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Modeling, Validation, and Operational Variables Optimization of a Solid Oxide Fuel Cell

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Abstract: Solid oxide fuel cells can generate electrical energy with electrical efficiency exceeding 50% and reduce pollutant emissions, particularly, when the fuel is hydrogen. They have numerous applications, such as stationary generation, aircraft, and hybrid plants producing hydrogen and electricity. This work uses a thermodynamics lumped model to obtain the voltage versus current density of an SOFC, and distinctively of other authors also use heuristic and deterministic optimization algorithms to determine the main operation variables to achieve maximum power for a single cell. Moreover, it also has a detailed discussion of the transport of each overpotential, particularly the concentration overpotential, along with a comprehensive set of equations for its calculation. It also connects the physical and chemical phenomena to the main modeling variables. Unlike other reviewed studies, the Butler-Volmer equation is solved using an implicit solution. The results demonstrate that higher pressures and temperatures improve power output, with both heuristic and deterministic algorithms producing similar results for maximum power. The model allows the SOFC to operate efficiently within a hybrid system and serves as a method for estimating key operating variables while assessing the influence of physical and chemical parameters on performance.

Key words: modeling, optimization, SOFC, single cell.

INTRODUCTION

Fuel cells can be described as devices that continuously work, producing electrical current by electrochemical combustion of gaseous fuel like hydrogen, methane, etc. (Wang et al. 2024, Tarôco et al. 2009). There are several types of fuel cells on the market (Qasem & Abdulrahman 2024), such as Proton-exchange membrane fuel cell and Solid oxide fuel cells (Hassan & Ticianelli 2018, Napoli et al. 2015, Carneiro et al. 2025). In addition, hydrogen can be obtained through different routes (Dawood et al. 2020, Costa et al. 2020, Campos et al. 2021).

Solid oxide fuel cells (SOFCs) convert chemical energy into electrical energy through chemical reactions between hydrogen (or hydrocarbons) and oxygen with the help of catalysts. The conversion process separates hydrogen into ions and electrons. The electrons are directed to flow through an external circuit, generating an electrical current, while the ions move through the electrolyte (Inci 2022). Figure 1 shows a simplified SOFC working scheme:

The reactions that occur in the case of SOFC, considering hydrogen as fuel, are described as follows in equations (1) to (3):





In an anodic reaction, two mols of electrons are produced for each mol of hydrogen, while for a cathodic reaction, four mols of electrons are consumed for each mol of oxygen.

The anode and the cathode are usually made of catalysts of the mentioned reactions; they are porous to allow the gases to be transported to the electrolyte interface (Jang et al. 2018). Nevertheless, the electrolyte should be a dense and compact material, avoiding mixtures of both gases while simultaneously being an excellent ionic conductor. This allows O^{2-} ions to be transported from the cathode to the anode, as shown in Figure 1. Many materials could be used in cell synthesis, but one of the most studied combinations is the anode made of a mixture of Ni with YSZ (zirconia stabilized with yttria), the electrolyte entirely made of YSZ and the cathode made of LSM (strontium doped with lanthanum manganite $LMnO_3$) or LSCF (Lanthanum strontium cobalt ferrite $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}$) Harboe et al. (2020). It is also possible to add extra layers, such as cathode current collectors and anode functional layers (Sarruf et al. 2020). It is shown in Figure 2 that the cell, assembly components, and cut view from the cell were made at LaMPaC – Materials and Fuel Cells Laboratory.

A single cell generates a relatively low power output, making it less suitable for practical applications. To address this issue, multiple cells are stacked together, forming a system known as a stack. Two components, usually metallic, are necessary to assemble a stack, called interconnectors and gaskets. In addition to allowing the referred association, the interconnector has channels to deliver and remove the gases from the electrodes (Gonçalves et al. 2024, Yi et al. 2024). Figure 3

