

Simulation and Characterization of SOFC Fuel Cell Model

Abstract. The SOFC fuel cell is one of the so-called solid electrolyte fuel cells that operate at high temperatures of 650 to 1200°C. This temperature level is necessary for the solid electrolyte to have sufficient ionic conductivity. This high temperature causes a very high heat exchange between the various components of the SOFC. In the 1-D model, the fuel cell is usually treated as a set of layers including interconnects, air channel, electrodes, electrolyte, and fuel channel both gas composition and flow rate in each channel are assumed to be constant, and their mean values are used in the simulation.

Streszczenie. Ogniwo paliwowe SOFC należy do tzw. ogniw paliwowych ze stałym elektrolitem, które pracują w wysokich temperaturach od 650 do 1200°C. Ten poziom temperatury jest konieczny, aby elektrolit stały miał wystarczającą przewodność jonową. Tak wysoka temperatura powoduje bardzo dużą wymianę ciepła pomiędzy poszczególnymi elementami SOFC. (Symulacja i charakterystyka modelu ogniwa paliwowego SOFC)

Keywords: SOFC, Fuel Cell, electrolyte, 1-D model, Layers.

Słowa kluczowe: SOFC, ogniwo paliwowe, elektrolit, model 1-D, warstwy.

Introduction

Fuel cells can directly convert chemical energy to electricity using electrochemical reactions and have higher efficiency than conventional, combustion-based power systems. The higher efficiency coupled with a reduction in harmful emissions makes them environmentally friendly power sources [1, 2]. Solid Oxide Fuel Cell (SOFC) systems use a ceramic electrolyte-based fuel cell and operate at high temperatures (> 650 °C). They are fuel-flexible and are particularly attractive for stationary and mobile applications [3, 4].

SOFC technology is a promising technology; it is essentially based on the use of a solid electrolyte (e.g. ceramic electrolyte) and a high temperature. Compared to low and medium temperature cells, it is potentially more interesting due to its high electrical efficiency (50% to 70%), less sensitivity to the type of fuel, the replacement of precious metals in the electrodes by other cheaper ones, possible internal reforming and the use of the heat produced (cogeneration) [5,6,7].

The principle is very simple since from a fuel such as a hydrogen and an oxidant such as oxygen, water and electricity are products. Beyond the ecological interest that these systems have, since they do not release any greenhouse gases, they highlight the potential of hydrogen as a vector of energy for the production of electricity but also the storage of energy in chemical form. The applications are essentially referred to be decentralized energy production with electrical powers provided that can go from a few kW to a few hundred kW for several hundreds of hours for residential and urban areas [8, 9].

The main characteristic of SOFC is therefore their operating temperature (700 to 1,000 °C), which is necessary to obtain a sufficient ionic conductivity of the ceramic electrolyte. This temperature has a double advantage. Firstly, it allows the direct use of hydrocarbons, which can be easily reformed without the need for a noble metal catalyst. Secondly, it produces a high level of heat that can be easily used in cogeneration, with an efficiency of up to 80%.

But it also has a disadvantage; the heating is long and complicates any use with short and repetitive cycles (as in the case of transport). For these reasons, the technology lends itself particularly well to decentralized electricity production and cogeneration (areas covering powers ranging from 1KW to several tens of MW) [10 11,12,13]. Thanks to its high efficiency and its potential capacity to operate directly with liquid hydrocarbons, it will also find an

outlet in naval propulsion. The development of this type of cell, due to its high operating temperature and the resolution of thermo-mechanical problems of material resistance, is quite complex. One of the particularities of the SOFC is its solid electrolyte, usually, zirconium (Zr2) doped with a mole of 8 to 10% yttrium (Y3+), which acts as a conductor for the oxygen anion (O2-).

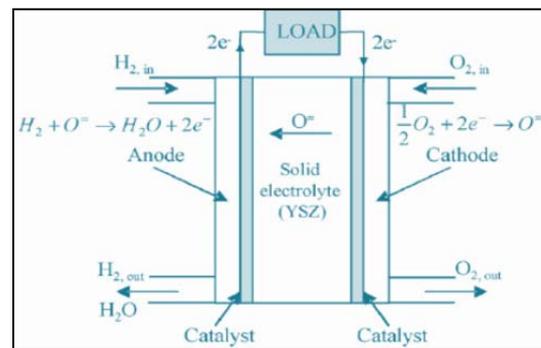


Figure.1: Schematic of a SOFC.

