THERMODYNAMIC OPTIMIZATION OF THE SOLID OXYDE FUEL CELL ELECTRIC POWER

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The object of the present work is the optimization study of the solid oxide fuel cell (SOFC) using a thermodynamic model; a particular attention is given to maximizing the produced power density by a single cell. In this study, the SOFC real delivered voltage is defined by the Nernst potentials and overpotentials due to the activation polarizations of the chemical reactions in the anode and the cathode, the losses due to the species concentration in these two electrodes (anode and cathode), and the ohmic losses caused by the Joule's effect in the electrolyte and both electrodes. The obtained results show that the SOFC power density is proportional to the variations of the operating temperature and the oxygen concentration in the oxidizer; conversely, it is inversely proportional to the evolutions of the fuel humidification and the thicknesses of the electrolyte, cathode and anode. The operating temperature and the electrolyte thickness are the most influential parameters on the power density; conversely, the cathode and anode thicknesses are the least influential parameters on the power density.

Keywords: SOFC, thermodynamic study, power density, optimization of fuel cells operation

1. Introduction

The fuel cell is one of clean energy production vectors. SOFC belongs to the fuel cell family, it is characterized by a high overall efficiency (90%), a solid electrolyte and a high operating temperature (600-1050°C). The high overall efficiency and operating capability of various fuels of the SOFCs gave a very good status between the renewable energies family. Current development research of SOFCs is focused on maximizing the energy produced by electrochemical cells or fuel cell systems and on reducing the high operating temperature that affecting the cell components in several ways to improve the lifetime of this technology.

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Several studies are carried out on this subject. The energetic production optimization of SOFCs has been conducted by several researchers in this domain using several optimization methods. The most widely used methods can be divided into three categories: deterministic, meta-heuristic and stochastic methods [1].

Wen et al. [2] have realized a numerical simulation in the microstructure level to optimize the electrical power of a single SOFC cell using a deterministic method. Goyal et al. [3] have used a deterministic method to optimize the solid oxide fuel cell combined with a proton exchange membrane fuel cell SOFC-PEMFC system power generation. Cheddie [4] has presented a thermo-economic study that is based on a stochastic method to obtain the energy production minimum cost of an indirectly coupled SOFC. Francois et al. [5] have proposed a real-time optimization according to a stochastic method to optimize SOFC electrical efficiency.

Moller et al. [6] have used a genetic algorithm based on a meta-heuristic method for optimization of several operating parameters of the coupled system, solid oxide fuel cell combined with a gas turbine (SOFC-GT), in an autonomous power system. Shi et al. [7] have studied the microstructure optimization by a meta-heuristic method to obtain the electrodes optimum porosity (pore size and porosity distribution) to maximize the cell output power.

In previous works [8-18] we have reported various studies of the SOFCs operation. In [8] the thermodynamic analysis was used to obtain the influence and behavior of all overpotentials (ohmic, concentration and activation) on the produced power density by SOFCs.

In [9], the thermoelectric performance of the intermediate temperature solid oxide fuel cell (IT-SOFC) has been obtained by a one-dimensional model based on the finite volume method. Heat is generated by the chemical loss due to the internal chemical reaction and the ohmic loss due to Joule's effect. In [14], the hydrogen consumption and the power density of the planar SOFC are studied by a one-dimensional model using the finite difference method. The influences of the input parameters, such as the operating temperature, operating pressure, flow rates and mass fractions of chemical species were analyzed.

In [10], the anode thickness influence on the water and hydrogen distribution has been evidenced in the planar SOFC heart using the finite difference method (FDM) in the perpendicular plane to the gas flow directions. In the reference [11] the effect of internal chemical reactions on the temperature field at an anode supported planar solid oxide fuel cell (AS-SOFC) was numerically studied by the aid of a two-dimensional mathematical model.

The reference [12] showed a numerical study of the determination and location of the maximum temperature in all cell parts (electrolyte, electrodes and interconnectors) of a planar AS-SOFC, in a perpendicular plane to the reactive gas

flow under the effects of different polarizations: concentration, ohmic and activation. The reference [13] represents an analysis of the thermal behavior during the SOFC operation. Heat production and its distribution in all porous and solid parts of a planar AS-SOFC under the effect of various overpotentials (activation, ohmic, chemical and concentration), in the perpendicular plane to the reactive gas flow direction were determined.

