Proceedings of ASME Turbo Expo 2011
GT2011
June 6-10, 2011, Vancouver, British Columbia, Canada

GT2011-45834

PERFORMANCE SIMULATION OF A HYBRID MICRO GAS TURBINE FUEL CELL SYSTEM BASED ON EXISTING COMPONENTS

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ABSTRACT

The objective of this work is the development of a simulation model for a hybrid Solid Oxide Fuel Cell (SOFC)/Micro Gas Turbine (MGT) system, flexible and robust enough, capable to predict the system performance under various operating conditions. The hybrid system consists of a high temperature SOFC, based on a tubular configuration developed by Siemens Power Generation Inc, and a recuperated small gas turbine (GT) validated using data for the Capstone C30. The design and off-design performance of the system is examined by means of performance maps. Moreover, operating parameters such as fuel utilization factor, steam to carbon ratio and current density are varied over a wide range and the influence on system performance is studied. The optimum operating conditions are discussed with regard to overall system performance under part load operation. The results show that high electrical efficiencies can be achieved making these systems appropriate for distributed generation applications.

NOMENCLATURE

F	Faraday constant
FC	Fuel cell
GT	Gas turbine
HS	Hybrid system
LHV	Lower heating value
MGT	Micro-gas turbine
N	Rotational speed
P	Pressure
R	Molar gas constant
SOFC	Solid oxide fuel cell
T	Temperature
TIT	Turbine inlet temperature
V	Voltage
W	Power
ΔG^o	molar Gibbs free energy of formation
η	Efficiency

Subscripts

Act	Activation
Conc	Concentration
des	design
DP	Design point
f	fuel
N	Nernst
Ohm	Ohmic
rel	relative

INTRODUCTION

The hybrid power generation systems based on micro-turbines and fuel cells are a promising technology combination which is expected to occupy a substantial portion of the energy market in the future.

Micro-turbines are appropriate for distributed generation as being well suited to meet the needs of small energy users with electricity and thermal power. The first generation of micro-turbines has been introduced to the energy market. Their size range from 25 to 80 kW with electrical efficiency of about 30%, [1]. Usually, they consist of singe stage radial compressors and turbines, a combustor, a highly effective recuperator and a high speed generator,[2]. The Micro-turbines can be coupled with thermally activated devices to produce either heating or cooling by using the exhaust heat and achieve high total efficiencies in the range of 75%, [3].

Solid Oxide Fuel Cells (SOFCs) are energy conversion devices that convert the chemical energy of a fuel to electrical energy and heating through electrochemical processes with high efficiency, [4]. The high operating temperature of SOFCs (800 – 900°C) makes them appropriate to be coupled with gas turbines and form the so called hybrid systems.

In hybrid systems the high temperature exhaust of the fuel cell is used to drive a gas turbine which provides the fuel cell air flow and supplementary power. This integration makes it possible to achieve efficiencies greater than either technology is capable independently. Integrating a fuel cell and a gas turbine is by no means trivial and a significant system-level effort has been made to understand hybrid system integration and thermodynamics. The most important concern is the smooth matching of a SOFC module with a gas turbine.[5, 17]

It can be seen from a literature review that only few papers are dealing with existing integrated systems or potential cooperation of existing subsystems. The present work aims to study the performance of a hybrid system consisting of existing GT and FC subsystems using appropriate models. Such an effort has its own value as it is based on validated technologies and the models could be verified against real data for both subsystems. To this end a model for the Capstone 30 kW recuperated gas turbine has been developed and compared against specification performance data.A reliable cell model resembling a high temperature SOFC, based on a tubular configuration developed by Siemens Power Generation Inc has also been validated with experimental data.

On the other hand, power systems are engineered to be operated under design-point conditions. Under real operating conditions however, design-point conditions can rarely be maintained due to the varying power (or load) levels that depend on the customer requirements and/or environmental changes. Besides, when existing subsystems are to be integrated, is almost certain that design operation of one subsystem implies non-design operation to another.

In these situations, it is necessary to operate the system under optimum part-load performance conditions. It is essential therefore for the models to represent efficiently the off-design operation of the system. To this end the models have been developed in a process simulation environment, such as Aspen Plus [18], supplying advanced and accurate thermodynamic calculations. The gas turbine and air compressor models were based on adequate maps. Although previous works using Aspen Plus exist for design point calculations [19] , it is the first time to our knowledge that specific off design models have been developed in this environment.