Single Cell Model

The ideal open circuit cell voltage is given by the Nernst equation:

$$(1) \quad V_{Nernst} = -\frac{\Delta G}{2F} - \frac{RT}{2F} \ln \left(\frac{P_{H_2O} P_{ref}^{0.5}}{P_{H_2} P_{O_2}^{0.5}} \right)$$

where ΔG is Gibbs free energy from the reaction and P_{ref} is the standard pressure 0.1 MPa. When a current is applied, the cell voltage drops due to Ohmic, activation and concentration losses, and thus the total voltage over the cell can be expressed as:

$$(2) \quad V = E_0 - iR - \eta_{Cathode} - \eta_{Anode}$$

where: E_0 : Nernst Potential of the reactions; R : Equivalent resistance value of the electrically conductive parts of the cell; $\eta_{Cathode}$: Polarization Losses in the cathode; η_{Anode} : Polarization Losses in the anode

In SOFC, it is often important to focus on Ohmic and concentration biases because high operating temperatures experience little activation polarizations. However, as the

lower limit of the SOFC operating temperature is approached (~800 °C), these polarizations become important. [14] The above equation is used to determine the SOFC voltage (in fact for the fuel cell voltage in general). This approach results in good agreement with particular experimental data (for which adequate factors have been obtained) and poor agreement for experimental working parameters other than the original ones. Moreover, most of the equations used to require the addition of many factors that are difficult or impossible to determine. This makes any process of optimizing the SOFC operating parameters as well as selecting the design architecture configuration very difficult. Due to these circumstances, a few other equations have been proposed: [15]

$$(3) \quad E_{SOFC} = \frac{E_{max} - i_{max} \eta_f \cdot r_1}{\frac{r_1}{r_2}(1 - \eta_f) + 1}$$

where: E_{SOFC} : Cell voltage; E_{max} : Maximum voltage given by the Nernst equation; i_{max} : Maximum current density (for a given fuel flow); η_f : Fuel utilization factor [15] [16]; r_1 : Specific ionic resistance of the electrolyte; r_2 : Specific electrical resistance of the electrolyte

The Losses SOFC Model

There are three major forms of polarization losses: activation, Ohmic, and concentration. A constant offset also contributes to the total polarization, which is the result of minor losses such as contact resistance, internal current, and leaks. Following [17], the offset was assumed to equal 0.07 V. The sum of the different polarizations results in the voltage drop from ideal Nernst potential to effective operating value. Since interconnect and electrodes are isopotential, the cell voltage is constant over the whole cell and can be estimated as:

$$(4) \quad V_{SOFC} = E_{Nernst}^i - V_{Act}^i - V_{Ohm}^i - V_{Con}^i$$

The total power drawn from the SOFC is calculated as:

$$(5) \quad P_{cell} = V_{SOFC} I_{SOFC}$$

Activation Loss Model

Activation losses occur at both the anode and cathode and derive from the fact that the reacting species in chemical reactions must overcome an energy barrier, i.e. the activation energy of the reaction. The activation loss shows a nonlinear current dependency related to a parameter known as the exchange current density, J_0 . For current densities $J < J_0$ the activation loss is low, typically in the order of 0.01 V, and for current densities $J > J_0$ the activation loss grows according to the Tafel equation: [19]

$$(6) \quad V_{Act}^i = \frac{RT_s^i}{\alpha(T_s^i)F} \left(\sinh^{-1} \left(\frac{J^i}{2J_0(T_s^i)} \right) \right)$$

Where α the charge is transfer coefficient and J_0 is the exchange current density.