Reference [15] showed a comparison of the heat distribution between two planar SOFC configurations (one with anode supported and the other one with electrolyte supported) depending on the gas supply temperature for both cases with and without the heat source (activation, ohmic, chemical and concentration). In [16], the effect of molar fractions of chemical species of the fuel (CH_4, H_2, CO, CO_2 and H_2O) on the heat distribution in the perpendicular plane to the reactive gas flow direction of the planar AS-SOFC was studied. The generation and absorption processes of heat due to the direct internal reforming are discussed. Reference [17] also showed the produced heat distribution by the direct internal reforming depending on the pressure and temperature of the fuel in all components of a planar AS-SOFC. In [18], a comparative study of the heat generation by the Joule's effect in the three geometric configurations of the planar SOFC (electrolyte supported, anode supported, and cathode supported) was presented.

In this work, we present a thermodynamic study of the solid oxide fuel cell. The maximum power density produced by SOFC is determined via the mathematical model which was implemented in FORTRAN language. The graphical method uses the SOFC physical and dimensional parameters: operating temperature, water and oxygen concentrations, electrolyte thickness, anode thickness and cathode thickness to optimize the delivered electric power.

2. Thermodynamic model

The SOFC operating voltage (V) is defined by the following difference:

$$V = E_{Nernst} - Losses, \tag{1}$$

E_{Nernst} is the SOFC theoretical voltage calculated from the Nernst potential between both anode and cathode, which represents the maximum voltage (open circuit voltage) of the SOFC; it is given by the following equation [19]:

$$E_{Nernst} = \frac{R.T}{n.F} ln(k) + \frac{R.T}{n.F} \left[ln \left(\frac{P_{H_2}.P_{O_2}^{0.5}}{P_{H_2O}} \right) \right], \tag{2}$$

R is the gas constant, T is the operating temperature, n is the transferred electrons number, F is the Faraday number, P_i is the partial pressure of each species i. The

parameter k is a constant related to the cell reaction, it is defined by the Arrhenius equation [19]:

$$k = A.e^{\frac{-E}{R.T}} , \qquad (3)$$

In equation (3) A is a constant and E is the activation energy, their values being 0.00144 and -246 kJ/mol, respectively [19].

The losses defined by equation (1) include three types of voltage losses due to activation, concentration and ohmic overvoltages.

2.1. Ohmic losses

These voltage losses in each SOFC constituent element are given by the product of the current density (i) and the corresponding electrical resistance (r_i) according to equation (4) [8, 18]:

$$\eta_{ohm} = i.r , \qquad (4)$$

The parameter r_i is the ratio of the thickness (e) of each component of the cell heart and its electrical conductivity (σ), equation (5) [8, 18]:

$$r_i = \frac{e_i}{\sigma_i} , \qquad (5)$$

The expressions of electrical conductivity of all parts of the SOFC (the two electrodes and electrolyte) are given in the Table 1.

Table 1

Electrical conductivity of cell components

Components	$\sigma\ [\Omega^{-1}.cm^{-1}]$	References
Electrolyte	$\sigma_{ele} = 3.34 \times 10^4 \exp(-10300/T)$	[8, 12, 18]
Cathode	$\sigma_{cat} = \dfrac{4.2 \times 10^7}{T} \exp(-1200/T)$	[8, 12, 18]
Anode	$\sigma_{an} = \dfrac{9.5 \times 10^7}{T} \exp(-1150/T)$	[8, 12, 18]

2.2. Activation losses

These voltage losses are due to the activation overpotentials at both electrodes. The activation overpotential expression for each electrode is given by equation (6) [8, 20]:

$$\eta_{Act,j} = \frac{R.T}{\alpha.n.F} . \sinh^{-1}\left(\frac{i}{2.i_{0,j}}\right), \quad j = anode, cathode\,, \tag{6}$$

The parameter α is the charge transfer coefficient and the parameter i_0 is the exchange current density of each electrode which varies exponentially with temperature, equation (7) [8, 20]:

$$i_{0,j} = k_j . \exp\left(-\frac{E_j}{R.T}\right), \quad j = anode, cathode\,, \tag{7}$$

where k and E are the pre-exponential factor and the activation energy for each electrode, respectively. Their values are given in Table 2.