The purpose of this paper is to study the influence of different sets of parameters controlling the system's operation such as load, rotational speed, fuel flow, turbine inlet temperature and cell temperature, on the performance of the hybrid system. Moreover, operating parameters such as fuel utilization factor, and steam to carbon ratio are varied over a wide range and the influence on system performance is also studied. In the following the developed models of micro-turbine, fuel cell and hybrid system are described and the full and part load performance of the hybrid system is presented and analyzed.

SYSTEM DESCRIPTION

The hybrid system incorporates a high temperature SOFC stack integrated with a single shaft gas turbine. The referred high temperature fuel cell represents the tubular SOFC type design developed from Siemens Power Generation Inc. Except for the fuel cell bundle the system contains an ejector which mixes the depleted fuel with the fresh fuel in order to supply steam to the shift and steam reforming reactions, an indirect internal reformer and an afterburner (Fig. 1).

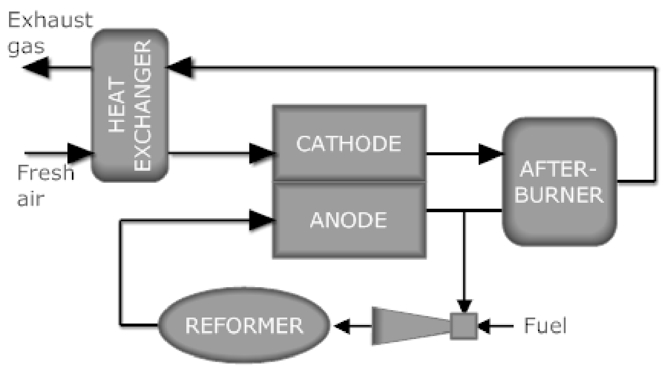

Figure 1 Simplified diagram of SOFC stack.

The selected gas turbine was the commercially available C30 micro turbine manufactured from Capstone. This recuperated gas turbine produces 30 kW of electrical power with 26% ± 2% (LHV) efficiency at ISO conditions. It consists from a centrifugal compressor, a recuperator, a combustion chamber, a radial turbine and a generator, [20]. All the rotating components are mounted on a single shaft which rotates at high rotational speed. Owing to the high rotational speed of the generator this system requires an inverter – power conditioner system in order to reduce the high frequency AC output to the desirable value.

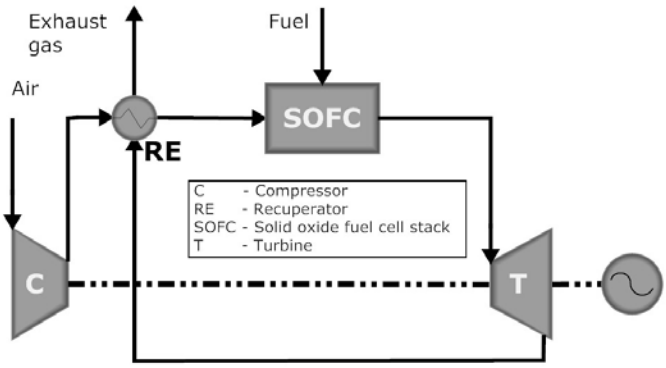

Figure 2 Hybrid system layout.

Figure 2 shows a simplified system layout, which have been come up from the recuperative gas turbine engine where the combustor has been substituted from a SOFC stack. The air enters from the compressor where its pressure raises. Thereinafter, the compressed air is preheated in the recuperator and is led in the SOFC stack where reacts electrochemically with the fuel (assumed to be natural gas). The hot exhaust gases from the fuel cell stack are expanded on the turbine and produces mechanical work for the compressor and electric generator. The hot gases at the exit of the turbine are used in order to preheat the supplied air to the stack.

MODEL DESCRIPTION

The system described above is simulated in Aspen Plus process simulator. The developed model is based on both existing built-in model blocks and development of specific user models. In the following the modeling methodology of each component of the system is described using the Aspen Plus terminology (words in italics).

Micro turbine model

As mentioned in the previous section the selected micro turbine resembles the Capstone C30, consisting of a compressor, a recuperator, a burner and a turbine.