Ohmic Loss Model

It is due to the resistance that meets the flow through the electrolyte and the electrical circuit, it is also due to the electrical resistance in the plates of dissemination (Backing). The Ohmic losses are expressed by the following equation.

$$(7) \quad V_{Ohm,k}^i = \frac{l_k}{\sigma_k(T_s^i)} J^i$$

$$V_{Ohm}^i = \sum V_{Ohm,k}^i \quad k = [Ano, Cath, Elec]$$

Conductivities are estimated utilizing correlations, proposed in the literature [17] for second-generation ceramic SOFC, in which the materials of anode, cathode, and electrolyte are, nickel-cermets, strontium-doped lanthanum manganite and yttria-stabilized zirconia, respectively:

$$\sigma_{an} = 1000$$

$$(8) \quad \sigma_{ca}(T_s) = c_1(T_s^i)^2 - c_2(T_s^i)^2 - c_3$$

$$\sigma_{el}(T_s) = c_4(T_s^i - 273)^2 - c_5(T_s^i - 273)^2 - c_6$$

Concentration Loss Model

At the level of the anode, there is a loss of potential due to the inability of the system to maintain, the initial concentration of reagents, then we have the formation of a concentration gradient. Many factors can contribute to the polarization of concentration, the low diffusion of the gas through the porous electrodes and the dissolution of the reagents. These losses are given by the following:

$$(9) \quad V_{Con}^i = -\frac{RT_s^i}{2F} \left[\frac{1}{2} \ln \left(1 - \frac{J^i}{J_{cs}} \right) + \ln \left(1 - \frac{J^i}{J_{as}} \right) - \ln \left(1 + \frac{P_{H_2}^i J^i}{P_{H_2O}^i J_{cs}} \right) \right]$$

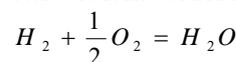
The anode and cathode limiting currents (i.e. J_{as} and J_{cs} respectively) are computed as function of species diffusion coefficients, following the approach proposed in [22].

Modelling and Simulation of the SOFC

This paper aims to present the model adopted to account for the physical phenomena in the cell. The first part of the paper is dedicated to the modelling principles applied to the chemical, thermal and electrical domains. The second part concerns the application of the modelling to the SOFC stack. The chemical and thermal modelling of the fuel cell is based on their formal analogy with the electrical domain. The temperature is similar to the voltage and the heat flow is similar to the current. Two heat sources within the cell are considered: endothermic or exothermic heat sources produced by chemical reactions and Ohmic heat sources. Furthermore, pressure is similar to voltage and flow is similar to current. The application of this analogy offers the possibility of representing physical laws within a system with electrical circuits. The use of such a representation allows the use of different techniques in the electrical domain: putting chemical and thermal models in series or in parallel, realization of the regulation of chemical or thermal quantities with the help of methods used in automation (e.g. pole compensation), ease and flexibility of integration of developed models in a global model (battery coupling or battery associated with the converter) The electrical model translates the electrochemical phenomena of each cell. The electrical model of the SOFC is based on the reversible Nernst voltage and the different voltage drops.

SOFC Output Voltage

The overall reaction in a solid oxide fuel cell is:



The Nernst equation used to calculate the reversible potential of the SOFC is:

$$(10) \quad E_{Cell} = E_{0,Cell} + \frac{R.T}{4.F} \ln \left[\frac{(P_{H_2}^{ch})^2 (P_{O_2}^{ch})}{(P_{H_2O}^{ch})} \right]$$

$E_{0,Cell}$: Consists of a constant term and a temperature-dependent term, as follows [23, 24]:

$$(11) \quad E_{0,Cell} = E_{0,Cell}^0 - K_E (T - 298)$$

$E_{0,Cell}$: The standard reference potential in the standard condition .298 K, 1 Atm.

$E_{0,Cell}^0$: Initial potential for cell.

The output voltage of the individual cells connected in series can be grouped together to obtain the output voltage of a SOFC Fuel Cell, taking into account ideal behaviour and constant temperature [25, 26, 27].

$$(12) \quad V_s = N_{Cell} V_{Cell} = E - V_{Act} - V_{Ohm} - V_{Con}$$

E_{cell} : The open circuit voltage can write as:

$$(13) \quad E_{cell} = N_{Cell} \left(E_{0,cell} + \frac{RT}{4F} \ln \left[\frac{(P_{H_2})^2 (P_{O_2})}{P_{H_2O}} \right] \right)$$

The output voltage of the SOFC Fuel Cell can also be calculated using the calculated voltage losses.

