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SOFC fuel cell heat production: Analysis

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Abstract

In the present work the effect of various heat sources on the temperature field within an Anode Supported Planar Solid Oxide Fuel Cell (ASP-SOFC) is studied. In order to describe the thermal behavior within the SOFC during its operation, the coupling of the mass and energy transport phenomena along with the electrochemistry is required. More precisely, the subject of the present analysis is the visualization of the temperature field and the location of the highest temperatures within an ASP-SOFC fed with hydrogen and air. The studied parameters are: i) the temperature values of the reactants and ii) the different types of the heat sources; due to the over potentials, the Joule effect and the water formation. The complex system of the governing equations is numerically solved with the finite differences method and the temperature field within each domain of the ASP-SOFC is calculated via a mathematical model implemented in FORTRAN language. The mathematical model predictions for the temperature gradient within the ASP-SOFC under the influence of the studied parameters are thoroughly discussed.

Keywords: Fuel cell, SOFC, heat, temperature, heat source

1. Introduction

In the literature there are many theoretical works concerning the study of the various heat sources effect on the heat transfer within a Solid Oxide Fuel Cell. More precisely, in the work of Y. Lu et al. [1], the effect of the heat source due to a) the chemical reaction, b) the irreversibility and c) the Joule effect

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was on a flat tube SOFC was studied via a three-dimensional numerical model. Q. Wang et al. [2] also, developed a mathematical model coupling the electrochemical kinetics with fluid dynamics in order to simulate the heat and the mass transfer within an anode-supported planar solid oxide fuel cell. The SOFC was fed with a fuel which was a mixture of hydrogen (H_2), steam (H_2O), carbon monoxide (CO), carbon dioxide (CO_2) and methane (CH_4). The authors studied the effect of the heat source due to the Ohmic resistance in the cathode, the electrolyte and the anode. The heat source due to the chemical reactions is at the anode. J. Ferguson et al. [3] developed a three-dimensional mathematical model of in order to study the heat transfer in a SOFC, taking into consideration the heat conduction at the solid parts of the cell; the anode, the cathode, the electrolyte, the anodic and the cathode interconnects. As it concerns the flow channels, they considered convection in the gas flow direction and conduction from the channels to the solid parts. The heat source term was the sum of two sources; the Ohmic heating and the heat source due to the chemical reactions. C. Chaisantikulwat et al. [4] demonstrated a mathematical model for the heat transport in a SOFC by conduction. The heat source term used in the mathematical model was the sum of three heat sources; i) the heat source due to Ohmic heating which applied to the entire solid structure, ii) the heat source generated by the activation loss applied at the interfaces electrode/electrolyte and iii) the heat source due to heat loss through entropy change in the electrochemical reactions applied at the interfaces anode/electrolyte. A. Pramuanjaroenkij et al. [5] developed a mathematical model for a planar solid oxide fuel cell. The heat source term is the sum of two sources: due to Joule effect and due to radiation heating. X. Zhang et al. [6] performed a numerical study on the thermal characteristics in a tubular solid oxide fuel cell with indirect internal reformer. The heat source of energy equation was the sum of the Ohmic heat term, the heat term due to the chemical reactions and the heat term due to radiation. K. Daun et al. [7] developed a two-dimensional mathematical model in order to simulate the heat transfer in a planar SOFC. The heat generated in the SOFC components was the sum of three heat sources; i) due to the electrochemical reactions applied to the interfaces electrolyte/electrode, ii) due to the cathode and anodic loss and iii) due to the Ohmic heating in the electrolyte due to the conduction of the oxygen ions. In the work of Chnani [8], the heat sources within the SOFC were principally due to the variation of the water entropy formation and the Ohmic loss, while the heat sources due to the activation and the concentration over potentials were neglected. It was found that the produced heat in the anodic and the cathode interconnections layers was very low and thus the study of the heat generation was focused only in the electrolyte and at the interfaces electrolyte/electrode. In the work of M. Suzuki et al. [11], the heat and the mass transfer taking into account the electrochemical reactions in an anode-supported flat-tube SOFC was studied by the aid of a three-dimensional mathematical model. The only heat source taken into account during the model formulation was the one due to the Ohmic losses and it was applied in the electrolyte, the electrodes and the interconnects.

