFR =17 kmol/h

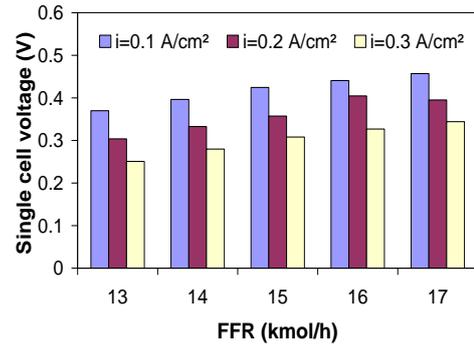


Fig.6. Cell voltage vs. FFR at various current densities for CPR = 17

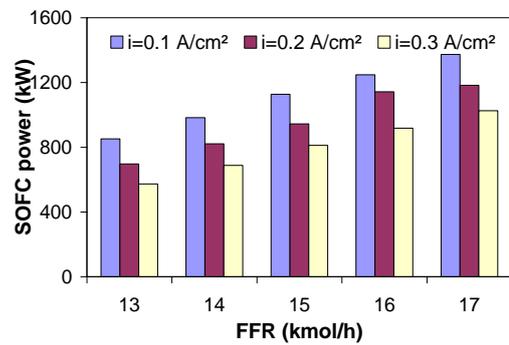


Fig.7. SOFC power vs. FFR at various current densities for CPR=17

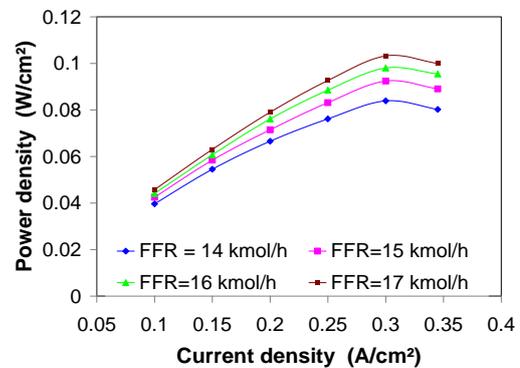


Fig.8. Power density vs. current density at various FFRs for CPR=17

Fig. 9 and 10 show the variation of GT power output with CPR at various current densities and FFR respectively. GT power also increases with CPR which is obvious but unlike the SOFC power, it increases with increasing current density. At a given FFR, GT power increases with current density. It was observed that with current density the SOFC stack temperature increases and due to subsequent burning of the residual fuel in the combustor, finally it results in higher turbine inlet temperature (TIT) and hence the GT produces more power. The stack temperature that increases with current density is presented in Fig. 11 for fixed FFR value of 17 kmol/h and fixed CPR of 17. Same is the reason that GT power increases with FFR at a given current density (Fig. 12). Consequently the net work output of the GT plant (W_{net}) which is the difference between the power developed by the GT and the compressor work required, also increases with CPR, current density and FFR. This is clearly shown in Fig. 13 and Fig. 14. W_{net} increases significantly with CPR initially but beyond certain CPR (a value of 8), the increase in W_{net} with CPR is found to be gradual.

The efficiency increases rapidly with CPR initially but remains almost constant thereafter beyond CPR value of 12. Further, the efficiency of the overall system is less at higher current density which is the case at all FFRs. With the increase in current density compressor power remains unchanged. However, although the GT power increases but the SOFC power decreases and the decrease in SOFC power is more significant compared to the increase in GT power, hence the efficiency of the overall system decreases at higher current density. With increase in FFR, since both the SOFC and the GT power increase, hence the overall system efficiency also increases as depicted in Fig. 16.

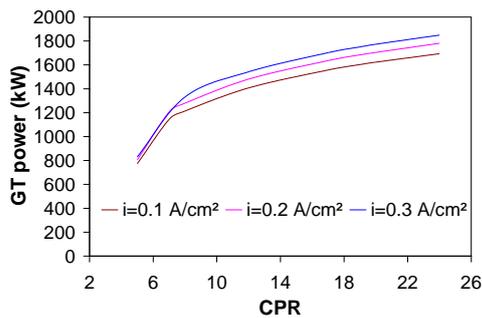


Fig.9. GT power variation with CPR at various current densities for FFR =17 kmol/h

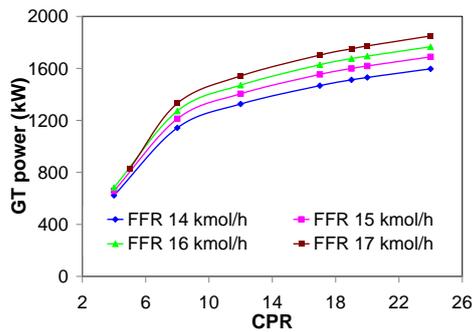


Fig.10. GT power variation with CPR at various FFRs for current density = 0.3 A/cm²

Fig. 15 shows the variation of overall SOFC-GT system efficiency with CPR at different current densities for a FFR value of 17 kmol/h.

