

Parametrical analysis of a tubular pressurized SOFC

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Abstract High temperature fuel cells of the solid oxide type (SOFC) are simple electrochemical devices that operate at 1000 °C and are capable of converting the chemical energy of natural gas to AC electric power at approximately 55-60% efficiency (net AC/LHV in atmospheric pressure). In this paper, a zero-dimensional model of a single tubular SOFC with internal reforming of hydrocarbons is proposed which has been both numerically implemented and parametrically analyzed.

Keywords: Fuel cell; Modelling, SOFC

Nomenclature

I_c	–	current produced by the fuel cell, A
g_e	–	cell current density, mA/cm ²
U_f	–	cell fuel utilization factor
U_a	–	cell air utilization factor
S/C	–	steam/carbon ratio
\dot{m}	–	mass flow rate, kg/s
\dot{n}	–	molar flux rate, kmol/s
M_k	–	molar mass of substance k , kg/kmol
\dot{L}	–	cell power output, W
\dot{Q}	–	external heat flux, W
i	–	specific enthalpy, kJ/kg
mi	–	molar enthalpy, kJ/kmol

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C_p	–	molar heat capacity, kJ/(kmol K)
T	–	temperature, K
pre_r	–	pre-reformer fraction, %
V_c	–	cell voltage, V
F	–	Faraday constant, $F = 96439$ C/mol
Δh	–	molar enthalpy change, kJ/kmol (reaction heat)
\dot{x}	–	CH ₄ rate of reaction, kmol/s (reforming)
\dot{y}	–	CO rate of reaction, kmol/s (shifting)
\dot{z}	–	H ₂ rate of reaction, kmol/s (electrochemical)
K	–	equilibrium constant
p	–	pressure, bar
A	–	cell active area, m ²
L	–	characteristic length of tubular cell, m
R_G	–	universal gas constant, Nm/(kmol K)
R	–	resistivity of material, Ω
ΔG	–	Gibbs free enthalpy change, J/kmol
SOFC	–	solid oxide fuel cell
LHV	–	lower heating value
CFM	–	Computational Flow Mechanics (based on 0D models)

Greek symbols

α_{rec}	–	fuel recirculation ratio
η_e	–	ejector efficiency, %
η_{el}	–	electrical efficiency (LHV)
ρ	–	electrical resistance, Ωcm

Subscripts

f	–	fuel
a	–	air, anode
c	–	cathode
k	–	chemical species
e	–	exhaust, outlet
i	–	inlet

1 Introduction

Among the SOFC technologies, tubular SOFC stacks with internal reforming have emerged as one of the most mature technology. In particular, they are promising for their high operating pressure and temperature that makes them suitable for integration with a gas turbine (Fig.1) in a hybrid cycle power system (cogeneration, trigeneration, etc)[1,2,3]. The tubular SOFC technology, mainly developed by Siemens-Westinghouse is based on a pressurized SOFC generator that operates on recuperative heated process air supplied by a compressor.

tained model must be easy to be integrated into the COM-GAS code, which has recently been used for complex thermodynamic and energy analysis.

2 The SOFC mathematic modelling

For the development of a 0D model the following main assumptions are employed to simplify the hybrid cycle calculations [3,4,8]:

- steady state operation is considered,
- gases do not leak outside the system,
- adiabatic cell – heat loss is negligibly small,
- relative pressure loss remains constant – therefore the momentum equation is reduced to the pressure drop,
- equilibrium of reforming and shift reactions,
- temperature of the anode outlet equal to the cathode stream temperature,
- internal distribution of temperature, gas composition and pressure in each component is not taken into account,
- O_2 ion transportation is responsible for electrical current flow,
- in the combustion chamber residual chemical species from the anode and injected methane are burned completely,

The fuel utilization U_f coefficient, the air utilization coefficient U_a and the pre-reformer fraction pre_r , and the fuel recirculation ratio α_{rec} are considered as input values. The current I_c ($A = C/s$) is easy to be evaluated since, when one mole of H_2 reacts with oxygen ($0,5 \cdot O_2^{2-}$) in one second, then the corresponding electric load is $2 \cdot 96439 A$. Sometimes, in the literature, instead of the fuel recirculation ratio, the steam/carbon ratio S/C is defined as the mole fraction of steam in the recirculated anode exhaust gas to all combustible species, which implicates that carbon is present in supplied fuel [2].

3 Solid oxide fuel cell model

In Figure 2 is shown the schematic of tubular SOFC that contains the mixer, the ejector pump, the pre-reformer, the SOFC tubular stack, the air preheated and the post-combustion chamber.

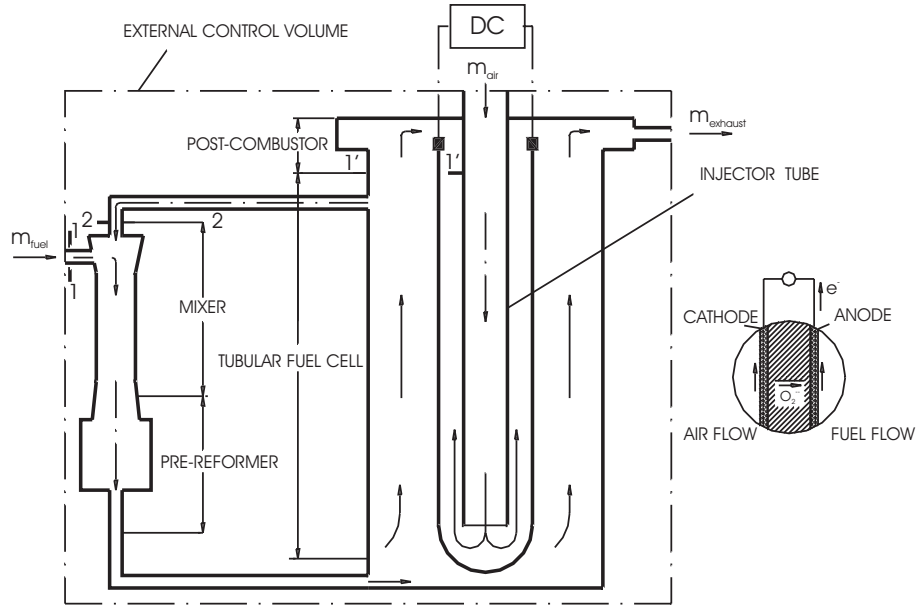


Figure 2. A lay-out of the tubular SOFC.