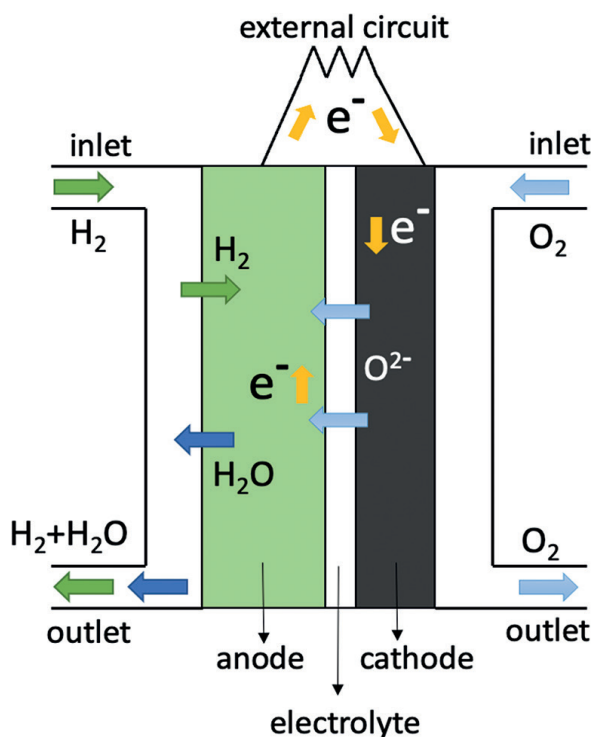


Figure 1. SOFC scheme (Andrade et al. 2022).

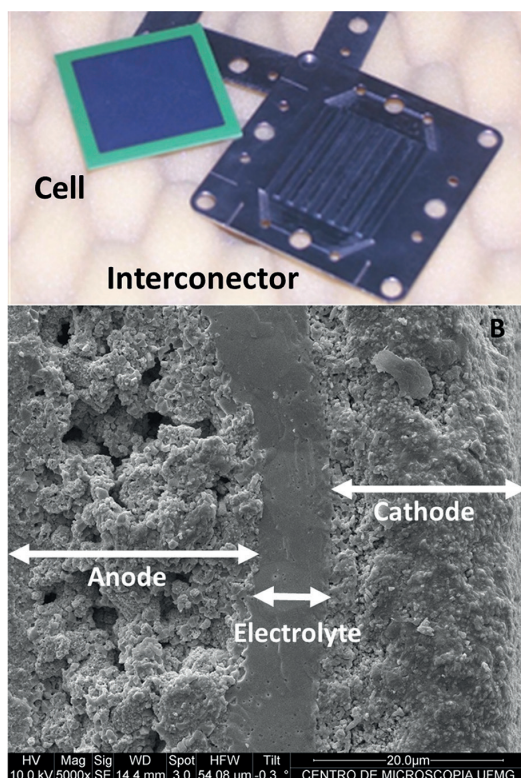


Figure 2. Cell, gasket, interconnector, and the cut view from the cell. Source: authors.

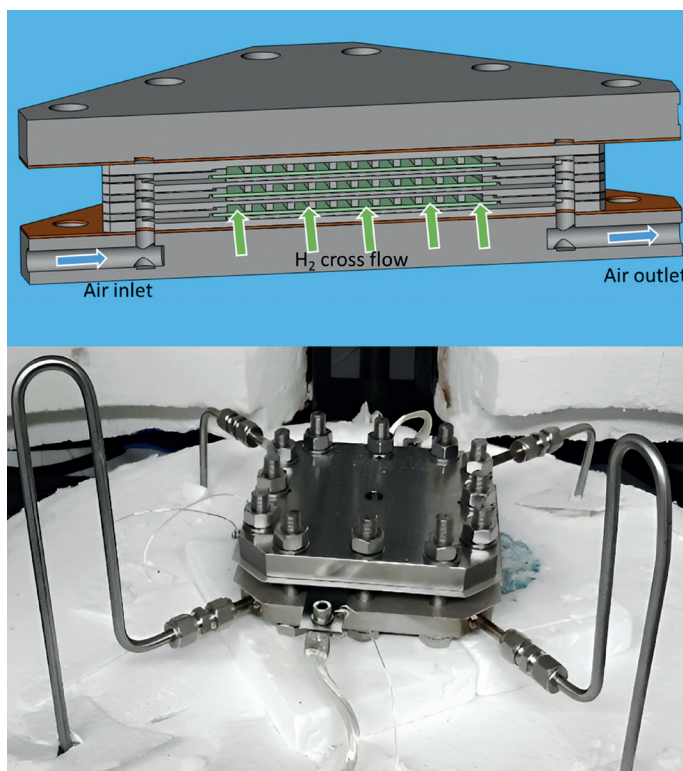


Figure 3. Stack cut view schematics and the actual image of the test chamber. Source: authors.

illustrates a three-dimensional cross-sectional view of a stack developed at LaMPaC and the same stack mounted inside a test chamber.