<div align="right"><i>Table 2</i></div>

Values of the pre-exponential factor and activation energy for the exchange current densities at both electrodes of SOFC

Anode		Cathode		References
k_{an} [A.m^{-2}]	E_{cat} [J.mol^{-1}]	k_{an} [A.m^{-2}]	E_{cat} [J.mol^{-1}]	
$6.54.10^{11} \dfrac{R.T}{2.F}$	$1.4.\,10^5$	$2.35.10^{11} \dfrac{R.T}{2.F}$	$1.37.\,10^5$	[8, 20]

2.3. Tension losses due to the concentration overpotentials

These losses are due to the inability of the system to maintain the initial species concentrations of the reactive gases in the electrolyte interfaces. Expression of concentration overpotential for each electrode is given by equation (8) [8, 21]:

$$\eta_{conc,j} = -\frac{R.T}{n.F} . \ln\left(1 - \frac{i}{i_l}\right), \quad j = anode, cathode\,, \tag{8}$$

where i_l is the limiting current of the anode and cathode, the chosen i_l values being respectively 2.99×10^4 and 2.16×10^4 A.m^{-2} [8, 21].

3. Results and discussion

A program in FORTRAN language that is based on the thermodynamic model equations has been developed locally. The code structure and procedure were described in [8]. The obtained results are presented in five sections. In the first we present the impact of operating temperature and current density on the

power density. In the second section, we show the influence of the oxygen concentration and the moisture content on the power density, for the different current densities. In the third section, we highlight the effect of the electrolyte thickness and the current density on the power density delivered by SOFC. As to the fourth section, the effects of the cathode thickness and the current density on the power density are exposed. Finally, the impacts of the anode thickness and current density on the power density are presented.

Fig. 1 shows the effect of the operating temperature and the current density on the power density of a supported electrolyte in the SOFC. The building materials are: nickel oxide–yttria stabilized zirconia (Ni-YSZ) for the anode, lanthanum strontium manganite (LSM) for the cathode and yttria stabilized zirconia (YSZ) for the electrolyte. The thicknesses of cell heart elements are identical to 100 μm for the electrodes and 50 μm for the electrolyte. The fuel is humidified hydrogen (low molar fraction X_{H2O} = 0.05), and the oxidizer is air (oxygen content X_{O2} = 0.21), the supply pressure being common for these both gases (1 bar).

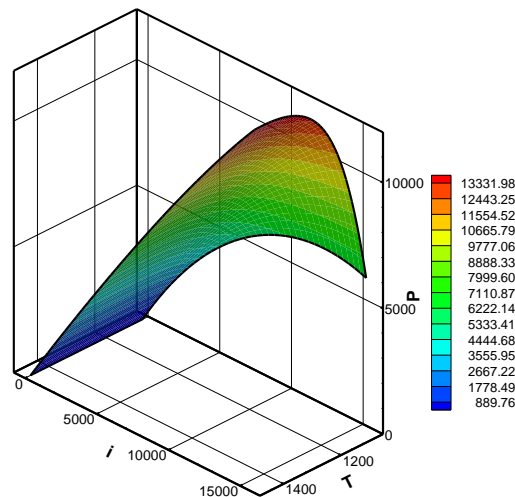Fig. 1. Power density P (W.m^{-2}) evolution vs. the operating temperature T (K) and current density i (A.m^{-2}).

It is clearly remarkable in Figure 1 that the maximum values of the power density are obtained for the maximum values of the current density. Figure 1 shows that the maximum values of the power density correspond to the maximum temperature values and the minimum values of the power density correspond to the minimum temperature values. Thus, we can consider that both voltage and power density are proportional to the operating temperature.

Fig. 2 shows the effect of the hydrogen water content and the oxidizer oxygen concentration on the SOFC power density. The building materials are Ni-