3.1 Basic balances within the external control volume

In order to verify the local balances for mixer, pre-reformer, SOFC stack and combustion chamber one must write down the following basic balances for the entire control volume.

Mass balance:

$$\dot{m}_{fuel} + \dot{m}_{air} = \dot{m}_{exhaust} \quad (1)$$

where the particular mass fluxes are defined to be:

$$\dot{m}_{fuel} = M_{CH_4} \cdot \dot{n}_{CH_4,f} + M_{H_2} \cdot \dot{n}_{H_2,f} + \dots = \sum_1^{f_k} M_k \cdot \dot{n}_{k,f} \quad (2)$$

$$\dot{m}_{air} = M_{N_2} \cdot \dot{n}_{N_2,a} + M_{O_2} \cdot \dot{n}_{O_2,a} + \dots = \sum_1^{a_k} M_k \cdot \dot{n}_{k,a} \quad (3)$$

$$\dot{m}_{exhaust} = M_{H_2O} \cdot \dot{n}_{H_2O,e} + M_{CO_2} \cdot \dot{n}_{CO_2,e} + \dots = \sum_1^{e_k} M_k \cdot \dot{n}_{k,e} \quad (4)$$

Above, the following denotations have been used:

- \dot{n}_k – the molar flux of substance k ,
- M_k – the molar mass of substance k .

Energy balance:

$$\dot{m}_{fuel} \cdot i_{fuel} + \dot{m}_{air} \cdot i_{air} - \dot{L}_{el} + \dot{Q}_{ex} = \dot{I}_{exhaust} \quad (5)$$

where:

- $\dot{m}_{fuel} \cdot i_{fuel}$ – the flux of physical and chemical enthalpy of the fuel,
- $\dot{m}_{air} \cdot i_{air}$ – the flux of physical enthalpy of the air,
- \dot{L}_{el} – the cell power output,
- \dot{Q}_{ex} – the flux of external heat (supplied or obtained),
- $\dot{I}_{exhaust}$ – the flux of enthalpy of exhaust flux gases.

3.2 Mixer

After clean up of sulphur components and mixing with primary steam, the pressurized natural gas is fed via a jet pump into the pre-reformer where the higher hydrocarbons and some percentage of methane are reformed. This is done with the help of steam coming from the stack outlet, which is re-circulated by the jet pump (ejector). Therefore the mixer is an ejector where the fuel and recycled anodic flow rate are mixed before entering the pre-reformer. The anodic flow is a gas at high temperature coming from the anode, which consists of CO, CO₂, H₂, H₂O and another chemical species, which are the products of reforming reactions occurring within the pre-reformer.

Writing mass and energy balances within the mixer we assume that, due to specific construction of the ejector, the recirculation number is known. It is usually equivalent to a steam/carbon ratio, which is defined as the mole fraction of steam in the recirculated anode exhaust gas to all combustible species, implicate carbon, in supplied fuel (Fig.2):

$$S/C = \frac{\dot{n}_{H_2O}^2}{\dot{n}_{CH_4}^1 + \dot{n}_{CO}^1} \quad (6)$$

Knowing S/C ratio one can calculate the fuel recirculation ratio α_{rec} which is used for definition of molar fluxes at inlet 2-2:

$$\dot{n}_k^{i,2} = \alpha_{rec} \cdot \dot{n}_k^{e,a}, \quad k = CH_4, H_2, H_2O, CO, CO_2 \quad (7)$$

where the superscript e means exhaust of the anodic part of the tubular fuel cell. If the index 1 refers to the fuel flow rate and index 2 refers to the recycled anodic flow rate the equations of mass and energy balance being the simple mixing process are:

Mass balance: (e – exhaust, i – inlet of the mixer)

$$\dot{n}_k^e = \dot{n}_k^{i,1} + \dot{n}_k^{i,2}, \quad k = \text{CH}_4, \text{H}_2, \text{O}, \text{CO}, \text{CO}_2 \quad (8)$$

Energy balance:

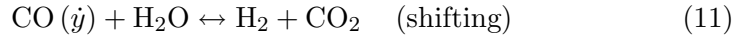
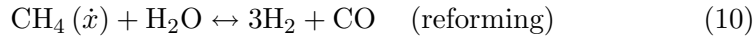
$$\sum_1^{f_k} \dot{n}_k^{i,1} \cdot m_i^{i,1} + \sum_1^{f_k} \dot{n}_k^{i,2} \cdot m_i^{i,2} = \eta_e \cdot \sum_1^{f_k} \dot{n}_k^e \cdot m_i^e \quad (9)$$

- $m_k^{i,1}$ – the molar enthalpy of inlet fuel,
- $m_k^{i,2}$ – the molar enthalpy of the exhaust anodic gas,
- m_k^e – the molar enthalpy of mixture.

In energy equation (9) the exhaust temperature T^e is the unknown to be calculated. Molar physical enthalpies are taken from the Janaf tables [10] or the idealization that $m_i = C_p \cdot T$. The nozzle isentropic efficiency of ejector is usually equal to $\eta_e = 0.92$.