Simulation and mathematical models are certainly useful for the development of various power generation devices; however, they are even more important when it comes to the development of fuel cells. This is due to the complexity of the cells and the systems based on them, and the difficulty of the experimental characterization of their internal operation. This complexity can be explained by the fact that in the fuel cell, electrochemical reactions are tightly coupled, and also by the fact that electrical conduction, ionic conduction, and heat transfer take place simultaneously. Therefore, a complete study of the cells needs a multidisciplinary approach. The simulation of these cells allows us to focus the experimental investigations to improve the accuracy of interpolations and extrapolations of results. In addition, mathematical models can serve as valuable tools for the design and optimization of fuel cell systems. Simulations are performed on various systems using various software packages. In this research investigation, researchers were interested in the simulation process performed on the SOFC fuel cell system using MATLAB /SIMULINK. The purpose of this simulation is to estimate the fuel cell required to produce a voltage corresponding to a given load and the evolution of the power and the different pressures as a function of the current density.

Tables.1: The Simulation Parameter [30, 31]

Parameter	Value	Units
Nominal power	15	Kw
N_{Cell}	350	/
SOFC array	2x2=4	/
SOFC array power rating	17x4=68	Kw
fuel airflow	12X10 ⁻³	Mol/s
fuel Water flow	1X10 ⁻⁴	Mol/s
fuel Hydrogen flow	0.9X10 ⁻³	Mol/s
T fuel	973	K
T air	973	K
Current Density	60	A/cm ²
V_{Out}	450	V

The Structure of a Static SOFC Model [28, 29, 30]

The modelling method was applied to a SOFC model with a block diagram developed by Matlab Simulink software to obtain the electrochemical characteristics of this SOFC and varied the parameters to understand the reliability of the fuel cell

Results and Discussion

A Static model for the SOFC has been developed in MATLAB/SIMULINK, based on the electrochemical and thermodynamic characteristics of the fuel cell discussed in the previous Works. The fuel cell output voltage, which is a function of temperature and load current, can be obtained from the mode (See Appendix).

Polarization Curve

Normally the thermodynamic potential equals a theoretical 1.18 V, but the open-circuit voltage (I = 0) equals 0.94 V.

This first reduction is linked to the irreversibility of the electrochemical reactions, including the reduction of the oxygen at the cathode. In addition, for the low current densities (figure.2), whereas, reactions on the electrodes, whose importance is linked to their kinetics; generate power surges of activation (figure.4).

Then, for the linear portion of the curve, these are the losses related to electronic resistors and internal ionic (figure.5), which decrease the voltage between electrodes.

Finally, for the high current densities, c is the kinetics of dissemination of gas through the electrodes which becomes the limiting factor. This phenomenon is the loss of concentration (figure.6).

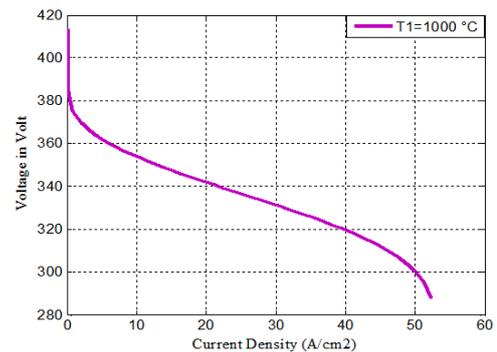


Fig..2 Current-Voltage characteristic of a Fuel Cell SOFC

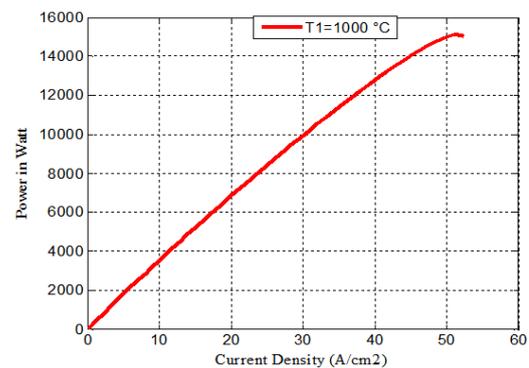


Fig. .3 Current-Power characteristic of a Fuel Cell SOFC

Figure.3 shows a polarization curve for the SOFC fuel cell. It can be seen that the characteristic starts with a no-load voltage at zero current. This behaviour is due to the effect of the polarizations which are directly connected to the current density. [32, 33].