The compressor is simulated in Aspen Plus using the *Compr* block, supplied with the performance map shown in Fig. 3. The map contains characteristics curves relating the efficiency and pressure ratio as a function of corrected mass flow and non-dimensional speed. The map was created through scaling of a representative one for centrifugal compressors to fit in our case. The performance map is supplied to the block through a written FORTRAN subroutine.

The recuperator is a two stream heat exchanger which allows the heat transmission from hot exhaust gases (hot stream) to the colder compressed air (cold stream). The recuperator is simulated using the *HeatX* block with shortcut calculation method selected and the hot inlet-cold outlet temperature difference as input. Also, the block is taking into account the pressure losses in the two streams.

The combustion chamber is modeled with the *RStoic* block which implements a stoichiometric reactor. The combustion chamber is assumed adiabatic with a small pressure drop. The reactions are assumed to reach equilibrium.

The turbine is simulated with a *User2* block, which is a driver for calling external subroutines developed in the FORTRAN programming language. The developed subroutine is based on the equations describing the turbine operation as well as mass and energy conservation equations. Also, it incorporates a turbine map (Fig. 4) which is adopted from [21].

The part load operation of the micro turbine is achieved by varying the rotational speed under constant turbine inlet temperature. This control method is preferred in micro turbines since it arises higher cycle efficiencies, [22].

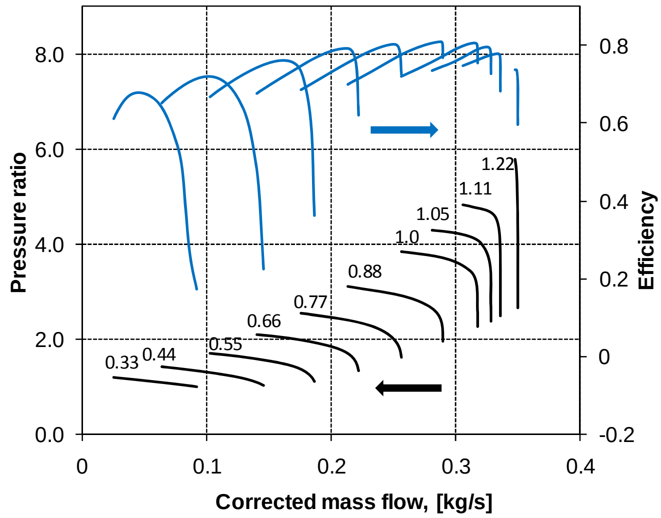

Figure 3 Compressor map.

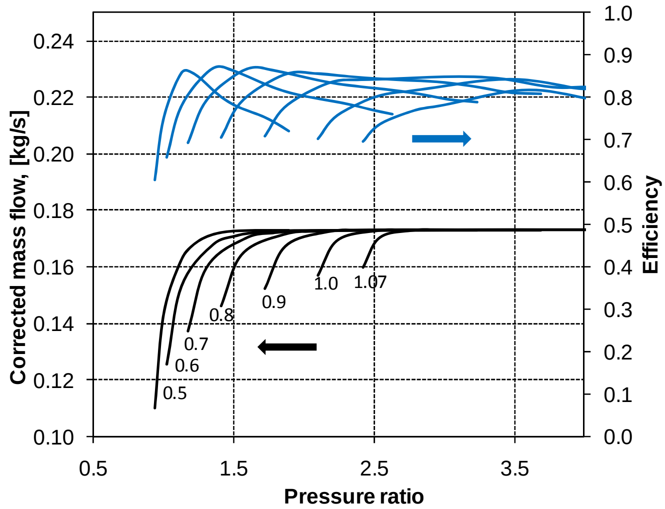

Figure 4 Turbine map.

Table 1 summarizes the assumptions of the developed model for the micro turbine. The presented data were found from the available literature[23].

Pressure ratio (DP)	3.6
Turbine inlet temperature	1117 K
Recuperator ΔP/P air/gas side (DP)	2%/3%
Recuperator hot inlet-cold outlet temp. difference	100 K
Combustion chamber ΔP/P (DP)	4%
Compressor isentropic efficiency (DP)	79.6%
Turbine isentropic efficiency (DP)	84%
Power condition system	96%
Mechanical efficiency	97%
Generator efficiency	96%

Table 1 Capstone C30 model assumptions.