YSZ for the anode, LSM for the cathode and YSZ for the electrolyte, and the cell heart elements thicknesses are identical to 100 μm for the electrodes and 50 μm for the electrolyte. The supply pressure is common for these both gases (1 bar). The SOFC operating temperature is 1073 K.
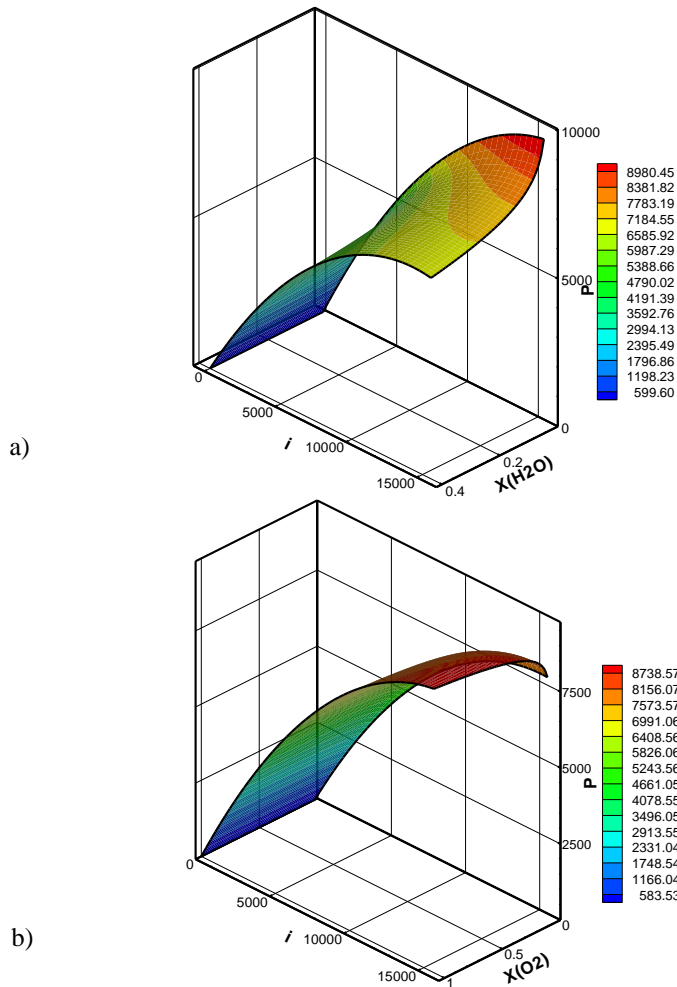

Fig. 2. Power density P (W.m^{-2}) evolution vs. species concentrations X (as mole fractions) and current density i (A.m^{-2}) at 1073 K for:
(a) water in the fuel; (b) oxygen in the oxidizer

Fig. 2.a shows that the maximum values of the power density correspond to the maximum values of the current density and to a minimum fuel humidification rate. The minimum values of the power density are obtained by a maximum fuel humidification rate, meaning that the power density of the solid oxide fuel cell is inversely proportional to the fuel humidification rate. Therefore,

the SOFC delivered voltage and voltage calculated from Nernst potential are inversely proportional to the fuel humidification rate.

In Fig. 2.b the maximum values of the power density are situated at the largest current density values. The maximum values of the power density correspond to the maximum oxygen concentration rate in the oxidizer and the minimum values of the power density correspond to the minimum oxygen concentration rate in the oxidizer. Therefore, the SOFC power density is proportional to the oxygen concentration in the oxidizer and also the SOFC delivered voltage and voltage calculated from Nernst potential are proportional to the oxygen concentration rate.

Fig. 3 shows the effect of the electrolyte thickness and the current density on the power density of a SOFC. The building materials are Ni-YSZ for the anode, LSM for the cathode and YSZ for the electrolyte. The thicknesses of the anode and cathode are of 100 μm .The fuel is humidified hydrogen (X_{H2O} = 0.05), and the oxidizer is air (X_{O2} = 0.21). The supply pressure is common for these both gases (1 bar). The SOFC operating temperature is 1073 K.

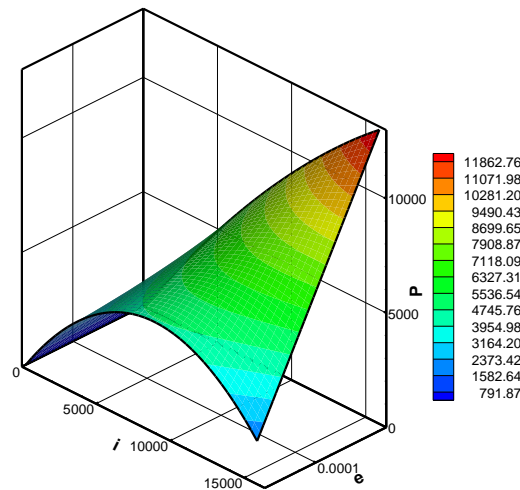Fig. 3. Power density P (W.m^{-2}) evolution vs. the electrolyte thickness e (m)
and current density i (A.m^{-2}) at 1073 K

It is clearly remarkable in Fig. 3 that the maximum values of the power density are obtained at the maximum values of the current density. Fig. 3 also shows that the maximum values of the power density correspond to the minimum electrolyte thickness. The minimum values of the power density correspond to the maximum electrolyte thickness. Thus, we can consider that both voltage and power density are inversely proportional to the electrolyte thickness.