Temperature Effect

Different temperatures, which are typical of SOFC, are shown in figure.4, figure.5. The activation voltage drop dominates the voltage drop in the low-current region figure.6. As load current increases, the Ohmic voltage drop increases fast and becomes the main contribution to the SOFC voltage drop figure.7. When load current exceeds a certain value, fuel cell output voltage will drop sharply due to the concentration voltage drop inside SOFC Figure.8. Figure.4 also shows the effect of temperature on SOFC V-I characteristics curve. SOFC output voltage is higher at a lower temperatures in the low current zone while the voltage is higher at higher temperature in the high current region.

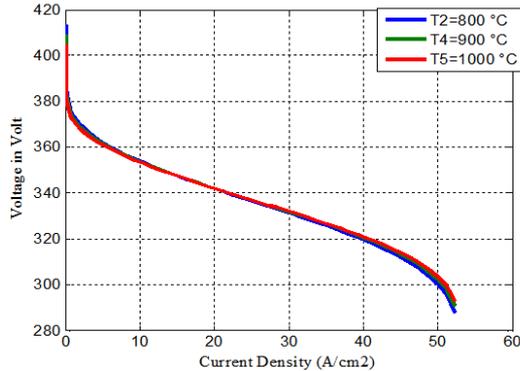


Fig.. 4 Current-Voltage characteristics for different temperatures values

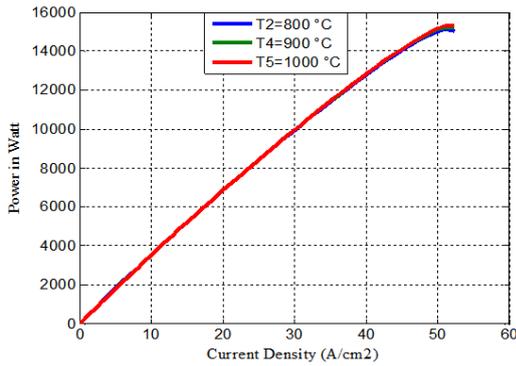


Fig..5 Current-Power characteristics for different temperatures values

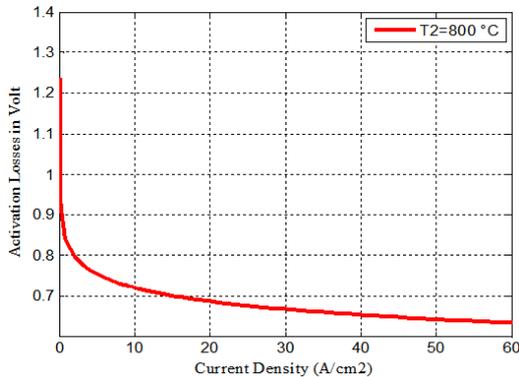


Fig. 6 Activation losses characteristics for different temperatures values

From this figure, it can be seen that increasing the temperature of the cell has a beneficial effect on the cell voltage, which is explained by the high ionic conduction of the cell (electrolyte plus electrodes) at higher temperatures (e.g. $T = 900^{\circ}\text{C}$ and $T = 1000^{\circ}\text{C}$) Figure.4. So, to ensure the proper functioning of the cell, it is necessary to increase the temperature [34, 35].