The model was validated using available data from the manufacturer. In Table 2 are presented the design point operating parameters as predicted from the developed model and compared with manufacturer's data.

	Capstone	AspenPlus	Error [%]
Power,[kW]	30	31.1	3.67
Fuel energy,[kW]	115.36	124.06	7.54
Air flow, [kg/s]	0.31	0.307	-0.97
EGT, [K]	549	562	2.37
Net eff., [%]	26±2	25.1	-

Table 2 Calibration results at 96000 rpm.

The model predicts also the part load operation of the engine with satisfactory accuracy as shown in Fig. 5.

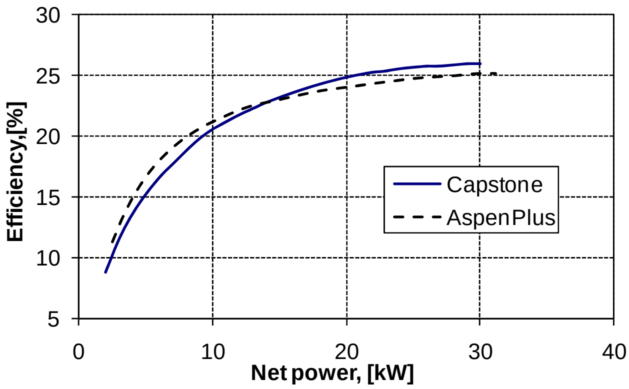

Figure 5 Part load performance of micro-turbine.

SOFC model

There are several works concerning the development of a simulation model for a SOFC. The models are either simplified bulk ones that predicts average values physical, chemical and electrochemical values [6, 8, 24, 25] or detailed which allow the evaluation of the distribution of all thermodynamic data within the fuel cell [26, 27]. The comparison of the two techniques is done in [28].

The SOFC model in this paper is a simplified bulk model which is developed using existing functions of AspenPlus software. The specific methodology has been used by many researchers [29-31].

Figure 6 presents the Aspen Plus flowsheet of the fuel cell stack model. In ejector the fresh desulfurized fuel is mixed with recycled anode gases containing depleted fuel (H_2 and CO) and electrochemical reaction products. The ejector is simulated with a *Mixer* block whilst the suction of the recycled depleted fuel stream is simulated with an *FSplit* block. The recycling process is modeled through a split fraction parameter which is calculated as a function of steam-to-carbon ratio. The mixed stream is introduced to the pre-reformer where the steam reforming (Eq. 1) and water-gas shift (Eq. 2) reactions take place and reform the higher hydrocarbons and a small amount of methane.

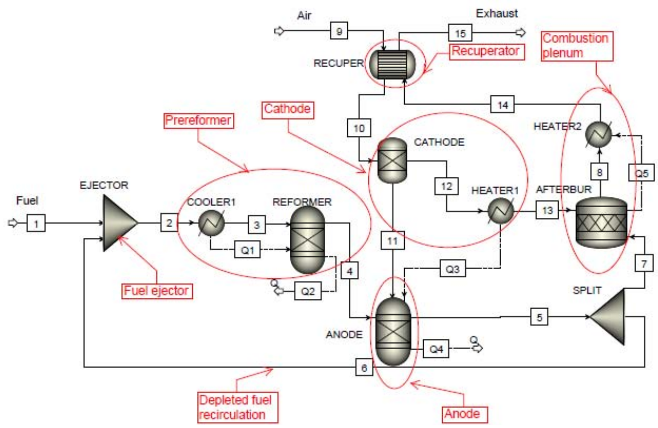

Figure 6 Simulation model of SOFC in Aspen Plus.

