MODELING AND SIMULATION OF AN ENERGY PRODUCTION SYSTEM WITH SOLID OXIDE FUEL CELL

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Abstract - Today's power demands and environmental concerns are stimulating the advancement of new power generation technologies. One of these technologies is that of the fuel cells. Fuel cells generate electricity from a simple electrochemical reaction in which an oxidizer, typically oxygen from air, and a fuel, typically hydrogen, combine to form a product, which is water for the typical fuel cell. Oxygen (air) continuously passes over the cathode and hydrogen passes over the anode to generate electricity, by-product heat and water. The fuel cell itself has no moving parts – making it a quiet and reliable source of power. This paper focuses on the modeling and simulation of a stack of Solid Oxide Fuel Cells (SOFC). The dynamic model has been made and implemented in the Matlab - Simulink environment. The efficiency of Solid Oxide Fuel Cells (SOFC) stack is expected to be about 50-60% in converting fuel to electricity, and about 80% in cogeneration applications.

Key words: fuel cells, clean energy, SOFC.

1. INTRODUCTION

Continuous growth in demand for conventional energy sources such as oil, natural gas and coal, adding environmental concerns stimulating the society to research and development the alternative energy sources. New technologies such as nuclear energy, wind energy, solar energy and fuel cells have all been shown to have promise as a possible future replacement for fossil fuels that provide most of its benefits and few of its harmful drawbacks

Fuel cells are a clean source of energy, generating electricity through an electrochemical reaction. The application of fuel cell technologies to advanced power generation systems signifies the most significant advancement in energy conservation and environmental protection for the next decade. This system produces performance projections of 60% or more efficiency while lowering pollutant levels such as nitrogen oxides (NO_X) and sulfur oxides (SO_X).

Fuel cells are classified primarily by the kind of electrolyte they employ. This classification determines the kind of chemical reactions that take place in the cell, the kind of catalysts required, the temperature range in which the cell operates, the fuel required, and other factors. These characteristics, in turn, affect the applications for which these cells are most suitable. There are several types of fuel cells currently under development, each with its own advantages, limitations, and potential applications.

The types of fuel cells, operating temperature, electrical efficiency, application and advantages are presented in Table. 1.

Table 1: Types of fuel cells

Fuel Cell Type	Common Electrolyte	Operating Temperature	System Output	Electrical Efficiency	Application	Advantages
Polymer Electrolyte Membrane (PEM)	organic polymer poly-perfluoro - sulfonic acid	50 - 100°C	<1kW – 250kW	53-58% (transportation) 25-35% (stationary)	-Backup power - Portable power - Small distributed generation - Transportation - Specialty vehicles	-Solid electrolyte reduces corrosion & electrolyte management problems - Low temperature - Quick start-up
Alkaline (AFC)	Aqueous solution of potassium hydroxide soaked in a matrix	90 - 100°C	10kW – 100kW	60%	- Military - Space	- Cathode reaction faster in alkaline electrolyte, leads to higher performance
Phosphoric Acid (PAFC)	Liquid phosphoric acid soaked in a matrix	150 - 200°C	50kW – 1MW (250kW module typical)	>40%	- Distributed generation	- Higher overall efficiency with CHP - Increased tolerance to impurities in hydrogen
Molten Carbonate (MCFC)	Liquid solution of lithium, sodium, and/or potassium carbonates, soaked in a matrix	600 - 700°C	<1kW – 1MW (250kW module typical)	45-47%	- Electric utility - Large distributed generation	- High efficiency - Fuel flexibility - Can use a variety of catalysts - Suitable for CHP
Solid Oxide (SOFC)	Yttrium stabilized zirconium	600 - 1000°C	<1kW – 3MW	35-43%	-Auxiliary power - Electric utility - Large distributed generation	-High efficiency - Fuel flexibility - Can use a variety of catalysts - Solid electrolyte reduces electrolyte management problems - Suitable for CHP

Two types of fuel cells are mostly used for cogeneration: solid-oxide fuel cells (SOFC) and molten carbonate fuel cells (MCFC).

Solid oxide fuel cells (SOFC) are operating at high temperatures that make them well suited for cogeneration process, but influence the entire system due to their dynamic character.

The drawbacks of the SOFC are the costs and short life time, associated with its materials that must accomplish the requirements imposed by the high operating temperature.