In the present work which is based on our previous works [14-15], the effect of various heat sources on the temperature field within an ASP-SOFC is studied by the aid of a mathematical model which combines the mass and the energy transport phenomena along with the electrochemistry. More precisely, the subject of the present analysis is the visualization of the temperature field and the location of the highest temperatures within the ASP-SOFC fed directly with hydrogen and air. The effect of the the temperature values of the reactants and the different types of the heat sources on the temperature distribution within the ASP-SOFC is analyzed.

2. Physical model

The schematic representation of the studied ASP-SOFC is illustrated in Figure 1. Moreover the boundary conditions and the location of the heat sources are also shown on the same figure.
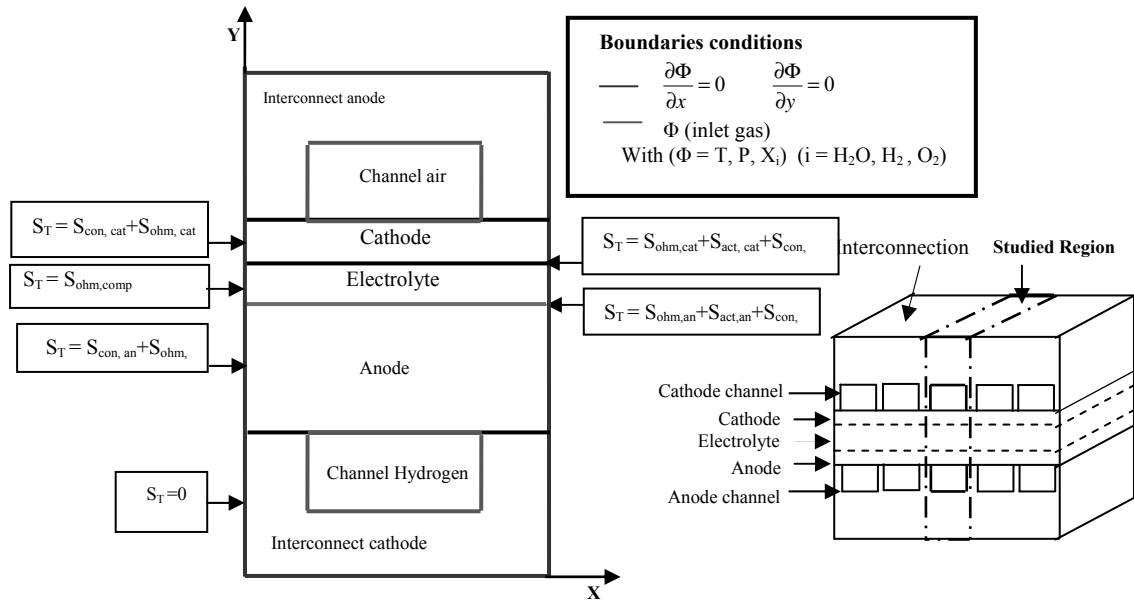
Fig.1: Physical model; Heat sources type and boundary conditions in SOFFC

3. Mathematical model

The planar SOFC temperature field is governed by the basic equations, such as the continuity conservation, the species conservation, the energy conservation and the electric potential equation. For the momentum, in the porous electrodes, the flow is modeled by using the Darcy's law. The generalized form of the steady governing equations is written as follows:

$$\operatorname{div}(\varepsilon\rho U\Phi) = \operatorname{div}(\Gamma_\Phi \operatorname{grad}\Phi) + S_\Phi \tag{1}$$