$$C_nH_m + nH_2O \leftrightarrow (m/2+n)H_2 + nCO \qquad (1)$$

$$CO + H_2O \leftrightarrow CO_2 + H_2 \qquad (2)$$

The pre-reformer is modeled using a combination of two Aspen Plus blocks: a *Heater* and an *Rgibbs* reactor. The reactor simulates the reforming reactions taking place in the pre-reformer and the *Heater* is used in order to determine the pre-reforming temperature. It is calculated using design specification which varies the temperature so as to nullify the net heat duty. Thereinafter, the pre-reformed fuel is fed to the anode side of the fuel cell, where the remaining methane is reformed and the carbon monoxide is shifted. It is a common approach to assume that H_2 is the only fuel that electrochemically reacts. In the SOFCs the following reactions occur:

$$0.5O_2 + 2e^- \rightarrow O^{2-} \quad \text{(Cathode half reaction)} \qquad (3)$$

$$H_2 + O^{2-} \rightarrow H_2O + 2e^- \quad \text{(Anode half reaction)} \qquad (4)$$

$$H_2 + 0.5O_2 \rightarrow H_2O \quad \text{(Overall reaction)} \qquad (5)$$

The fresh air is preheated in the recuperator which is modeled with a *HeatX* block and simulates the heat transfer from the hot exhaust gases to the colder fresh air. The preheated air is supplied to the cathode side of the fuel cell to supply the requisite oxygen for the electrochemical reaction. The cathode is simulated with the separator module *Sep* which separates the required oxygen for the electrochemical reaction. The residual air and the not-recycled depleted fuel are fed to the combustion plenum where complete combustion of the remaining fuel occurs. The combustor is modeled using a couple of Aspen Plus blocks, an *RStoic* block which simulates the reactions taking place and a *Heater* which adds the generated heat into the exhaust.

Although the above set up of the SOFC simulation model is similar to the one used by Zhang et al. [31], the two approaches differ concerning the voltage calculation. In Zhang et al. model, the voltage calculations were done using an experimental performance characteristic curve and semi empirical relationships to predict the actual operating voltage in various operating conditions. The experimental curve corresponds to design condition for operating the fuel cell in ambient pressure and a given temperature (1000 K).

As in the present work the fuel cell is supposed to be pressurized and to operate at off design conditions, more accurate equations that consider the fundamental phenomena and fuel cell geometry were implemented. The voltage calculation is done by calculating the reversible Nernst voltage

$$V_N = -\frac{\Delta G^o}{2F} + \frac{RT_{SOFC}}{2F} \ln \frac{P_{H_2} P_{O_2}^{\ 0.5}}{P_{H_2O}} \quad (6)$$

and then subtracting the ohmic, activation and concentration losses

$$V = V_N - (V_{Ohm} + V_{Act} + V_{Conc}) \quad (7)$$

The ohmic losses are calculated using the equations presented by Song et al. [27], which are based on realistic electron/ion paths and assume uniform ionic flux. The activation losses are estimated by the equations given in Achenbach [32]. Finally, the concentration losses are calculated using Chan et all. [33] equations, that take into account the ordinary and Knudsen diffusion phenomena and develops a methodology to estimate the polarization effects.

This approach requires information for the geometry and material properties. The data used for the simulations in this paper, were taken from Doherty et al. [29]

Table 3 summarizes the assumptions used for the developed fuel cell model.

Active area (1152 cells)	96.1 m^2
Afterburner efficiency	100%
DC to AC inverter efficiency	96%
Overall fuel utilization factor	0.85
Ejector fresh fuel pressure ratio	3
S/C ratio	2.5
SOFC thermal losses	2%
Total SOFC stack pressure losses	4%
Cell operating temperature	1183 K

Table 3 Assumptions for the fuel cell model at design point.

Validation of the SOFC model was done with the available literature data. The comparison of the expected and predicted values is shown in Table 5.

	Expected,[31]	Model
Air utilization factor	0.19	0.20
Voltage, [V]	0.70	0.692
Current density, [A/m^2]	1800	1806

Table 4 SOFC model validation.

Hybrid system model

The two independent models developed for the gas turbine and the SOFC stack are merged into a single one in order to investigate the integrated hybrid system.

Figure 7 presents the hybrid system as it is implemented in AspenPlus software. It contains the compressor thermodynamic model ('COMP'), the recuperator model ('RECUP') and the turbine model ('TURB') which are developed for the gas turbine. The burner model of the gas turbine is replaced with the model developed for the SOFC stack ('FC'). The fuel cell model (Fig. 6) is imported into a *Hierarchy* block in order to simplify the model flowchart. The *Hierarchy* block offers the ability to group complex parts of a simulation code in order to simplify its presentation. In the specific case, the air and the exhaust gas of the fuel cell (Fig. 6) are connected with the streams 3 and 4 (Fig. 7) respectively. Similarly the fuel stream is connected with stream 7.