Generally, generating electricity using fuel cells is silent, pollution free, highly reliable, and efficient (Fernandes et al. 2018). Moreover, SOFCs can be used in many situations, such as stationary generation, aircraft, trains, hybrid power plants, and fast charging stations (FCS) for battery electric vehicles (BEVs) (Wahedi & Bicer 2020, Andrade et al. 2022, Siddiqui & Dincer 2019). Many design works of hybrid power plants and FCS were done through optimization algorithms, some genetic algorithms, and energy balance (Rahman et al. 2016, Domínguez-Navarro et al. 2019).

Several optimization algorithms are commonly found in the literature for estimating unknown electrochemical parameters or for obtaining the best operational conditions and performance maps (Li et al. 2024, Waeber et al. 2024).

Yang et al. (2020) performed an extensive review considering the use of seventeen metaheuristic optimization algorithms, including genetic algorithms, for adjusting electrochemical parameters in SOFCs. In the end, a comparative table was obtained to assist in choosing the most convenient algorithm for each type of case.

Kele et al. (2022) used a modified metaheuristic algorithm called the Cat Optimization Algorithm (CAO), implemented on MATLAB, to obtain seven unknown electrochemical parameters. Other algorithms, such as the Converged Grass Fibrous Root Optimization Algorithm (CGFROA), the Modified African Vulture Optimization algorithm (MAVO), the Chaotic Binary Shark Smell Optimization (BSSO), and the Coyote Optimization Algorithm (COA), were also compared.

Saberi Mehr et al. (2024) used a genetic algorithm implemented in MATLAB to optimize a hybrid plant for electricity and hydrogen production. The plant would use a PEM and SOFC electrolyzer operating in conjunction with PV panels and biomass gasifiers. The optimization was performed in several scenarios, such as maximum electricity production, minimum cost, and maximum exergy efficiency. The authors found that combined exergy efficiency of the plant was up to 43%.

Experimental techniques in association with numerical adjustments have also been employed (Waeber et al. 2024). Zotto et al. (2024) performed several potentiometric and electrochemical impedance spectroscopy (EIS) experiments with a unit cell, varying the temperature (650, 700, and 750 °C) and also the hydrogen inlet ratio to water (15, 25, 50, 75, and 90 %) to then validate a lumped parameter model and perform numerical adjustments to obtain unknown parameters, such as the charge transfer coefficients. From the EIS results, it was also possible to infer the main reaction processes that occurred in the cell.

Hafsi et al. (2024), based on experimental results of polarization curves for temperatures between 700°C and 800°C, calibrated a lumped parameter model to predict the maximum operating current density of a unit cell. Like the other authors, they adjusted the unknown parameters using a deterministic MATLAB optimization algorithm (fmincon). The model showed excellent agreement with the experimental data and was able to predict current densities of up to 2 A/cm².

Several authors choose to use simplified models for activation and concentration overpotentials. For activation overpotential, it is common to find studies that assume the charge transfer coefficient equal to 0.5 Kele et al. (2022), Alsarraf et al. (2022), Alzahrani & Dincer (2018), Hafsi et al. (2024). For the concentration overpotential, the constant limit current is often used instead of the detailed calculation by diffusion (Zotto et al. 2024, Yang et al. 2020, Kele et al. 2022). A further discussion about this variable can be found together in equation (30). Another observation is that there are works that do not include mass balance in the calculations (Hafsi et al. 2024, Zotto et al. 2024).

The objective of this work is to evaluate the maximum electrical power generated by a SOFC as a function of gas partial pressure, operating temperature, and current. It uses a heuristic optimization algorithm, known as the genetic algorithm (GA), and a deterministic algorithm, both already implemented in MATLAB software. The adopted physical-chemical model consists of lumped parameters that allow simple and fast calculus. Furthermore, the reactions between species are computed using Faraday's law, which allows the mass balance in the cell to be carried out. A more detailed approach for calculating the activation and concentration overpotential, similar to those employed by other authors, is applied to calculations (Li et al. 2024). The model used in this study is validated based on experimental results available in the literature. In any case, the present work allows the reader a didactical introduction to the electrochemical processes that occur in SOFCs.

MATERIALS AND METHODS

This section presents the equations necessary for formulating the objective function, along with the selected algorithms employed to maximize power output. The calculation of the electrical power generated by solid oxide fuel cells (SOFCs) involves a series of interrelated equations. These are introduced in a logical sequence consistent with the underlying computational procedure.

First, calculating the variation in Gibbs free energy of the reaction is necessary, as demonstrated in equation (4) (O'Hayre et al. 2016).

$$\Delta G^{\circ} = \Delta H^{\circ} - T_{SOFC} \Delta S^{\circ} \quad (4)$$

Where ΔG° is the variation in Gibbs free energy under standard conditions [J/mol]; ΔH° is the variation in enthalpy under standard conditions [J/mol]; ΔS° is the variation in entropy under standard conditions [J/mol-K]; T_{SOFC} is the operating temperature of the SOFC [K].