3.3 Pre-reformer

From the mixer the gaseous mixture enters the pre-reformer, which is a typical catalytic reactor where hydrogen and carbon dioxide are produced from methane and steam. The reforming/shifting reactions are as follows [5]:



It is common to assume that only a part of mole fraction of methane takes the reforming reaction. Therefore, in order to calculate the molar part of flux of methane \dot{x} , which reacts in the reforming reaction, it is necessary to know a typical value of percentage of methane, which is able to react in the reformer (for example $pre_r = 10 - 15\%$).

$$\dot{x} = pre_r \cdot \dot{n}_{\text{CH}_4}^i \quad (12)$$

where: $\dot{n}_{\text{CH}_4}^i$ (pre-reformer) $\equiv \dot{n}_{\text{CH}_4}^e$ (mixer).

The CO-shift reaction is considered to reach thermodynamic equilibrium, with an equilibrium constant calculated at outlet pre-reformer temperature T^e

$$K_{p,shift}(T^e) = \frac{\dot{n}_{H_2} \cdot \dot{n}_{CO_2}}{\dot{n}_{H_2O} \cdot \dot{n}_{CO}} \quad (13)$$

Let \dot{y} denote the moles of CO, which react in the shifting reaction. Then using the definition of equilibrium reaction one can calculate \dot{y} .

Then, keeping in mind that the energy balance for the reformer should include additional input and output contribution due to reforming reaction Δh_{ref} and to shift reaction Δh_{shift} , we write down both balances as follows:

Mass balance:

$$\dot{n}_{CH_4}^e = \dot{n}_{CH_4}^i - \dot{x}, \quad (14)$$

$$\dot{n}_{H_2}^e = \dot{n}_{H_2}^i + 3 \cdot \dot{x} + \dot{y}, \quad (15)$$

$$\dot{n}_{H_2O}^e = \dot{n}_{H_2O}^i - \dot{x} - \dot{y}, \quad (16)$$

$$\dot{n}_{CO}^e = \dot{n}_{CO}^i + \dot{x} - \dot{y}, \quad (17)$$

$$\dot{n}_{CO_2}^e = \dot{n}_{CO_2}^i + \dot{y}. \quad (18)$$

Energy balance:

$$\begin{aligned} & \dot{n}_{CH_4}^i \cdot m_{CH_4}^i + \dot{n}_{H_2}^i \cdot m_{H_2}^i + \dot{n}_{H_2O}^i \cdot m_{H_2O}^i + \dot{n}_{CO}^i \cdot m_{CO}^i + \\ & + \dot{n}_{CO_2}^i \cdot m_{CO_2}^i - \dot{x} \cdot (\Delta h_{ref}) - \dot{y} \cdot (\Delta h_{shift}) = \\ & = \dot{n}_{CH_4}^e \cdot m_{CH_4}^e + \dot{n}_{H_2}^e \cdot m_{H_2}^e + \dot{n}_{H_2O}^e \cdot m_{H_2O}^e + \\ & + \dot{n}_{CO}^e \cdot m_{CO}^e + \dot{n}_{CO_2}^e \cdot m_{CO_2}^e \end{aligned} \quad (19)$$

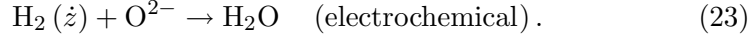
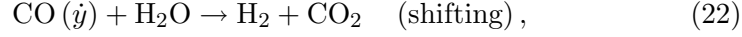
This last equation allows us to calculate the outlet temperature of gases T^e . The value of the equilibrium constant $K_{p,shift}$ is approximately given by [4]

$$\log K_{p,shift} = A \cdot T^4 + B \cdot T^3 + C \cdot T^2 + D \cdot T + E \quad (20)$$

with the constant coefficients given in Table 1.

3.4 Tubular Fuel Cell (anodic side)

Leaving the adiabatic pre-reformer the gas/steam mixture is fed to an internal reforming zone where all methane is reformed, using the heat of the electrochemical reaction zone for this endothermic reaction. The reformed gas enters the reaction zone (Fig. 2) at the closed end of the cell. The reactions considered inside the cell (anode side) are as follows:



The unknowns \dot{x} , \dot{y} , \dot{z} can be calculated from the assumption of equilibrium reactions. However, \dot{z} is known from the given value of the fuel utilization coefficient U_f [8].

$$U_f = \frac{\dot{z}}{\dot{n}_{\text{H}_2}^i + \dot{n}_{\text{CO}}^i + 4 \cdot \dot{n}_{\text{CH}_4}^i} \quad (24)$$

where 4 is the number of H_2 moles generated by each CH_4 mole (three by the reforming and one by the shift reaction). The variable \dot{z} is the number of H_2 moles, which react in electrochemical reaction. The variable \dot{x} is the number of CH_4 moles, which react in the reforming reaction. All methane reacts in this reaction. To evaluate the CO mole (\dot{y}) the equilibrium constants $K_{p,shift}$ should be put as a known function of temperature [7]:

$$K_{p,shift}(T^e) = \frac{\dot{n}_{\text{H}_2} \cdot \dot{n}_{\text{CO}_2}}{\dot{n}_{\text{H}_2\text{O}} \cdot \dot{n}_{\text{CO}}} \quad (25)$$

where the equilibrium constant $K_{p,shift}$ can be directly correlated to the temperature as [4]:

$$\log K_{p,shift} = A \cdot T^4 + B \cdot T^3 + C \cdot T^2 + D \cdot T + E \quad (26)$$