The results presented in Fig. 4 show the effect of the anode thickness and current density on the power density variation. The building materials are Ni-YSZ

for the anode, LSM for the cathode and YSZ for the electrolyte. The anode and electrolyte thickness are respectively 100 μm and 50 μm. The fuel is the humidified hydrogen (X_{H2O} = 0.05), and the air (X_{O2} = 0.21) is the oxidant, the supply pressure is common for the fuel and air (1 bar). The cell operating temperature is identical to 1073 K.

Fig. 4 shows that the maximum values of the power density correspond to the maximum values of the current density. The maximum values of the power density are obtained by a minimum cathode thickness values and the minimum values of the power density are obtained by a maximum cathode thickness values. Thus, we can state that the power density of the solid oxide fuel cell is inversely proportional to the cathode thickness.
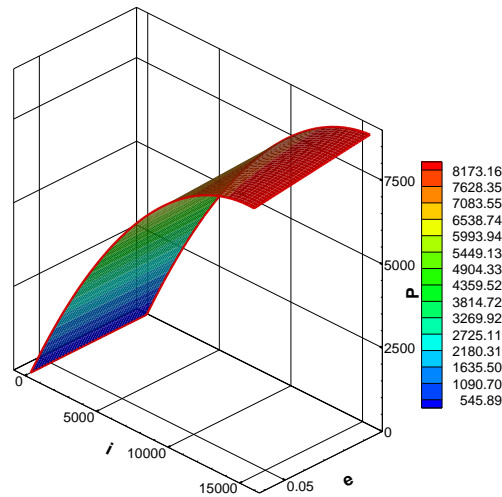

Fig. 4. Power density P (W.m^{-2}) evolution vs. the cathode thickness e (m)
and current density i (A.m^{-2}) at 1073 K

Fig. 5 shows the effect of the anode thickness and the current density on the SOFC power density, the building materials are Ni-YSZ for the anode, LSM for the cathode and YSZ for the electrolyte, the cathode and electrolyte thickness are respectively 100 μm and 50 μm. The fuel is humidified hydrogen (X_{H2O} = 0.05), and the oxidizer is air (X_{O2} = 0.21) is the oxidizer. The supply pressure is common for these both gases (1 bar). The SOFC operating temperature is 1073 K.

The maximum values of the power density are situated at the largest current density values. The maximum values of the power density correspond to the minimum anode thickness values and the minimum values of the power density correspond to the maximum anode thickness values. The SOFC real delivered voltage is inversely proportional to the anode thickness. SOFC power density is also inversely proportional to the anode thickness.
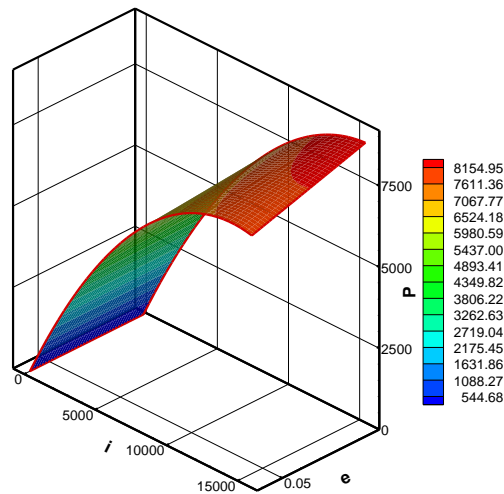
Fig. 5. Power density P (W.m^{-2}) evolution vs. the anode thickness e (m)
and current density i (A.m^{-2}) at 1073 K

6. Conclusions

The solid oxide fuel cell is an electrochemical device that converts the chemical energy of a reaction to the thermal and electrical energies. In the present study an optimization study of the produced electric power by SOFCs is presented. A program in FORTRAN language that is based on the thermodynamic model equations has been developed locally. According to the analysis of the obtained results, it appears that the realized code can be used as a design tool for the optimization of the produced electric power by SOFCs. The main obtained results of this work are:

-The SOFC power density is proportional to the operating temperature and the oxygen concentration in the oxidizer.

-The SOFC power density is inversely proportional to the fuel humidification and the thicknesses of electrolyte, cathode and anode.

-The operating temperature and the electrolyte thickness are the most influential parameters on the power density; conversely, the cathode and anode thicknesses are the few influential parameters on the power density.

R E F E R E N C E S

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