Where 'Φ' is a generalized variable, 'Γ_Φ' is the diffusion coefficient and 'S_Φ' is the source term for the general variable 'Φ'. For the continuity equation, $\Phi = 1$, $\Gamma_\Phi = 0$ and $S_\Phi = 0$. For other control equations, 'Φ' is replaced by the mass fraction of each species Xi [$\Phi = X_i$ with $i = (H_2, O_2, H_2O)$ and $\Gamma_\Phi = \rho D_{(eff,j)}$ with j = (an, cat)], the temperature T for energy equation [$\Phi = T$ and $\Gamma_\Phi = \lambda_j$ with j = (an, cat, int)] and the pressure P for pressure equation [$\Phi = P$, $\Gamma_\Phi = \kappa.\rho/\mu$ and $S_\Phi = 0$]. The heat source terms locations are visualized in Figure 1.

The heat sources taken into account in the present work are: the heat source due to the ohmic over potentials, the heat sources due to irreversibility (activation and concentration over potentials) and the heat source due to the chemical reaction. The physical properties data of the cell components as well as the properties of air and hydrogen are illustrated in Table 1-2. The expressions for the calculation of the source terms are illustrated in Table 3-4.

4. Results & Discussion

As it was previously mentioned, the mathematical model predicts the temperatures distribution within an ASP-SOFC with Ni-YSZ as anode, YSZ as electrolyte and LSM as cathode. It is well known that most of the SOFCs are operated in the temperature range from 873 K up to 1173 K.

Table 1: Air and hydrogen composition and properties [1] and [7]		
Properties	Air	Hydrogen
ρ [Kg.m-3]	0.399	0.255
Cp [J.Kg-1.K-1]	1.129	1.673
μ [Kg.m-1.S-1]	2.3.10-5	2.3.10-5
X_{O2}	0.8	0
X_{H2}	0	0.9
X_{H2O}	0.2	0.1
P [bar]	2	2

Table 2: Physical properties of the solid parts [2] and [5]				
Parameters	Anode	electrolyte	cathode	interconnects
ε %	50	/	50	/
D [m2. s-1]	3.5.10-5		7.3.10-6	
$\mathcal{K}$ [m2]	10-12	/	10-12	/
λ [W.m-1.K-1]	6.2	2.7	9.6	9.6
ρ [Kg.m-3]	3030	5160	3310	8030
Cp [J.Kg-1.K-1]	595	606	573	502
γ [Ω-1.m-2]	6,54.1011	/	2,35.1011	/
E [j.mol-1]	140.103	/	137.103	/
e [mm]	0.2	0.05	0.05	0.3

Thus, in the present study the temperature values used for the feed hydrogen and the feed air in the anode and the cathode channels are $TH_2 = T_{air}= 873$ K and $TH_2 = T_{air}= 1173$ K, while the cell current density is 20000 (A/m^2). The analysis of the temperature field is performed under the effect of the heat source due to: i) the Ohmic over potentials, ii) the irreversibility (concentrations and activation over potentials), and iii) the chemical reaction (heat source due to the water formation). According to the heat source term that is taken into account during the model formulation the temperature fields of the ASP-SOFC are as follows: At the absence of the heat source, it is shown that the maximum temperature values are located in the channels (Figure 2).

The effect of the heat source due to the Ohmic over potential (Joules effect) is remarkable for the lower gasses temperature T=873K. The maximum temperature gradient reached value is 2.2 K. The maximum temperature (T_{max}) location is in the electrolyte Figure 3a. At higher temperature T=1173K this effect becomes negligible, as it can be seen in Figure 3b. The very small increase of the temperature (0.1 K) is also found in the electrolyte.