The paper deals with the realization of accurate dynamic models of the hybrid system components in order to estimate the effect of the operating parameters on the characteristics of the SOFC, but also on the entire hybrid system. The components of the system will be presented in detail, together with the Simulink-Matlab diagram of the electro-thermal model of each of them.

2. SOLID OXIDE FUEL CELL

To generate a substantial level of power the single cells must be bundled together into a stack. An interconnector is then used to connect a cathode of one cell to the anode of the next one. This results in an electrical series configuration, so that summing each cell's voltage is the stack voltage and each cell carries the same current. A second function of the interconnector is to keep the gaseous reactants separate and to direct their flow by the cells. A grooved design creating reactant stream flow channels is often used to accomplish this. The interconnect material varies amongst fuel cell manufacturers, but stainless steel is typical. The interconnectors add a substantial amount of mass and thermal capacitance to the stack. Therefore, they are an important factor in the thermal response of a stack.

Solid oxide fuel cells (SOFC) use a hard, non-porous ceramic compound as the electrolyte. Since the electrolyte is a solid, construction of the solid oxide fuel cell does not have to be in the plate-like configuration typical of other fuel cell types. It is expected that solid oxide fuel cell efficiency at converting fuel to electricity is between 50 and 60 percent. In co-generation or combined heat and power (CHP), applications where the waste heat is captured and utilized, the overall system fuel use efficiencies can reach 80-85%.

Solid oxide fuel cells (SOFC) have become very important due to their main advantages: high operating temperature (600-1000ºC) and high efficiency. The high operating temperature allows the internal reforming and can be used in a cogeneration system with a gas turbine. The CH_4 that has not entirely reacted in the fuel cell is burned in a combustor and the exhaust gases are expanded in the gas turbine.

The electrochemical reactions inside the fuel cell are [1]:

Anode
$$H_2 + O^{2-} \rightarrow H_2O + 2e^-$$
$$CO + O^{2-} \rightarrow CO_2 + 2e^- \quad (1)$$

Cathode
$$\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-} \quad (2)$$

Global reaction
$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O + Heat + Electricity \quad (3)$$

The structure of a solid oxide fuel cell is presented in Figure 1.

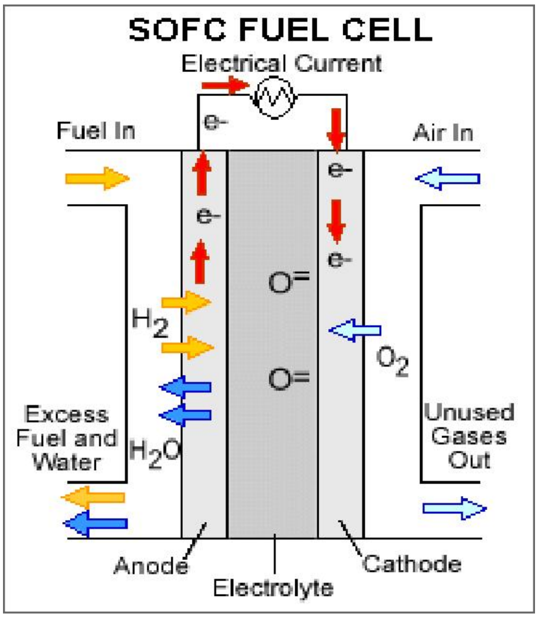

Fig. 1. Solid Oxide Fuel Cell

The SOFC fuel cell in case operates with CH_4 reformed inside the fuel stack thanks to the very high temperature conditions. The steam reforming equation and the water-gas shift equation occur at high temperature to produce H_2 that reacts at anode.

Steam reforming equation
$$CH_4 + H_2O \rightarrow 3H_2 + CO \quad (4)$$

Water-gas shift reaction
$$CO + H_2O \overset{x}{\longleftrightarrow} H_2 + CO_2 \quad (5)$$

The composition of the exhaust gases from the fuel cell without considering equation (5) would not be the true exhaust composition.

The CO shift equilibrium is applied to the resulting gas composition and the equilibrium constant, function of the molar concentrations and depending on the fuel cell outlet temperature, is:

$$K = \frac{[H_2 + x]\cdot[CO_2 + x]}{[CO - x]\cdot[H_2O - x]}$$

Knowing the equilibrium constant *K*, the extent of the reaction in the forward direction *x* is calculated and the moles of every product, accounting the water gas shift equilibrium, are determined. The resulted effluent gases are expanded in the bottoming cycle gas turbine.