For the part load operation of the hybrid system the rotational speed of the gas turbine is manipulated in order to control the amount of the supplied air. The fuel flow is also manipulated in order to maintain the fuel cell temperature constant.

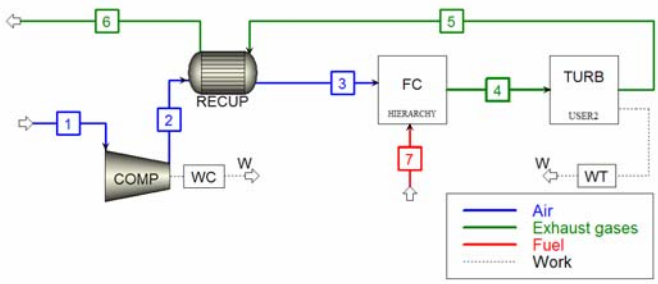

Figure 7 AspenPlus simulation model for hybrid SOFC/GT system.

The following assumptions are made to simplify the hybrid system analysis:

- Steady state operation is considered
- There are not gas leakages from the system
- The fuel supplied to the system is natural gas (CH_4 81.3%, C_2H_6 2.9%, C_3H_8 0.4%, C_4H_{10} 0.2%, N_2 14.3%, CO 0.9%)
- The operating cell voltage in each fuel cell is constant
- The distributions of temperature, pressure and gas compositions are neglected
- The fuel has always the required pressure and the fuel compression work is not taken into account.

The power output of the hybrid system is estimated as:

$$W_{HS} = W_{SOFC} + W_{GT} \quad (8)$$

The power generation efficiency is defined as

$$\eta_{HS} = \frac{W_{HS}}{\dot{m}_f LHV} \quad (9)$$

SIMULATION RESULTS

In Table 5 are summarized the predicted design point data of the hybrid system.

Total power,	181 kW
SOFC power	149.5 kW
GT power	31.5 kW
Fuel consumption	7.483 g/s
Air flow	0.295 kg/s
Exhaust gas temperature	581 K
Efficiency	63 %
Fuel cell efficiency	52 %

Table 5 Hybrid system design point data.

Part load performance

Figure 8 presents the efficiency of the hybrid system under part load conditions when turbine inlet and cell operating temperatures and fuel utilization factor are kept constant at design values. It is obvious that the system efficiency increases as the produced power decreases. This is expected since the system operates with variable rotational speed [34]. In this control strategy the amounts of air and fuel are manipulated in order to meet the power requirements. The reduction of fuel flow causes the fuel cell to operate at lower current densities which result in lower polarizations losses and increases the fuel cell efficiency. The decrease in air flow enhances the recuperator effectiveness since there is excess area for the fluids to exchange thermal energy. The augmentations of the fuel cell efficiency and recuperator effectiveness contribute to higher overall system efficiencies. At the same figure the fuel flow schedule with the load could be considered as an optimum strategy for maintaining critical parameters such as TIT and T_{sofc} at design levels.

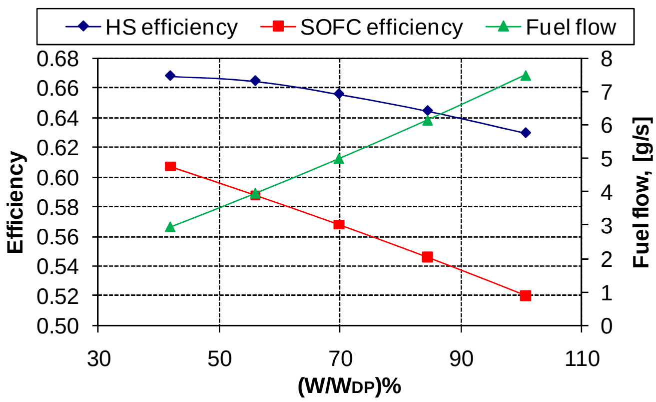

Figure 8 Part load performance of hybrid system.

When the system operates at part load conditions the contribution of the gas turbine to the total system output power decreases (Fig. 9). This occurs since the gas turbine performance deteriorates sensibly (Fig. 5) at part load conditions and on the other hand the SOFC stack operates more efficiently.