Activation over potentials is located either at the interfaces of the electrodes/electrolyte [4] or in the electrodes [1, 13]. In the present case, the visualization of the temperature field is obtained under the heat of irreversibility resulting from: the heat source due to the concentration over potential and due to the activation over potential applied at the interfaces of the electrodes/electrolyte. According to the model predictions presented on Figure 4, it is found that the maximum temperatures are located in the electrolyte due to its fine thickness. When the gases temperature values are 873K, the maximum temperature gradient value is 0.5K within the electrolyte. Thus, it can be concluded that the feed gases play the role of a cooler for the electrolyte, Figure 4a. When feed gases temperature value is 1173K, any increasing is noted; however there is a change in the pace of the temperature distribution cf. Figure 4b. At higher temperatures both the activation and the concentration over potentials are reduced, due to the improved kinetics of the reactions and the better diffusivity of the species respectively.

The effect of the heat source due to the chemical reaction, in other words the formation of water on the temperature distribution within the ASP-SOFC is illustrated in Figure 5. Based on the model predictions it can be concluded that the maximum temperature gradient value is located in the interface between the anode and the electrolyte and at both sides at the ends of this interface. From these hot sites heat is transmitted to the other parts of the cell. It is also noticed that the absolute temperature raise at the above mentioned hot sites is smaller when the cell is fed with the gases at high temperature.

Table 3: Various expressions of the heat sources

Heat Source	SΦ expressions	η and Q_{chem} expressions	References
Heat source due to the Ohmic over potential	$S_{ohm} = \dfrac{\eta_{Ohm}}{\delta}.i$	$\eta_{Ohm} = \dfrac{e_j}{\sigma_j}.i$, j = (comp, an, cat), σ_j : (Table 4)	[2-4] [10]
Heat source due to activation over potentials	$S_{act,i} = \dfrac{\eta_{act,i}}{\delta}.i$ i = an, cat	$\eta_{act,i} = \dfrac{R.T}{\alpha.n.F}\ln\left(\dfrac{i}{i_{0,i}}\right)$, $i_{0,i} = \gamma_i\left(\dfrac{RT}{2.F}\right).\exp\left(\dfrac{-E_i}{RT}\right)$	[11-12]
Heat source due to concentration over potentials	$S_{con,i} = \dfrac{\eta_{con,i}}{\delta}.i$	$\eta_{con,an} = -\dfrac{R.T}{2.F}\ln\left(1-\dfrac{i}{i_{l,an}}\right) + \dfrac{R.T}{2.F}\ln\left(1+\dfrac{P_{H_2,car}}{P_{H_2O,car}}.\dfrac{i}{i_{l,an}}\right)$ $\eta_{con,cat} = -\dfrac{R.T}{4.F}\ln\left(1-\dfrac{i}{i_{l,cat}}\right)$ $i_{l,an} = \dfrac{2F.P_{H_2,car}.D_{eff,an}}{R.T.e_{an}}$, $i_{l,cat} = \dfrac{4F.P_{O_2,a}.D_{eff,cat}}{\left((P-P_{O_2,a})/P\right)R.T.e_{cat}}$	[5]
Heat source due to the chemical reaction	$S_{chem} = \dfrac{Q_{chem}}{2F}.\dfrac{i}{\delta}$	$Q_{chem} = -\Delta H_{f,H_2O} - 2FV$, $\Delta H_{f,H_2O} = -\left(240506 + 7.3835T\right)$ $V = E_{ideal} - \left(\eta_{ohm} + \eta_{con} + \eta_{act}\right)$ $E_{ideal}(T) = E^0(T) - \dfrac{RT}{n_eF}\ln\left[\dfrac{X_{H_2O}}{X_{H_2}X_{O_2}^{0.5}}\right]$ $E^0(T) = 1.2723 - 2.7645\times10^{-4}T$	[8], [11]

Table 4: Electric conductivities

SOFC component	σ [Ω-1 cm-1]
Electrolyte	$\sigma_{éle} = 3.34\times10^4\exp\left(-10300/T\right)$
Cathode	$\sigma_{cat} = 4.2\times10^7/T\exp\left(-1200/T\right)$
Anode	$\sigma_{an} = 9.5\times10^7/T\exp\left(-1150/T\right)$