and the constants value are [7]: and temperature T is taken as the outlet temperature T^e . The outlet temperature T^e is calculated by means of an iteration until the compatibility of the right and left side of the energy balance (32). The **mass balance** between inlet and exit (see Fig. 2) of anodic side SOFC is given to be:

$$\dot{n}_{\text{CH}_4}^e = \dot{n}_{\text{CH}_4}^i - \dot{x} = 0, \quad (27)$$

Table 1

Shifting constants

Shifting	
A	$5.470 \cdot 10^{-12}$
B	$-2.574 \cdot 10^{-8}$
C	$4.637 \cdot 10^{-5}$
D	$-3.915 \cdot 10^{-2}$
E	13.209

$$\dot{n}_{\text{H}_2}^e = \dot{n}_{\text{H}_2}^i + 3 \cdot \dot{x} + \dot{y} - \dot{z}, \quad (28)$$

$$\dot{n}_{\text{H}_2\text{O}}^e = \dot{n}_{\text{H}_2\text{O}}^i - \dot{x} - \dot{y} + \dot{z}, \quad (29)$$

$$\dot{n}_{\text{CO}}^e = \dot{n}_{\text{CO}}^i - \dot{y} + \dot{x}, \quad (30)$$

$$\dot{n}_{\text{CO}_2}^e = \dot{n}_{\text{CO}_2}^i + \dot{y}. \quad (31)$$

The **balance of energy** on the anodic side is given by:

$$\begin{aligned} & \dot{n}_{\text{CH}_4}^i \cdot mi_{\text{CH}_4}^i + \dot{n}_{\text{H}_2}^i \cdot mi_{\text{H}_2}^i + \dot{n}_{\text{H}_2\text{O}}^i \cdot mi_{\text{H}_2\text{O}}^i + \dot{n}_{\text{CO}}^i \cdot mi_{\text{CO}}^i + \\ & + \dot{n}_{\text{CO}_2}^i \cdot mi_{\text{CO}_2}^i - \dot{L}_{el} - \dot{x} \cdot (\Delta h_{ref}) - \dot{y} \cdot (\Delta h_{shift}) + \\ & - \dot{z} \cdot (\Delta h_{el}) = \dot{n}_{\text{CH}_4}^e \cdot mi_{\text{CH}_4}^e + \dot{n}_{\text{H}_2}^e \cdot mi_{\text{H}_2}^e + \dot{n}_{\text{H}_2\text{O}}^e \cdot mi_{\text{H}_2\text{O}}^e \\ & + \dot{n}_{\text{CO}}^e \cdot mi_{\text{CO}}^e + \dot{n}_{\text{CO}_2}^e \cdot mi_{\text{CO}_2}^e \end{aligned} \quad (32)$$

where:

- \dot{L}_{el} – the cell electrical power,
- $\Delta h_{ref}, \Delta h_{shift}, \Delta h_{el}$ – the heat of reactions, respectively,

The cell electrical power

The cell electrical power is calculated as the product of cell current I_c and the cell electrodes voltage V_c

$$\dot{L}_{el} = I_c \cdot V_c \quad (33)$$

Since, when one mole of H_2 reacts in one second the corresponding current generated is $2 \cdot 96439 \text{ A}$. Thus:

$$I_c = 2 \cdot \dot{z} F \quad (34)$$

where $F = 96439$ C/mol is the Faraday constant.

Usually, in the literature the smaller quantity is used- the current density $i_c = I_c/A$ (1000-2000 A/m²) where $A = 834$ cm² is the electrode area of tubular Siemens-Westinghouse SOFC [1].

The evaluation of electrodes voltage V_c is most difficult part of modelling process. In general, calculation of the cell voltage is performed as a function of the current density, operating temperature, operating pressure and reactant and products composition. Then, the voltage V_c is calculated as a difference between the reversible ideal Nernst potential V_{oc} and irreversible potential V_{irr} :

$$V_c = V_{oc} - V_{irr} \quad (35)$$

Since the cell Nernst voltage decreases from inlet to the outlet of the cell due to the change in partial pressures of the chemical species, an average value between the inlet V_{oc}^i and the exit V_{oc}^e should be calculated as the cell Nernst potential:

$$V_{oc} = \frac{V_{oc}^i + V_{oc}^e}{2} \quad (36)$$

where the Nernst potential is given [4]:

$$V_{oc} = \frac{-\Delta G}{2 \cdot F} + \frac{R_G \cdot T}{2 \cdot F} \ln \frac{p_{H_2} \cdot p_{O_2}^{0.5}}{p_{H_2O}}$$

The Nernst potential is reduced, when the electrical cell circuit is closed due to the following irreversibilities:

$$V_{irr} = (R_{OHM} + R_{ATTIV}) \cdot I_c$$

where:

- R_{OHM} – ohmic resistance of the cell elements,
- R_{ATTIV} – polarization resistance of the electrodes.

In the literature [7÷9] the ohmic losses are calculated from the Ohm equation $R_{OHM} = \rho \cdot L/A$ that needs the evaluation of the electrons path throughout each element of the cell (anode, electrolyte, cathode and interconnections), (L, A – characteristic length and area). The resistance is described by the Bessette closures [7]:

$$\begin{aligned} \rho &= 0.008114 \cdot e^{(600/T)} && \text{(cathodic electrode),} \\ \rho &= 0.00294 \cdot e^{(10350/T)} && \text{(electrolyte, yttria stabilized zirconia YSZ),} \\ \rho &= 0.00298 \cdot e^{(-1392/T)} && \text{(anodic electrode).} \end{aligned} \quad (39)$$

The electrode polarization effects can be evaluated using the Achenbach closure [6,7]:

$$R_{ATTIV} = \frac{R_{att,a}}{A_a} + \frac{R_{att,c}}{A_c} \quad (40)$$

where:

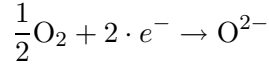
$$R_{att,c}^{-1} = K_c \cdot \frac{4 \cdot F}{R_G \cdot T} \cdot \left(\frac{p_{O_2}}{p_{ref}} \right)^m \cdot e^{-\left(\frac{E_{a,c}}{R_G \cdot T} \right)} \quad (41)$$

$$R_{att,a}^{-1} = K_a \cdot \frac{2 \cdot F}{R_G \cdot T} \cdot \left(\frac{p_{H_2}}{p_{ref}} \right)^m \cdot e^{-\left(\frac{E_{a,a}}{R_G \cdot T} \right)} \quad (42)$$

and $E_{a,c} = 160$ kJ/mole, $E_{a,a} = 110$ kJ/mole, p_{ref} – reference pressure, $K_c = 1.49 \cdot 10^{10}$, $K_a = 2.13 \cdot 10^8$, $m = 0.25$ [6, 7].

3.5 Tubular Fuel Cell (cathodic side)

The cathode reaction of SOFC is described by the equation:



A part of oxygen $\left(\frac{\dot{z}}{2}\right)$ contained within preheated air diffuses through the electrolyte to anode. Usually, similar to combustion process, the above reaction needs to feed much more oxygen [13,14]:

$$\dot{n}_{O_2}^{i,\min} = \frac{\dot{z}}{2 \cdot U_a} \quad (44)$$

where U_a , the air utilization factor, has a value given by experiments. Therefore, the balances of air components on the cathodic side are:

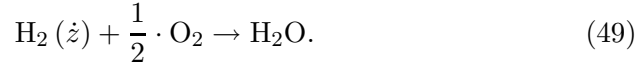
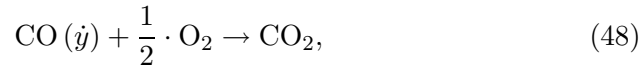
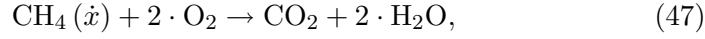
$$\dot{n}_{N_2}^e = \dot{n}_{N_2}^i, \quad (45)$$

$$\dot{n}_{O_2}^e = \frac{\dot{z}}{2 \cdot U_a} - \frac{\dot{z}}{2}. \quad (46)$$

The choice of U_a (15-25%) depends on several exploitation problems as a deactivation of cathode and strong thermal stresses within electrodes.

3.6 Post-combustion chamber

On the outlet anode side $(1 - \alpha_{rec}) \cdot \dot{n}_e$ flux gases contains not only pure steam and carbon dioxide but also unburned CH_4 (if $\text{CH}_4 \neq 0$), H_2 , CO . Therefore, this unburned gases after mixing with exit air can be burnt in stoichiometric manner:



The heat produced in the above reactions is used to preheat the air flow entering the cell from the cathodic side. Thus, if $\dot{x}, \dot{y}, \dot{z}$, as previously denote the mole flux of CH_4 , CO and H_2 , then it is simple to write an approximate balance of mass and energy.

Mass balance: (a – anodic side, c – cathodic side)

$$\dot{n}_{\text{O}_2}^e = \dot{n}_{\text{O}_2}^{i,c} - 2 \cdot \dot{x} - \frac{1}{2} \cdot \dot{y} - \frac{1}{2} \cdot \dot{z}, \quad (50)$$

$$\dot{n}_{\text{H}_2}^e = \dot{n}_{\text{H}_2}^{i,a} - \dot{z}, \quad (51)$$

$$\dot{n}_{\text{CH}_4}^e = \dot{n}_{\text{CH}_4}^{i,a} - \dot{x}, \quad (52)$$

$$\dot{n}_{\text{H}_2\text{O}}^e = \dot{n}_{\text{H}_2\text{O}}^{i,a} + \dot{n}_{\text{H}_2\text{O}}^{i,c} + 2 \cdot \dot{x} + \dot{z}, \quad (53)$$

$$\dot{n}_{\text{CO}}^e = \dot{n}_{\text{CO}}^{i,a} - \dot{y}, \quad (54)$$

$$\dot{n}_{\text{CO}_2}^e = \dot{n}_{\text{CO}_2}^{i,a} + \dot{n}_{\text{CO}_2}^{i,c} + \dot{x} + \dot{y}, \quad (55)$$

$$\dot{n}_{\text{N}_2}^e = \dot{n}_{\text{N}_2}^{i,c}. \quad (56)$$

Balance of energy:

$$\begin{aligned} & \dot{n}_{\text{CH}_4}^{i,a} \cdot m_{\text{CH}_4}^{i,a} + \dot{n}_{\text{H}_2}^{i,a} \cdot m_{\text{H}_2}^{i,a} + \dot{n}_{\text{H}_2\text{O}}^{i,a} \cdot m_{\text{H}_2\text{O}}^{i,a} + \dot{n}_{\text{CO}}^{i,a} \cdot m_{\text{CO}}^{i,a} + \\ & + \dot{n}_{\text{CO}_2}^{i,a} \cdot m_{\text{CO}_2}^{i,a} + \dot{n}_{\text{N}_2}^{i,c} \cdot m_{\text{N}_2}^{i,c} + \dot{n}_{\text{O}_2}^{i,c} \cdot m_{\text{O}_2}^{i,c} + \dots + \\ & - \dot{x} \cdot (\Delta h_{\text{CH}_4}) - \dot{y} \cdot (\Delta h_{\text{CO}}) - \dot{z} \cdot (\Delta h_{\text{H}_2}) = \sum_1^{eK} \dot{n}_K^e \cdot m_{\text{K}}^e(T^e), \end{aligned} \quad (57)$$

$k = \text{H}_2, \text{H}_2\text{O}, \text{CO}, \text{CO}_2, \text{CH}_4, \text{O}_2, \text{N}_2$

The above group of equations allows to calculate the temperature and compositions of the mixture exiting the SOFC module.