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The electrochemical model of the fuel cell is based on the material balance equation. The variation of the concentration for each reactant and product reaction can be written as function of the input, output and the reaction molar flows and partial pressures, according to the following equation (considering for example the hydrogen) [2], [3]:

$$\frac{d}{dt} p_{H_2} = \frac{R \cdot T}{V_{an}} \left(q_{H_2}^{in} - q_{H_2}^{out} - q_{H_2}^{react} \right) \tag{6}$$

where p_{H_2} is the partial pressure of the hydrogen, $q_{H_2}^{in}$ is the inlet flow [kmol/s], $q_{H_2}^{out}$ is the outlet flow [kmol/s] and $q_{H_2}^{react}$ is the hydrogen flow that reacts [kmol/s].

For an orifice that is choked, it can be considered that molar flow of any gas is proportional to its partial pressure inside the channel, according to the expressions:

$$\frac{q_{H_2}}{p_{H_2}} = K_{H_2} \tag{7}$$

$$\frac{q_{H_2O}}{p_{H_2O}} = K_{H_2O} \tag{8}$$

where q_{H_2} and q_{H_2O} are the molar flows through the anode valve, p_{H_2} and p_{H_2O} are the partial pressures, K_{H_2} and K_{H_2O} are valve molar constants.

The molar flow $q_{H_2}^{react}$ can be calculated with:

$$q_{H_2}^{react} = \frac{N \cdot I}{2 \cdot F} = 2 \cdot K_r \cdot I \tag{9}$$

where K_r is a constant defined for modeling purposes [4], [5].

Replacing in equation (6) the output molar flow given by equation (7), the reaction molar flow given by equation (9) and applying the Laplace transformation, the partial pressure of hydrogen has the following expression:

$$p_{H_2} = \frac{1/K_{H_2}}{1 + \tau_{H_2} \cdot s} \left(q_{H_2}^{in} - 2 \cdot K_r \cdot I \right)$$
$$\tau_{H_2} = \frac{V_{an}}{K_{H_2} \cdot R \cdot T} \tag{10}$$

where τ_{H_2} ,expressed in seconds, is the value of the system pole associated with the hydrogen flow.

Similar expressions can be written also for H_2O and O_2. For the case of O_2 the partial pressure is given by:

$$p_{O_2} = \frac{1/K_{O_2}}{1 + \tau_{O_2} \cdot s} \left(q_{O_2}^{in} - K_r \cdot I \right) \tag{11}$$

Applying Nernst's equation and considering the Ohmic losses associated with the fuel cell, the output voltage of the stack is:

$$V = N \cdot \left(E_0 + \frac{R \cdot T}{2 \cdot F} \ln \frac{p_{H_2} \cdot p_{O_2}^{0.5}}{p_{H_2O}} \right) - r \cdot I \tag{12}$$

where E_0 is the standard reversible cell potential and $r = 0.126\ \Omega$ is the resistance associated with the Ohmic losses.

3. COMPRESSOR DYNAMIC MODEL

In the hybrid system, the compressor supplies the air containing the oxygen needed for the cathode of the fuel cell. The equations that model the compressor are based on the perfect gas equation and polytrophic transformations.

For the compressor, the equation that gives the flow through a nozzle for a uniform polytrophic compression is, [6]:

$$q_{air} = A_{C0} \cdot \frac{p_i}{\sqrt{R_a \cdot T_i}} \cdot \left\{ \frac{2 \cdot m_a}{\eta_{\infty C} \cdot (m_a - 1)} \left[\left(\frac{p_e}{p_i} \right)^{\frac{2}{m_a}} - \left(\frac{p_e}{p_i} \right)^{\frac{m_a + 1}{m_a}} \right] \right\}^{\frac{1}{2}} \tag{13}$$

where A_{C0} [m^2] is the compressor exit area, $\eta_{\infty C}$ - compressor polytrophic efficiency, R_a [J/kg·K] - air gas constant, $m_a = \frac{\gamma_a}{\gamma_a - \eta_{\infty C} \cdot (\gamma_a - 1)}$ - the polytrophic exponent, $\gamma_a = \frac{c_{pa}}{c_{va}}$ - ratio of air specific heats (constant).