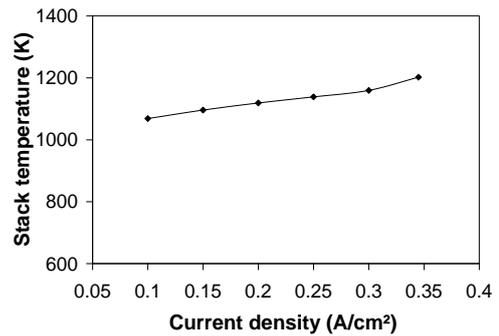


Fig.11. SOFC stack temperature variation with current density at FFR=17 kmol/h and CPR =17

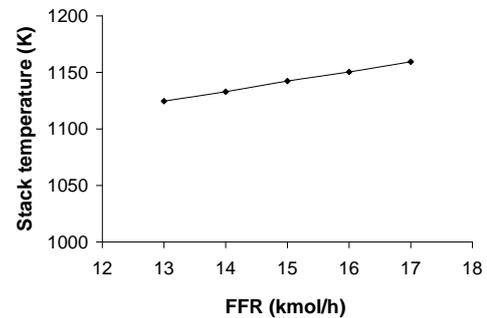


Fig.12. SOFC stack temperature variation with FFR at current density = 0.3 A/cm² and CPR =17

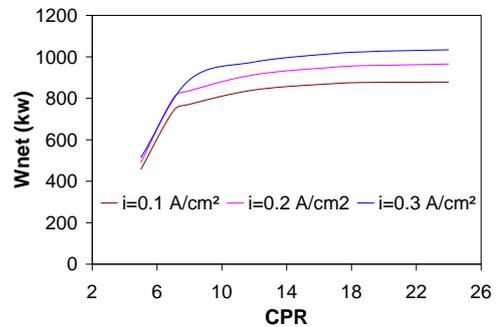


Fig.13. Net GT power as function of CPR at various current densities for FFR=17 kmol/h

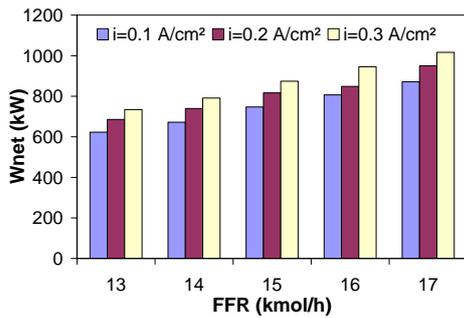


Fig.14. Net GT power as function of FFR at various current densities for CPR=17

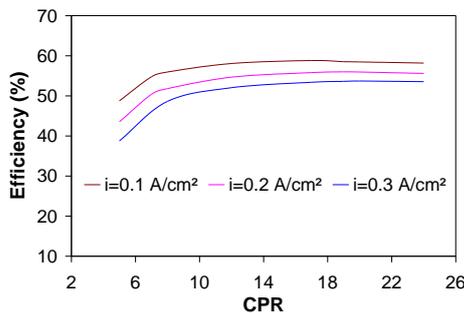


Fig.15. Efficiency variation with CPR at various current densities for FFR= 17 kmol/h

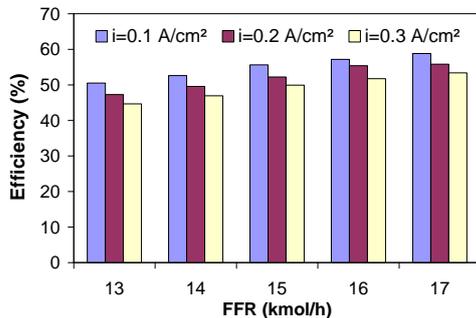


Fig.16. Efficiency variation with FFR at various current densities for CPR =17

Further, simulation of conventional recuperated GT plant has been performed with the same operating conditions to compare the performance of the hybrid SOFC-GT plant against the conventional GT plant (without including the SOFC). The efficiency results of the two plants with and without SOFC are illustrated in Fig 17. It can be seen from Fig. 17 that the hybrid SOFC-GT plant offers superior performance over the conventional plant particularly at higher CPR. At CPR value of 3, the efficiency of both the plants is nearly the same while at CPR 4, the efficiency of the conventional plant is optimum and it is higher than that of the hybrid plant. The efficiency gain in case of the hybrid system becomes significant only at higher CPR (at CPR 5 and more). As for instance, for plant operation with FFR of 17 kmol/h and SOFC current density at 0.3 A/cm², the efficiency of the hybrid system is predicted to be 52.04% at CPR 12 as against an efficiency of 28.94% of the conventional GT plant with a gain of almost 80%.