4 Geometrical-loading data and SOFC calculation

The mathematical model of the SOFC presented above has been implemented in the Lahey Fortran 90 and Borland Delphi (similar to the COM-GAS code). In order to calculate SOFC module we have to know input values such as:

- air mass flow rate and temperature,
- pressure of the cell,
- fuel recirculation ratio,
- air utilization factor, fuel utilization factor,
- percentage of methane, which reacts in the pre-reformer.

The program calculates the composition and the temperature of the exhaust gas for each discussed part of the SOFC module, using these input parameters. Next, the program calculates the electrical current, the voltage and the electrical efficiency (LHV) of the SOFC module.

It is assumed that:

- single tubular cell, $A = 1036 \text{ cm}^2$,
- fuel temperature, $T_f = 873 \text{ K}$,
- air temperature, $T_a = 473 \text{ K}$,
- pressure of the cell, $p = 1 \text{ bar}$,
- fuel recirculation ratio, $\alpha_{rec} = 0.235$,
- percentage of methane, which react in the pre-reformer, $pre_r = 0.15$,
- the fuel utilization factor, $U_f = 0.85$,
- the air utilization factor, $U_a = 0.25$,
- inlet mixture composition, $\text{CH}_4 - 17.1\%$; $\text{CO}_2 - 4.36\%$; $\text{CO} - 2.94\%$;
 $\text{H}_2 - 26.26\%$; $\text{H}_2\text{O} - 49.34\%$

and then changing the parameters \dot{m}_f , U_f , α_{rec} , U_a respectively, one calculate the SOFC module. Then, next calculation one has changed pressure of the cell.

5 Results of the parametric analysis

In the first calculation, SOFC module parameters (single cell) for different values of fuel mass flow (presented in Tab. 2 and Fig. 3 and Fig. 4) have been calculated. In the case of all examples of calculations the determined factors are constant.

Table 2

Results of calculations for single cell for different values of fuel mass flow and U_f .

Changed parameters	\dot{m}_{fuel} [kg/s]	\dot{m}_{air} [kg/s]	T [K]	U_f [-]	U_a [-]	α_{rec}	S/C	pre_r	g_e [mA/cm ²]	V_c [V]	\dot{L}_{el} [kW]	η_{el} [-]
\dot{m}_{fuel}	0,0000098	0,00015	1194,9	0.85	0.250	0,235	1.80	0.15	105,3	0,749	0,082	0,594
	0,0000163	0,00025	1238,8						175,5	0,735	0,134	0,583
	0,0000229	0,00035	1269,7						245,8	0,725	0,185	0,575
	0,0000294	0,00045	1294,1						316,0	0,717	0,235	0,569
	0,0000360	0,00055	1314,8						386,2	0,711	0,284	0,564
U_f	0,0000299	0,00035	1390,6	0,65	0.250	0,235	1,56	0.15	258,4	0,654	0,175	0,417
	0,0000278		1350,2	0,70			1,63		255,1	0,677	0,179	0,459
	0,0000259		1316,6	0,75			1,69		251,9	0,695	0,182	0,499
	0,0000243		1289,7	0,80			1,75		248,8	0,712	0,183	0,538
	0,0000229		1269,7	0,85			1,80		245,8	0,725	0,185	0,575
	0,0000216		1258,6	0,90			1,86		242,8	0,736	0,186	0,610

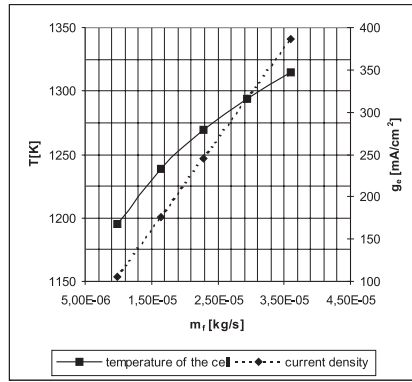


Figure 3. Increase of temperature of the cell with increase of fuel mass flow.

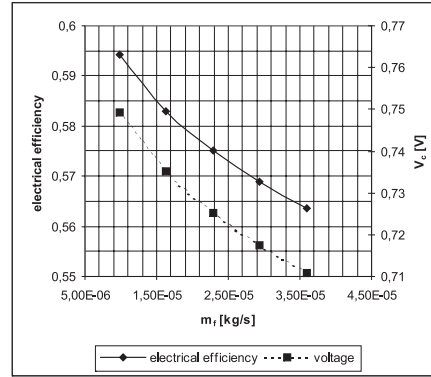


Figure 4. Decrease of the LHV and the cell with increase of fuel mass flow.

Increase of the fuel mass flow causes increase of temperature of the cell and decrease of electrical efficiency (LHV) and the cell voltage (Figs. 3 and 4).

In the second example, calculations of the single cell for the different fuel utilization coefficient value U_f and constant air mass flow for which temperature of single cell is equal to 1273 K were done. The other coefficients remain the same (Tab.2).

The fuel utilization factor has a decisive effect on the electrical efficiency of the SOFC module, because it determines the number of mole of hydro-

gen, which reacts in the electrochemical reaction. This reaction is mainly responsible for the value of current. With increasing U_f , the temperature of the fuel cell decreases, because more of hydrogen is utilized in the electrochemical reactions. Also with increasing U_f the voltage has to increase and the current decreases in the cell, what is shown in Fig. 5 and Fig. 6.