The exhaust temperature of air can be obtained from:

$$T_e = T_i \cdot \left(\frac{p_e}{p_i} \right)^{\frac{\gamma_a - 1}{\gamma_a \cdot \eta_{\infty C}}} \tag{14}$$

With the help of the above expressions, the perfect gas isentropic enthalpy can be written as:

$$\Delta h_C = c_{pa} \cdot T_i \cdot \left(\left(\frac{p_e}{p_i} \right)^{\frac{R}{c_{pa}}} - 1 \right) = h_C(t_2) - h_C(t_1) \tag{15}$$

where Δh_C [kJ/kg] is the isentropic enthalpy variation corresponding to a compression from p_i to p_e, and $h_C(t_1)$, $h_C(t_2)$ [kJ/kg] are the enthalpies of the exhaust air, respectively the inlet air.

The efficiency of the compressor is given by:

$$\eta_C = \frac{1-\left(\frac{p_e}{p_i}\right)^{\frac{\gamma_a - 1}{\gamma_a}}}{1-\left(\frac{p_e}{p_i}\right)^{\frac{\gamma_a - 1}{\gamma_a \cdot \eta_{\infty C}}}} \quad (16)$$

Knowing the air flow (13), the isentropic enthalpy (15) and the compressor efficiency (16), the electrical power consumed by the compressor is:

$$P_C = \frac{q_{\text{air}} \cdot \Delta h_C}{\eta_C \cdot \eta_{trans}} \quad (17)$$

where P_C [kW] is the compressor power consumption and η_{trans} is the transmission efficiency from turbine to compressor.

4. GAS TURBINE DYNAMIC MODEL

The exhausted un-reacted fuel of the fuel cell is combusted in the gas turbine, increasing in this way the electrical efficiencies and reducing the impact of the power plant on the environment.

Gas turbines used in hybrid systems together with SOFC are subject of many studies and output power of the entire system has continuously increased in the past years. Special care should be given to the operation parameters of the gas turbine that affect the dynamic behavior of the system. Thus, a suitable model of the gas turbine is very important in order to establish the optimal operation and control strategies of the hybrid system.

For a gas turbine, the flow equation that gives the stream through a nozzle for a uniform polytrophic expansion is [6]:

$$q_{\text{TG}} = \text{A}_{\text{TG0}} \cdot \frac{p_{\text{i}}}{\sqrt{R_g \cdot T_i}} \cdot \left\{ \frac{2 \cdot m_{TG}}{\eta_{\infty TG} \cdot (m_{TG} - 1)} \left[\left(\frac{p_{\text{e}}}{p_{\text{i}}}\right)^{\frac{2}{m_{TG}}} - \left(\frac{p_{\text{e}}}{p_{\text{i}}}\right)^{\frac{m_{TG}+1}{m_{TG}}} \right] \right\}^{\frac{1}{2}} \quad (18)$$

where q_{TG} [kg/s] is the inlet gas mass flow to the turbine, $\eta_{\infty TG}$ - the gas turbine polytrophic efficiency, A_{TG0} [m^2] - turbine exit area; R_g [J/kg·K] - combustion gases constant; $m_{TG} = \frac{\gamma_g}{\gamma_g - \eta_{\infty TG} \cdot (\gamma_g - 1)}$ - the combustion gases polytrophic index, $\eta_{\infty TG}$ - the turbine polytrophic efficiency, $\gamma_g = \frac{c_{pg}}{c_{vg}}$ - ratio of combustion gases specific heats.

The exhaust temperature of gases can be obtained from:

$$T_e = T_i \cdot \left(\frac{p_e}{p_i}\right)^{\eta_{\infty TG} \cdot \frac{\gamma_g - 1}{\gamma_g}} \quad (19)$$

The above expressions allow writing the perfect gas isentropic enthalpy change equation:

$$\Delta h_{TG} = c_{pg} \cdot T_i \cdot \left(\left(\frac{p_e}{p_i}\right)^{\frac{R_g}{c_{pg}}} - 1 \right) = h_{TG}(t_2) - h_{TG}(t_1) \quad (20)$$

where: Δh_{TG} [kJ/kg] is the isentropic enthalpy variation corresponding to an expansion from p_i to p_e, and $h_{TG}(t_1)$, $h_{TG}(t_2)$ [kJ/kg] are the enthalpies of the exhaust gases, respectively the inlet gases.