In order to verify that the two systems can be combined safely, the fuel cell cathode temperature difference is checked. Tarroja et al. [9] suggest that this temperature difference must remain under 200 K in order to avoid high thermal stresses within the fuel cell and possible failure.

Figure 9 indicates that the temperature rise in the fuel cell cathode side (i.e. the temperature difference between the inlet and outlet of the stack) remains below that limit.

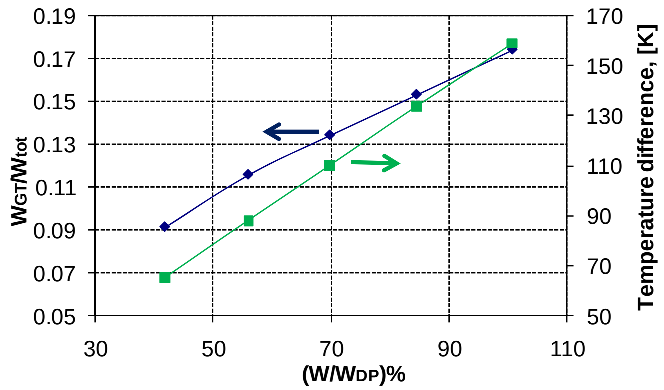

Figure 9 Gas turbine to total power output and fuel cell cathode temperature rise at part load conditions.

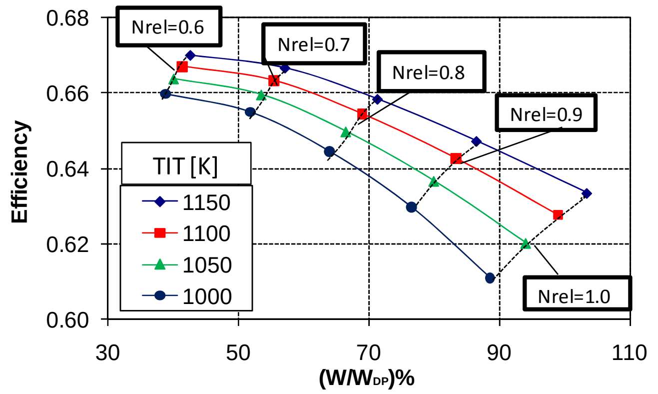

Figure 10 Effect of turbine inlet temperature in part-load performance.

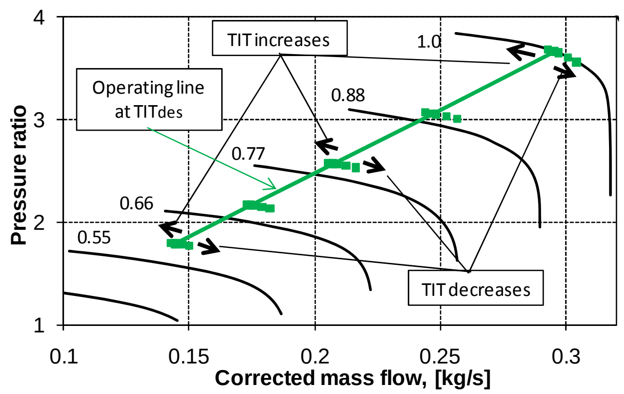

Figure 11 Compressor operating line.

Effect of turbine inlet temperature

In Fig. 10 is presented the part load behavior of the system for various values of turbine inlet temperature (the fuel cell operating temperature and fuel utilization factor remain constant). The system works more efficiently for the higher values of turbine inlet temperature in either case of constant speed or load.

The turbine inlet temperature affects the matching of the turbomachinery components resulting in changes of the air flow and pressure ratio of the compressor. In Fig. 11 are presented the corresponding operating points of Fig. 10 on the compressor map. It is observed that as the turbine inlet temperature increases, the risk of compressor surge increases, too. Thus, the turbine inlet temperature must remain below a certain limit in order to ensure the safe operation of the system.