Conclusions

In the present work, the effect of various heat sources on the temperature field at an ASP-SOFC components (electrodes, electrolyte and interconnects) is studied. More precisely, the location of the highest temperatures within the ASP-SOFC fed with hydrogen and air was found. The studied parameters were a) the temperature values of the reactants and b) the different types of the heat sources. The results of the present analysis showed the remarkable effect of the heat source when the cell is operated at low temperatures, T = 873 K. The cell operation at higher temperature eliminates the effect of the heat source. In the case that no heat source is considered, the maximum temperatures within the cell are the temperatures of the feed reactants and they exist in the flow channels. The highest temperature raises are caused by the heat source due to the chemical reaction, at both high and low feed temperatures. Furthermore, it was found that no significant raise in temperature is noted in the case of the heat source

due to concentration and activation over potentials. Finally, the Joule effect has a considerable effect especially at low gas temperatures.
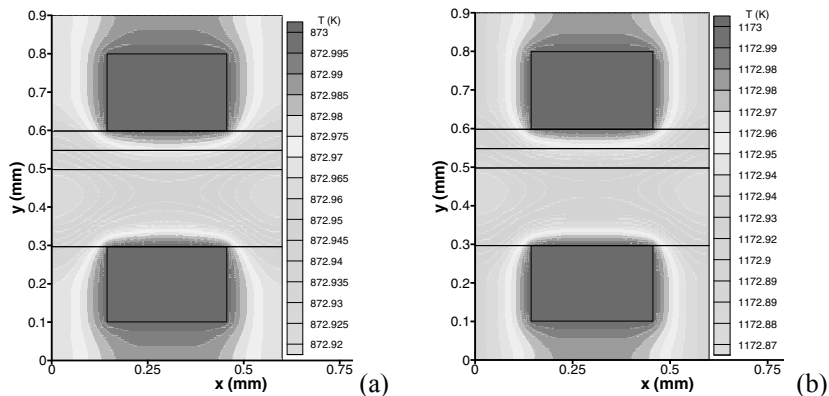

Fig. 2: ASP-SOFC Temperature field: Heat source absence. (a): T = 873 K, (b): T = 1173 K
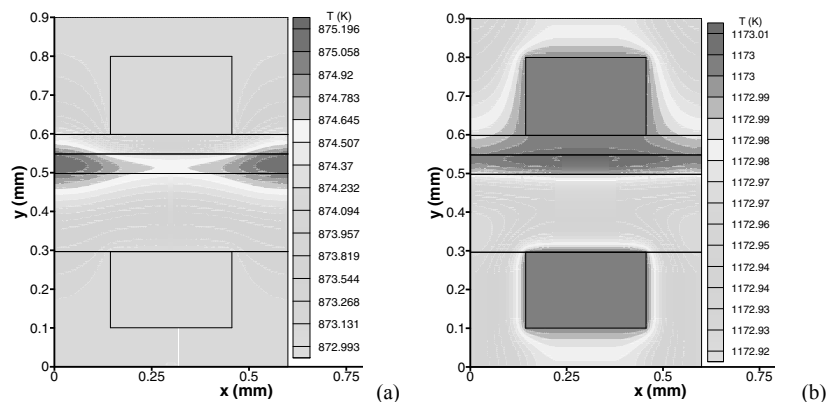