The efficiency of the gas turbine is defined by [7], [8], [9]:

$$\eta_{TG} = \frac{1-\left(\frac{p_e}{p_i}\right)^{\eta_{\infty TG} \cdot \frac{\gamma_g - 1}{\gamma_g}}}{1-\left(\frac{p_e}{p_i}\right)^{\frac{\gamma_g - 1}{\gamma_g}}} \quad (21)$$

The mechanical power delivered by the gas turbine depends on the isentropic enthalpy and efficiency by:

$$P_{TG} = \eta_{TG} \cdot q_{\text{TG}} \cdot \Delta h_{TG} \quad (22)$$

where: P_{TG} [kW] is the total mechanical power delivered by the gas turbine.

The mechanical power produced by the gas turbine that is delivered to the generators is:

$$P_{mec} = P_{TG} - P_C \quad (23)$$

5. SYSTEM CONFIGURATION

The system under study is illustrated in Figure 2. The fuel cells stack has a capacity of 220 kW, containing 2304 cells, and the electrical generation efficiency is 64% (AC / low heating value). The air is supplied to the compressor and the exhaust is preheated before being provided to the cathode of the fuel cell.

The heat exchangers increase the temperature of the natural gas before supplying it to the anode. Inside the fuel cell the CH_4 is internally reformed and the exhaust gases from the anode are burned together with additional fuel in the combustor.

The exhaust gases are than expanded in a gas turbine that delivers the mechanical power to the electric generator. The turbine exhaust gases are used, in a heat exchanger, to preheat the air exiting the compressor, the fuel supplied and water for district heating. The output DC power of the fuel cell is delivered to a generic load through an inverter.

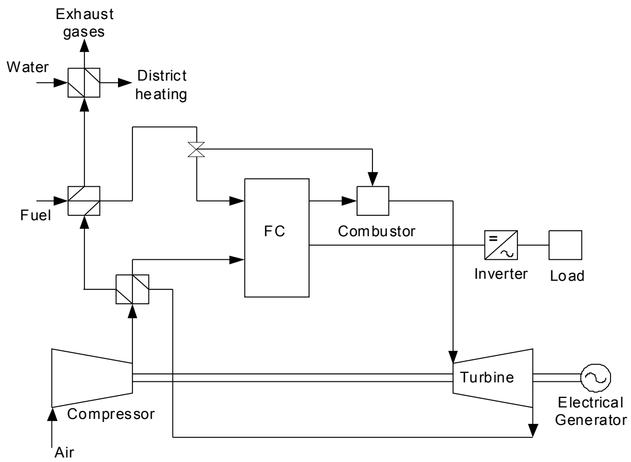

Fig. 2. System configuration layout

6. MATLAB – SIMULINK DYNAMIC MODELS

The dynamic models of the components for the system configuration under study were implemented taking into consideration the electro-chemical, thermal and electrical operating equations.

The Matlab – Simulink model of the cathode processes of the SOFC represents the electrochemical equations associated to the cathode side of the fuel cell, delivering the masses of H_2O (proportional with the humidification coefficient), N_2 and O_2, and the partial pressure of O_2. The inputs of the model are the electrical current, the excess air coefficient, the humidification coefficient, and the inlet air temperature and pressure.

The Matlab – Simulink model of the anode side of the fuel cell, implementing the processes associated with the fuel, delivers the flows of effluent of the reforming and water-gas shift reaction processes. The inputs of the model are the electrical current, the fuel utilization coefficient and the temperature of the inlet fuel. The effluent from the anode is combusted together with additional fuel and the high temperature exhaust gases are expanded in the gas turbine. The variation of electrical power generated by the SOFC stack is presented in Figure 3.

The Matlab – Simulink model of the compressor implements the equations (12) – (17). The enthalpy is expressed by a third order degree polynomial function [6], [10]. The inputs of the model are the air temperature, pressure and flow rate. The outputs of the model are the exhaust air temperature, the mechanical power consumed, the heat, and the exhaust pressure.

The Matlab – Simulink model of the gas turbine deals with the equations (18) - (23), where the inputs are the mass flows of the combustor exhaust gases, the heat of the gases, and the pressure of the inlet turbine gases. As outputs, the temperature and pressure of the exhaust gases, the electrical power, and the produced heat were considered.