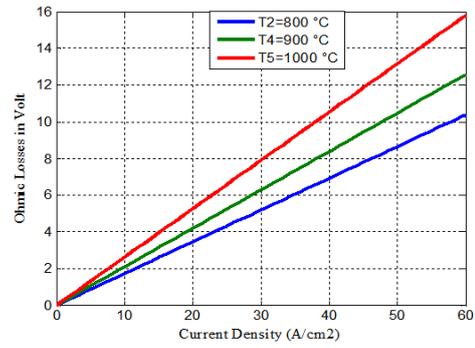


Fig. 7 Ohmic losses characteristics for different temperatures values

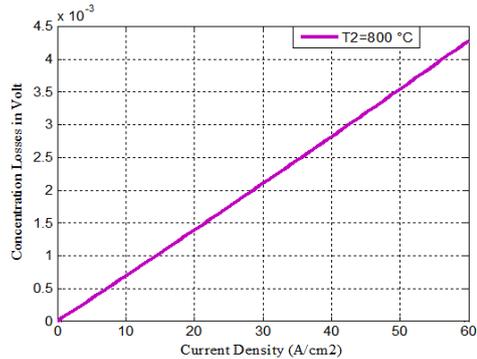


Fig. 8 Concentration losses characteristics for different temperatures values

Pressure Effect Variation of H2 Pressure

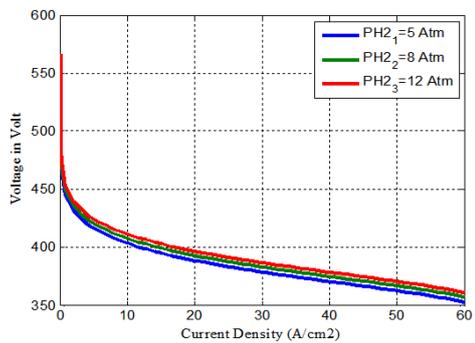


Fig.. 9 Current-Voltage characteristics for different pressures H2 values

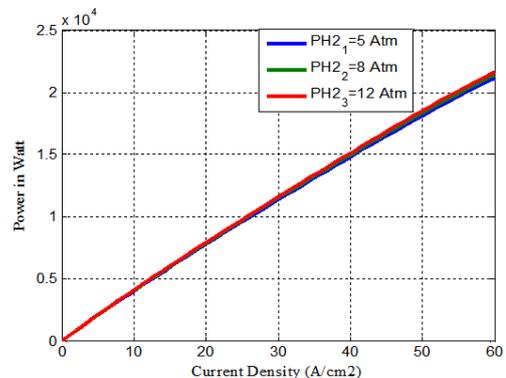


Fig.. 10 Current-Power characteristics for different pressures H2 values

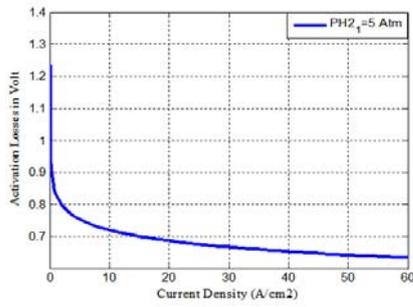


Fig. 11 Activation losses characteristics for different pressures H2 values

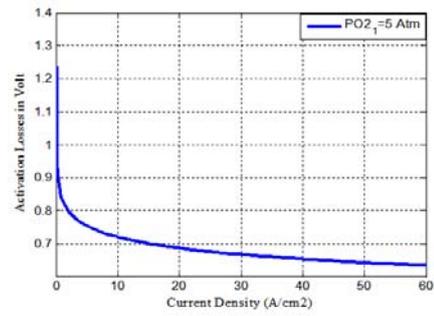


Fig.16 Activation losses characteristics for different pressures O2 values

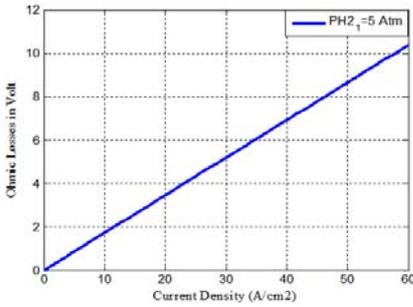


Fig. 12 Ohmic losses characteristics for different pressures H2 values

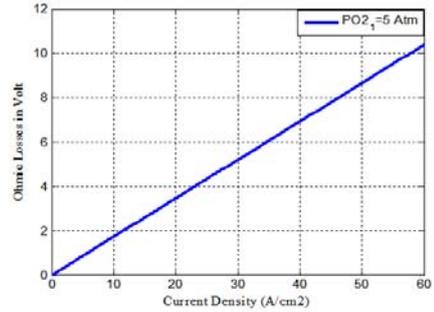


Fig.17 Ohmic losses characteristics for different pressures O2 values

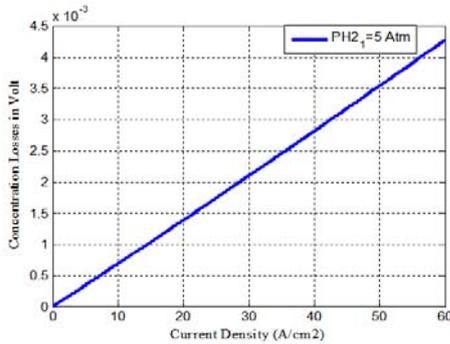


Fig. 13 Concentration losses characteristics for different pressures H2 values

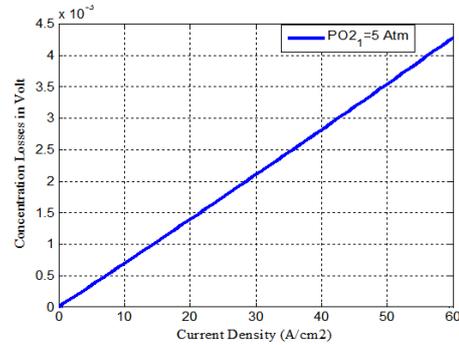


Fig.18 Concentration losses characteristics for different pressures O2 values

Variation of O2 Pressure

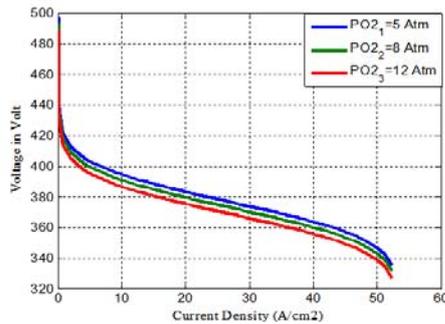


Fig. 14 Current-Voltage characteristics for different pressures O2 values

Variation of H2O pressure

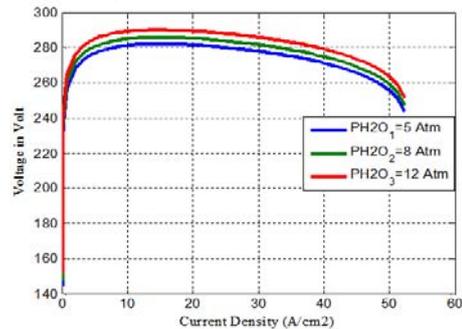