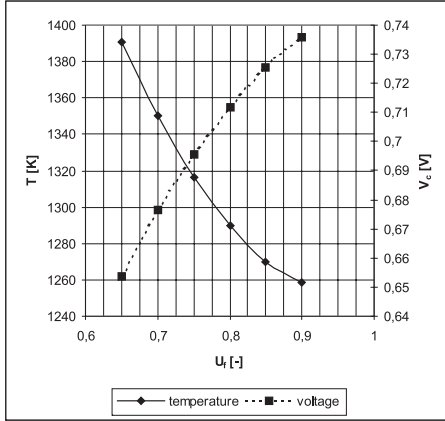


Figure 5. Temperature and voltage of the cell for different values of U_f .

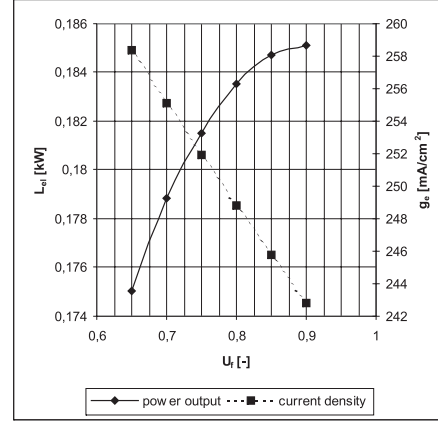


Figure 6. The cell power output and current density for different values of U_f .

In the following example for the constant air mass flow and the fuel mass flow and different values of fuel recirculation coefficients α_{rec} (Fig. 7 and Fig. 8) calculations were done. With the growth of α_{rec} temperature of the cell increases, because recirculated stream consists of more combustible elements, which are burnt during post-combustion. Voltage of the single cell is almost constant, but current is bigger for higher values of α_{rec} . Thus, the cell power output increases. For higher values of α_{rec} , recirculated stream consists of more steam, so the S/C values are bigger (Tab. 3).

As it is shown in Fig. 9 and Fig. 10, the growth of value U_a causes the growth of temperature in the fuel cell, as bigger coefficients U_a require more fuel supply. For bigger U_a the voltage of the cell is lower and the current is greater. However, the single fuel cell has more power output.

In the last example, for air mass flow and fuel mass flow given in Tab. 2, calculations for pressure $p = 10$ bar were performed (Fig. 11).

For higher pressure in the fuel cell more voltage and electrical efficiency

Table 3

Results calculations of single cell for different values of α_{rec} and U_a .

Changed parameters	\dot{m}_{fuel} [kg/s]	\dot{m}_{air} [kg/s]	T [K]	U_f [-]	U_a [-]	α_{rec}	S/C	pre_r	g_e [mA/cm ²]	V_c [V]	\dot{L}_{el} [kW]	η_{el} [-]
α_{rec}	0,0000229	0,00035	1268,0	0,85	0,250	0,205	1,51	0,15	244,6	0,725	0,184	0,572
			1269,7			0,235	1,80		245,8	0,725	0,185	0,575
			1271,7			0,265	2,13		246,9	0,725	0,186	0,578
			1273,6			0,295	2,48		248,1	0,725	0,187	0,581
			1276,4			0,325	2,86		249,3	0,725	0,188	0,583
U_a	0,0000137	0,00035	1192,4	0,85	0,15	0,235	1,8	0,15	147,5	0,740	0,113	0,587
	0,0000183		1233,7		0,20				196,6	0,732	0,149	0,581
	0,0000229		1269,7		0,25				245,8	0,725	0,185	0,575
	0,0000275		1302,1		0,30				294,9	0,719	0,220	0,570
	0,0000320		1331,5		0,35				344,1	0,714	0,255	0,566

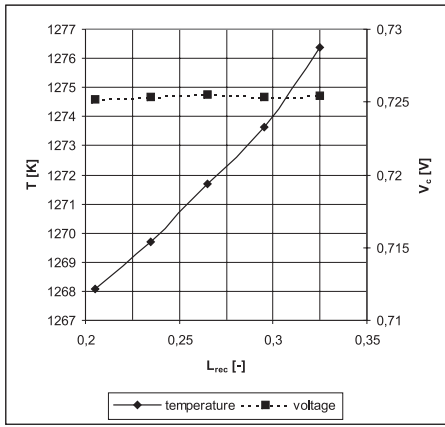


Figure 7. Temperature and voltage of the cell for different values of α_{rec} .

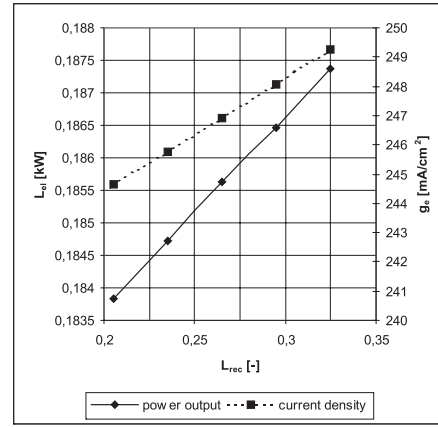


Figure 8. The cell power output and current density for different values of α_{rec} .

is obtained, which is shown in Fig. 11.

6 Conclusions

The mathematical model of tubular SOFC module with internal reforming has been presented. In spite of its zero-dimensional description the model gives very well approximated results [11]. Using this model one can expect, that the fuel cell has the biggest electrical efficiency for the

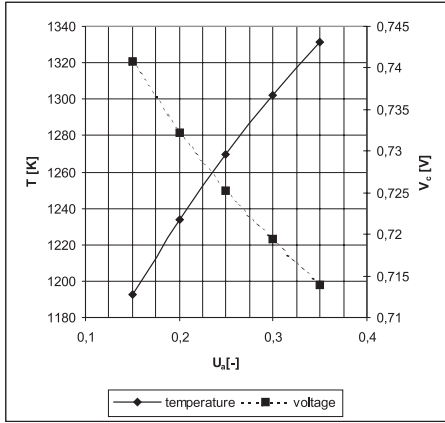


Figure 9. Temperature and voltage of the cell for different values of U_a .