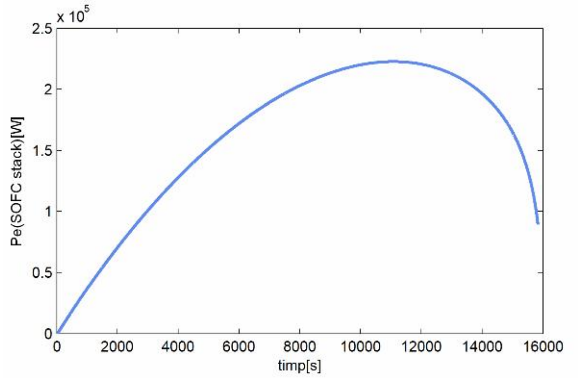

Fig. 3. Variation of electrical power generated by the SOFC stack

Figure 4 shows that, for a decrease of the current through the fuel cells from 438kA to 50kA (and in correspondence a decay of the current density), the cell voltage increases and the electric power (generated kW/inlet flow of fuel) is reduced.

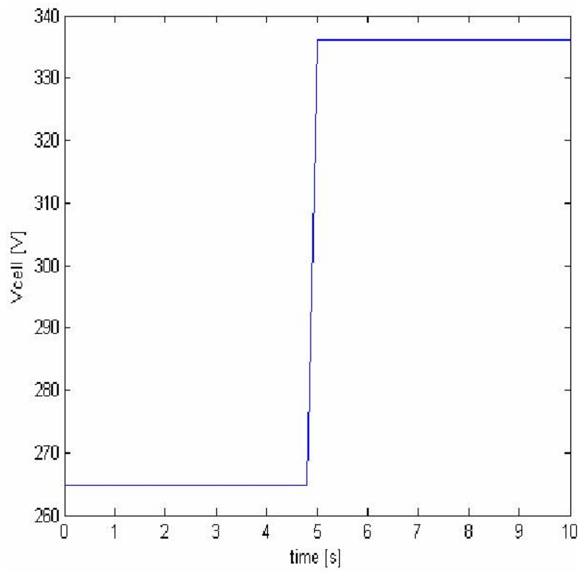

Fig. 4: Variation of the cell voltage for the fuel cell current step

In correspondence with the current decrease, the air utilization factor is reduced proportionally. The variations of the fuel cell current and of the air utilization factor allow controlling the power generated by the fuel cell.

In case of the SOFC inlet air flow reduction, simultaneously with the decrease of the fuel cell current, the exhaust temperature of the gas turbine connected to the fuel cell will increase. Hence, the temperature of the gases entering the heat exchangers will increase and in consequence warmer gases are delivered to the fuel cell. The variation of the temperature of the gases exhausted from the turbine is shown in Figure 5.

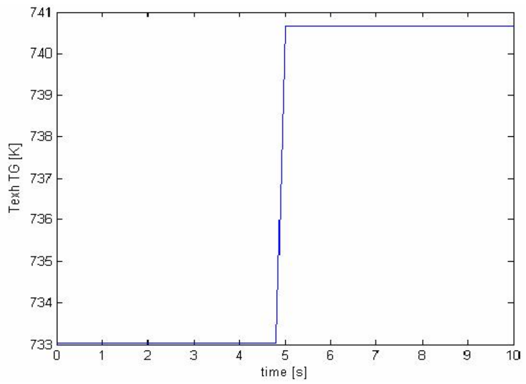

Fig. 5. Variation of the exhaust gas turbine temperature with the inlet air flow of the SOFC

The variation of the fuel cell operating pressure determines the increase of the electrical power generated by the turbine and compressor assembly, as it can be seen in Figure 6. Figure 7 shows, for the variation of the cell operating pressure, the exhaust temperature of the gas turbine.

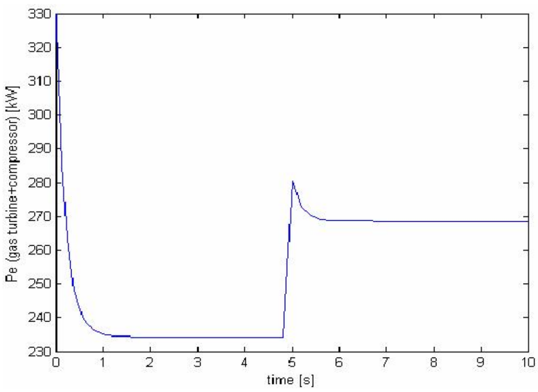

Fig. 6. Variation of electrical power generated by the ensemble gas turbine – compressor with the operating pressure of the fuel cell