Fig. 19 Current-Voltage characteristics for different pressures H2O values

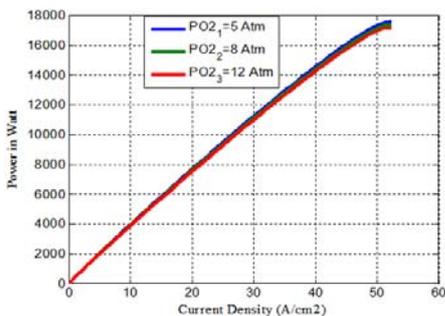


Fig. 15 Current-Power characteristics for different pressures O2 values

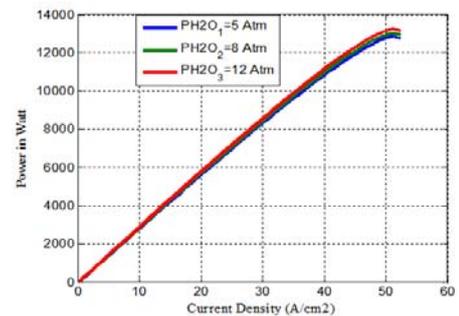


Fig. 20 Current-Power characteristics for different pressures H2O values

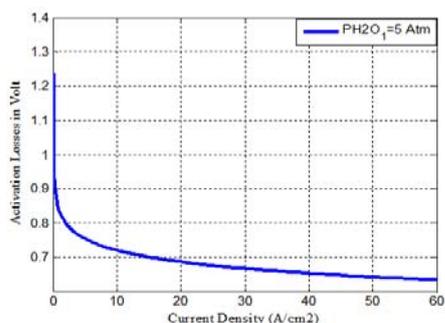


Fig. 21 Activation losses characteristics for different pressures H2O values

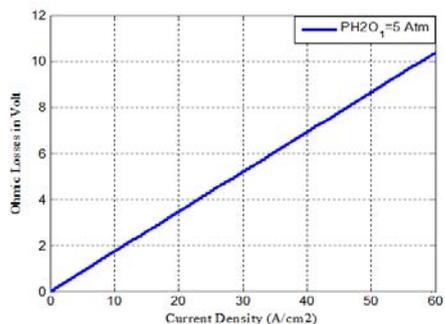


Fig. 22 Ohmic losses characteristics for different pressures H2O values

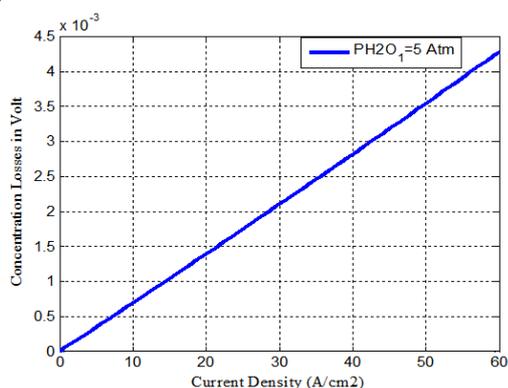


Fig. 23 Concentration losses characteristics for different pressures H2O values

The polarization curves, the curves of activation, Ohmic, and concentration overvoltage at different pressures for 800°C are shown in Figures 9,10,11,12, and 13 respectively. For flooding fault, the pressure effect corresponding to the hydrogen and oxygen at the fuel cell inlet is measured. As the pressure of hydrogen and oxygen increases, the activation losses decrease and reduce the rising current density, as shown in Figure 14,15,16,17 and figures18. Furthermore, the increasing pressure reduces the concentration losses and improves the current density, as shown in Figures 19,20,21,22 and figure23. Generally, the increase in pressure at inlet improves the fuel cell voltage and power density as shown in Figure 19. For the normal operation of the