Fig. 3: ASP-SOFC Temperature field: Heat source effect due to Ohmic over potentials, (a): T = 873 K, (b): T = 1173 K
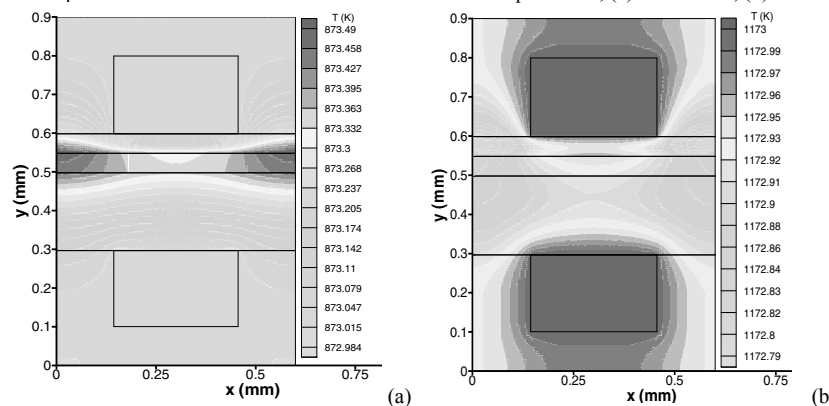

Fig. 4: ASP-SOFC Temperature field: Heat source effect due to activation and concentration over potentials, (a): T = 873 K and (b): T = 1173 K
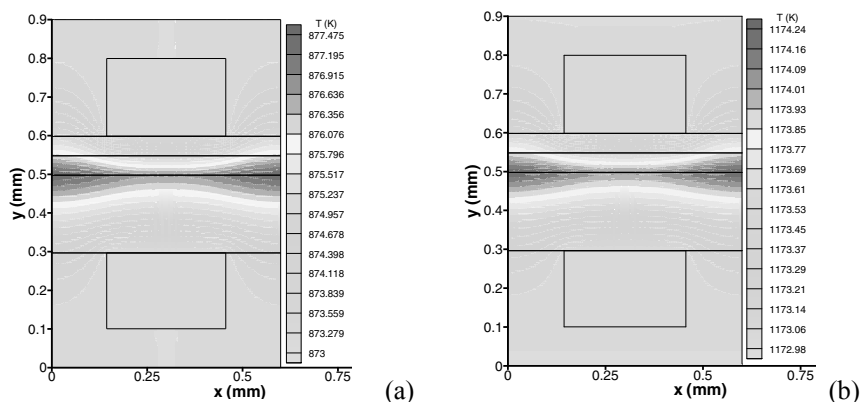
Fig. 5: Temperature field of an ASP-SOFC: Heat source effect due to the chemical reaction (a): T = 873 K, (b): T = 1173 K

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Nomenclature

Cp	fluid specific heat at constant pressure	$[J.Kg^{-1}.K]$
D_{eff}	effective diffusion coefficients	$[m^2.s]$
e	thickness of each component	$[\mu m]$
$E°$, E_{ideal}	standard potential, ideal potential	$[V]$
Ei	activation energy of anode and cathode	$[J.mol^{-1}]$
F	faraday constant	$[C.mol^{-1}]$
i_0	exchange current density	$[A.m^2]$
i	current density	$[A.m^2]$
p	pressure	$[Pa]$
p_k	partial pressure of the species k	$[Pa]$
R	perfect gas constant	$[J.mol^{-1}.K]$
S	heat source	$[W.m^3]$
T	temperature	$[K]$
V	cell Tension	$[V]$
U	velocity	$[m.s^{-1}]$
X	species mass fraction (i=H2, H2O, O2) , O2)	/
ΔH	enthalpy Variation	$[J.mol^{-1}]$
δ	zone thickness e where heat is produced	$[mm]$
σ	electrical conductivity	$[\Omega^{-1}.m^{-1}]$
η	over potential	$[V]$
γ	exponential factor	$[A.m^{-2}]$
α	charge transfer Coefficient	/
λ	thermal conductivity	$[W.m^{-1}.K^{-1}]$
ρ	density	$[Kg.m^{-3}]$
ε	porosity	%
$\kappa\,[m^2]$	permeability	$[m^2]$
μ	viscosity	$[Kg.m^{-1}.S^{-1}]$
an, cat, ele	Anode, cathode, electrolyte	
Ohm, act, con, chem, T, tot	Ohm, activation, concentration, chemical, thermal, total	