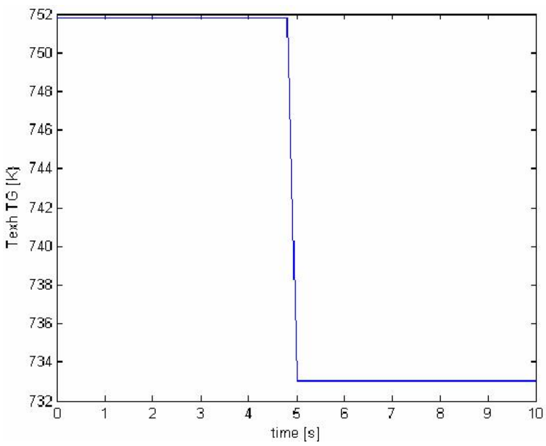

Fig. 7. Variation of the exhaust gas turbine temperature fuel cell operating pressure

CONCLUSIONS

Hybrid cycles comprising high temperature fuel cells, such as the solid oxide fuel cells (SOFC), are very promising for generating electric power in the future, initially at the small to medium scale (250 kW to 20 MW), and later in large scale central plants (>100 MW).

The hybrid gas turbine fuel cell systems have demonstrated lower environmental impact and higher efficiency compared to conventional combustion driven power plants. Lower carbon dioxide emissions can be achieved through higher fuel-to-electrical efficiencies, while NO_x and other criteria pollutant emissions are greatly reduced by primary electrochemical conversion of the fuel versus the combustion process of conventional plants.

In this paper, the dynamic models of a solid oxide fuel cell – gas turbine system components in Matlab-Simulink environment are developed. The fuel cell was represented creating the cathode and anode processes models in order to better manage the behavior of the fuel cell at operating parameters variations. The cathode model includes the internal reforming and the water-gas shift reaction for obtaining the true composition of the effluent gases. The compressor and gas turbine models include the calculation of air and combustion gases enthalpies, respectively.

The operating parameters study (electric current of the fuel cell, air utilization factor, inlet air flow, fuel cell pressure) showed that these ones have an important influence not only on the operation of the fuel cell, but also on the operation of the gas turbine, and in consequence on the power delivered by the hybrid system SOFC – gas turbine.

REFERENCES

[1] D. J. Hall and R. G. Colclaser, "Transient modeling and simulation of tubular solid oxide fuel cells," IEEE Trans. Energy Conversion, vol. 14, pp. 749–753, Sept. 1999.

[2] Fuel Cell HandBook, 5th ed., EG&G Services Parsons Inc., U.S. Department of Energy, 2000.

[3] J.F. Blackburn, G. Reethof, J.L. Shearer Eds., Fluid Power Control, 1960.

[4] J. Padullés, G.W. Ault, and J. R. McDonald, "An integrated SOFC plant dynamic model for power system simulation," Journal of Power Sources, pp. 495–500, 2000.

[5] K. Sedghisigarchi, A. Feliachi, "Dynamic and transient analysis of power distribution systems with fuel cells - part I: Fuel-Cell Dynamic Model", IEEE Trans. Energy Conversion, vol. 19, pp. 423–428, June 2004

[6] LĂZĂROIU Gh., Modeling and simulating thermal power plants, Ed. Printech, Bucharest, 1998, pag. 190-203.

[7] LĂZĂROIU Gh., LAZĂROIU G.C., On modeling and simulation of electrical generators, Rev. Roum. Sci. Techn. - Électrotechn. et Énerg., 49, 2, Bucharest, 2004, pag. 217-225.

[8] LĂZĂROIU Gh., On modeling and simulating steam turbines, Rev. Roum. Sci. Techn. - Électrotechn. et Énerg., 47, 2, Bucharest, 2002, pag. 229-246.

[9] Gheorghe LAZAROIU, Umberto DESIDERI, Dana RĂDOI, Optimization of a SOFC Systems: Influence of Design Operation Parameters on System Efficiency, 3rd International Conference on Energy and Environment 2007, U.P.B. Sci. Bull., Series C, Vol. 69, No.4, 2007, pp. 83-90.

[10] K. Raznjevic, Tables and thermodynamic diagrams, Technical Editure, Bucharest, 1978