cell, this pressure is maintained at 1 Atm. During, flooding conditions, the pressure at the inlets automatically increases, resulting in cell failure. Hence, efficient monitoring of the cell is necessary for the reliable operation of the cell.

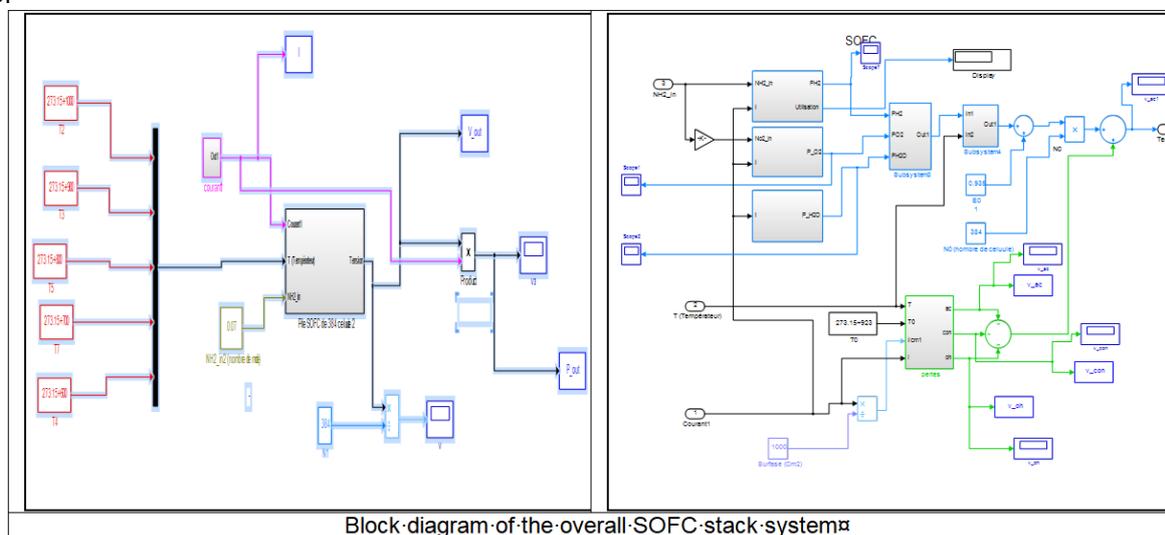
Conclusion

In the context of this work, a macroscopic modelling tool has been implemented thanks to the analogy between the electrical and thermal domains. This method constitutes a simple, scalable, and efficient modelling tool. Once the component library has been completed, we will have a complete tool for studying and optimizing the architecture of fuel cell systems, taking into account the different energy flows: electrical and thermal. Finally, we look at cogeneration systems using solid oxide fuel cells (SOFC).

As discussed in the abstract and introduction, modeling all relevant physics in a fuel cell system requires a flexible tool capable of including several physical domains in the same model. The equation based language and possibility for causal models allows for physical models, which is very useful if components are to be reused in multiple system designs with different purp.

Appendix

We model the fuel cell system with the electrochemical equations in a matlab simulink program. Here is the total diagram of the SOF



Block diagram of the overall SOFC stack system

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