Effect of SOFC temperature

The SOFC temperature is one of the most important operating parameters for fuel cells and hybrid systems since has significant effects in power and efficiency. Fig. 12 presents the effect of SOFC temperature on various operating parameters and a comparison with the effect of turbine inlet temperature on the same parameters. The results are arisen by varying either the T_{SOFC} or TIT by 1% and calculating the deviation of the performance parameters from their values at the design case. The higher cell temperature contributes to higher fuel consumption which increases the fuel cell power production. The air mass flow, practically is not affected when the turbine inlet temperature remains constant. This fact contributes to higher oxygen utilization factors. The current density increases because of the higher amount of fuel flow. There is also an increment in the cell voltage since there are lower voltage losses. Finally, as it can be seen the increment of SOFC temperature leads to more efficient operation in both SOFC stack and total efficiency.

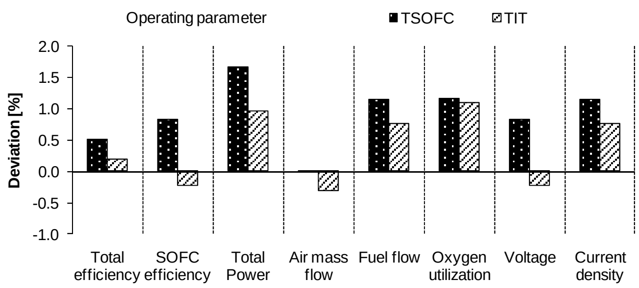

Figure 12 Effect of SOFC and turbine inlet temperature on various parameters.

The turbine inlet temperature effect on system operating parameters is smaller compared with the effect of SOFC temperature. The results show that the total power increases, as the micro-turbine produces more power. Although, the system efficiency increases, the SOFC stack efficiency decreases since higher amount of thermal energy is rejected out of stack and more fuel is consumed in order to maintain higher stack exhaust temperature. The decrease of the air flow entering the compressor is due to the turbomachinery components re-matching. The increased fuel consumption and the lower air mass flow lead to higher values of oxygen utilization factor. The current density increases since the fuel utilization factor remains constant and the fuel flow increases. The voltage decreases due to the increment of activation, concentration and ohmic losses.

Effect of fuel utilization factor

Figure 13 illustrates the effect of fuel utilization factor on various operating parameters and at different speed levels. The hybrid system responds similarly as in the case of varying the SOFC temperature. The only difference is that reduction of fuel cell voltage occurs due to higher current density which leads to higher voltage losses. Similar findings were observed when the effect of steam to carbon ratio was examined. The increment of that parameter deteriorates the system performance because the amount of the recycled fuel affects the partial pressures of gaseous components and causes a decrease in open circuit voltage (Eq. 5).

The effect of fuel utilization factor is increased at part load operation since the increment of that operating parameter has a positive impact on fuel cell efficiency. The fuel cell efficiency is higher in part load operation and so the benefit in system performance is higher.

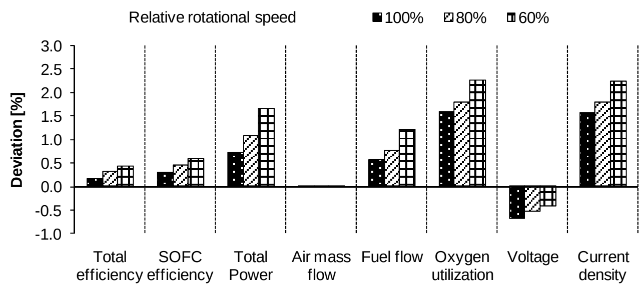

Figure 13 Effect of fuel utilization factor on various operating parameters.

CONCLUSIONS

A simulation model for a hybrid SOFC/GT system based on existing devices is developed, using the AspenPlus process simulator.

The micro turbine is modeled and calibrated using the available manufacturer data for Capstone C30. The model incorporates typical performance maps for the compressor and turbine and is able to predict the part load performance of the engine.

The fuel cell model was developed based on available literature data for Siemens-Westinghouse tubular SOFC design. The voltage calculations were done by taking into account the fundamental phenomena taking place and fuel cell geometry.

The two independent models are incorporated into a single one and performance data for the resulted hybrid system were presented and discussed. It was also studied the effect of main operating parameters on the system performance.

The simulations shown that the two existing systems can be coupled safely together, achieving thus high electrical efficiency. The size of the proposed hybrid system and its efficient operation make it an attractive solution for distributed generation applications.

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