The SOFC integrated into the GT system not only produces electric power but also acts as a regenerator that preheats the fuel and air stream before entering the combustor. This leads to higher efficiency in respect of the hybrid plant. However, CPR has a very little effect on the hybrid cycle system efficiency than for a conventional GT system. Moreover, SOFC operation at higher pressure would require careful attention due to leakage of gases from the fuel cell interior to outside and also from one chamber to the other. Use of high quality sealing materials might reduce this problem.

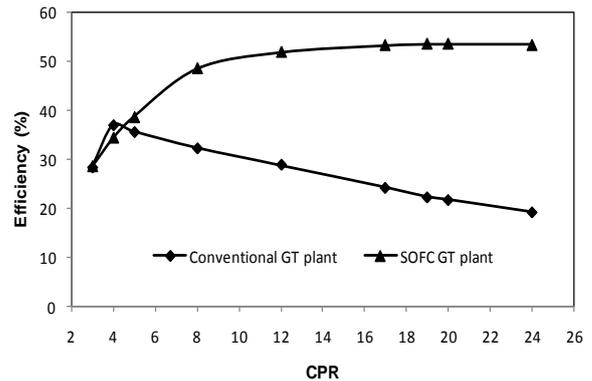


Fig.17. Comparison of efficiency at various CPRs, between a conventional GT (without an SOFC) and hybrid SOFC-GT plant at the same operation conditions

5. CONCLUSIONS

A simple methane fed hybrid IRSOFC-GT system has been simulated with the help of a mathematical model. The following conclusion can be made based on the simulation results obtained.

- (i) The compressor power requirement increases with CPR, but varies very little with the FFR and current density.
- (ii) The IRSOFC voltage and the power output on the other hand remains invariant with CPR but decreases with increase in current density. With increase in FFR however, the SOFC power increases due to increase in cell voltage and current. A complete opposite trend is observed in case of GT power output variation with current density. The GT power increases with current density mainly due to increase in the SOFC stack temperature and resulting TIT. Both the GT power and W_{net} increase with increase in FFR.
- (iii) The efficiency of the hybrid system is therefore better at higher FFR and hence it is the maximum at FFR of 17 kmol/h. But the predominant effect of lower SOFC power over higher GT power at higher current density finally lowers the system efficiency when current density increases. Further, the efficiency although increases with CPR initially but varies asymptotically beyond a CPR value of 12 which indicates insignificant effect of pressure on system efficiency at higher CPR.

(iv) The efficiency values of the hybrid system is found to be more than 50% in many test cases at higher CPR, FFR and also at relatively lower CPR and FFR at lower current density.

(v) The comparison between the conventional GT plant without the SOFC and the hybrid system at same operating conditions shows better performance with respect to the hybrid plant at CPR values of 5 and higher.

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NOMENCLATURE

Symbol

| | | |
|-------------------|---|-------------------|
| A | Constant | |
| B | Constant | |
| E | Reversible open circuit voltage | (V) |
| E _{act} | Activation energy | J/kmol |
| F | Faraday's constant | |
| G ⁰ | Gibbs free energy | kJ/kmol |
| h | Enthalpy | A/cm ² |
| i | Current density | A |
| I | Total current | A/cm ² |
| i _L | Limiting current density | |
| K _p | Equilibrium constant | bar |
| p | pressure | W |
| P | Power | kW |
| Q | heat transfer | kW |
| Q _{rxn} | heat generated during electrochemical reaction | kJ/kmolK |
| R | Universal gas constant | ohm |
| R _{act} | Resistance | kJ/kmolK |
| S | Entropy | K |
| T | Temperature | |
| U _f | Fuel utilization factor | V |
| V | Actual cell voltage | V |
| V _{act} | Activation over-potential | V |
| V _{conc} | Concentration overpotential | V |
| V _{ohm} | Ohmic overpotential | |
| z | Number of moles of hydrogen utilized in fuel cell | |

Subscripts

| | |
|------|--------------------|
| an | Anode |
| ca | Cathode |
| cell | Fuel cell |
| r | Reforming reaction |
| s | Shifting reaction |

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