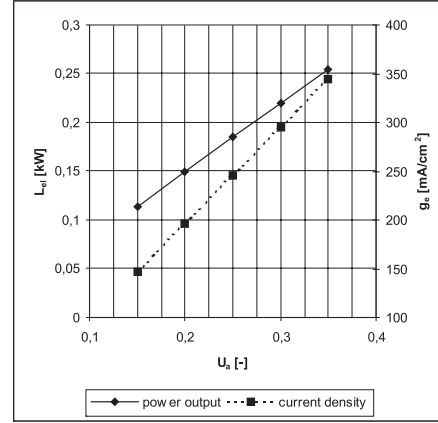


Figure 10. The cell power output and current density for different values of U_a .

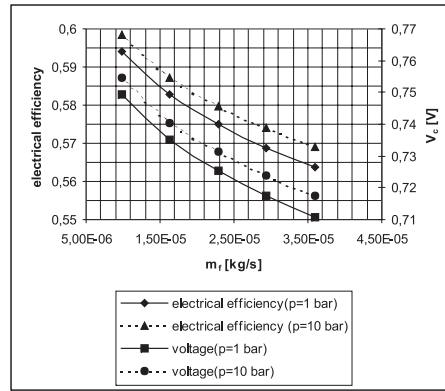


Figure 11. Single fuel cell parameters for different pressure.

higher fuel utilization factor. In the literature the optimum value has been approximated to yield about $U_f=0.85$. The fuel cell has bigger electrical efficiency for the higher pressure, so it can be used with gas turbine in a hybrid system. Electrical efficiency (LHV) for the real parameters has been approximated by about 50-60%. The parametric analysis of the tubular SOFC module behavior yields a detailed insight on the influence of each

variable on the cell efficiency and electric power output important for a future optimal design hybrid fuel cell – gas turbine systems [1]. The presented model of the solid oxide fuel cell will be integrated to the COM-GAS code and in the future it will be used for a complex thermodynamic and energy analysis of installations based on gas turbines and SOFC modules.

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References

- [1] VEYO S.E., SHOCKLING L. A., DEDERER J. T., GILLETT J. E., LUNDBERG W. L.: *Tubular solid oxide fuel cell/ gas turbine hybrid cycle power systems*, Status, ASME J. of Eng. for Gas Turbines and Power, 124, 2002, 845-849.
- [2] RAO A.D., SAMUELSEN G.S.: *Analysis strategies for tubular solid oxide fuel cell based hybrid systems*, ASME J. of Eng. for Gas Turbines and Power, 124, 2002, 503-509.
- [3] KIMIJIMA S., KASAGI N.: *Performance evaluation of gas turbine-fuel cell hybrid micro generation system*, Proc. ASME TURBO EXPO, GT-2002-30111, 2002, 1-10.
- [4] MASSARDO A.F., LUBELLI F.: *Internal reforming solid oxide fuel cell-gas turbine combined cycles: Part A-Cell Model and cycle thermodynamic analysis*, ASME J. of Eng. for Gas Turbines and Power, 122, 2000, 27-35.
- [5] CHOW A., WYSZYNSKI M. L.: *Modeling the monolithic exhaust converter/fuel reformer reactor-a zonal approach*, SAE Paper 880282, 2002, 1-23.
- [6] GEMMEN R. S., ROGERS W. A., PRINKEY M.T.: *Application of a computational fluid dynamics code to fuel cells – integrated SOFC fuel cell and post oxidizer*, www.fluent.com, TN128, 2002, 1-10.
- [7] BESSETTE N. F.: *Modeling and Simulation for SOFC Power Systems*, PhD Dissertation, Georgia Institute of Technology, 1994, 1-212.
- [8] CAMPANARI S.: *Thermodynamic model and parametric analysis of a tubular SOFC module*, J. of Power Sources, 92, 2001, 26-34.
- [9] IWATA M., HIKOSAKA T., MORITA M., IWANARI T., ITO K., ONDA K., ESAKI Y., SAKAKI Y., NAGATA S.: *Performance analysis of planar – type unit SOFC considering current and temperature distributions*, Solid State Ionics, 132, 2000, 297-308.
- [10] TOPOLSKI J.: *Combustion diagnosis within combined gas-steam cycles*, PhD Dissertation, Institute of Fluid-Flow Machinery, PAF, Gdańsk, 2002, 1-204 (in Polish).
- [11] TOPOLSKI J., LEMAŃSKI M., BADUR J.: *Mathematical model of the pressurized SOFC with the COM-GAS code*, Heat and Power Problems Conf., 1-10, Warszawa, 12-13.12.2003, (in Polish).
- [12] BADUR J., LEMAŃSKI M.: *Inverted Brayton Cycle- an efficient tool for recovery of waste heat*, Energetyka Ciepłota i Zawodowa, 221, 2003, 46-48 (in Polish).

- [13] LEMAŃSKI M.: *Detailed balances of enthalpy and chemical species in the tubular SOFC*, Report of the IFFM, No. 3175/2003, 1-26 (in Polish).
- [14] ZANON F., LAZZARETTO A.: *A tubular solid oxide fuel cell model*, <http://www.efpe.org>
- [15] <http://www.siemenswestinghouse.com/en/fuelcells/hybrids/index.cfm>