The open circuit voltage (OCV) is the maximum theoretical electrical potential a fuel cell can operate, can be determined using the Nernst expression, as shown in equation (5) (Fryda et al. 2008, O'Hayre et al. 2016).

$$V_{nernst} = -\frac{\Delta G^{\circ}}{nF} + \frac{RT_{SOFC}}{nF} \ln \left[\frac{\left(\frac{P_{H_2}}{P_{ref}}\right) \left(\frac{P_{O_2}}{P_{ref}}\right)^{1/2}}{\left(\frac{P_{H_2O}}{P_{ref}}\right)} \right] \quad (5)$$

Where V_{nernst} is the open circuit voltage [V]; ΔG° is the variation in Gibbs free energy under standard conditions [J/mol]; R is the universal gas constant and equal to 8.314 [J/K-mol]; F is the Faraday constant and equal to 96,485 [C/mol]; n is the number of electrons that participate in the reaction per mol of reagent, equal to 2; P_{H_2} is the partial pressure of hydrogen delivered to the anode [Pa]; P_{O_2} is the partial pressure of oxygen supplied to the cathode [Pa]; P_{H_2O} is the partial pressure of water produced on an anode [Pa]; P_{ref} is the reference pressure; in this case, the atmospheric pressure [Pa] is used; T_{SOFC} is the operating temperature of the SOFC [K].

Usually, on a planar SOFC, the current density is related to the total current produced and to the effective surface area of the cathode, as shown in the equation (6):

$$J = I/A \quad (6)$$

Where J is the current density [A/m²]; I is the total produced current [A]; A is the effective surface area of the cathode [m²].

The effective surface area of the cathode is defined by the designer and is a fraction of the total cell area. Many different sizes are reported in the literature: 0.8 x 5.6 cm² (Costamagna et al. 2004), 5 x 5 cm² (Haanappel et al. 2009, Cammarata et al. 2022, Bae et al. 2005), 10 x 10 cm² (Bae et al. 2005, Jang et al. 2018) and 12 x 8 cm² (Jang et al. 2018).

In practice, the open-circuit voltage is lower than expected due to various irreversible processes that occur during fuel cell operation, e.g., activation overpotential, ohmic overpotential, and concentration overpotential. In this way, the practically produced voltage (V) by SOFC can be calculated using equation (7) (Rosner et al. 2020, Bianchi et al. 2020):

$$V = V_{nernst} - \eta_{activation} - \eta_{ohmic} - \eta_{concentration} \quad (7)$$

Where V is the closed-circuit potential [V]; $\eta_{activation}$ is the activation overpotential [V]; η_{ohmic} is the ohmic overpotential [V]; $\eta_{concentration}$ is the concentration overpotential [V].

The activation overpotential corresponds to the energy barrier that separates reactants from products. Only reactant species with energy equal to or greater than this barrier can take part in the charge transfer reactions represented by equations (1) and (2). Hence, the activation overpotential

can be calculated by the implicit solution of the Butler-Volmer equation, as it is impossible to isolate the overpotential for a given current density and each electrode, as described by equations (8) and (9). After this, both found overpotentials should be summed according to equation (10): (Yonekura et al. 2011b, Vijay & Tadé 2017, Rosner et al. 2020, Fu et al. 2021):

$$J = J_{o,anode} \left\{ e^{\left[\frac{\alpha_{anode} n F}{RT_{SOFC}} \right] \eta_{activation,anode}} - e^{\left[\frac{(1-\alpha_{anode}) n F}{RT_{SOFC}} \right] \eta_{activation,anode}} \right\} \quad (8)$$

$$J = J_{o,cathode} \left\{ e^{\left[\frac{\alpha_{cathode} n F}{RT_{SOFC}} \right] \eta_{activation,cathode}} - e^{\left[\frac{(1-\alpha_{cathode}) n F}{RT_{SOFC}} \right] \eta_{activation,cathode}} \right\} \quad (9)$$

$$\eta_{activation} = \eta_{activation,anode} + \eta_{activation,cathode} \quad (10)$$

Where $\eta_{activation}$ is the activation overpotential [V]; α_{anode} and $\alpha_{cathode}$ are the dimensionless charge transfer coefficients [-]; n is the number of electrons that participate in the reaction per mol of reagent, equal to 2 for the anode and equal to 4 for the cathode; $J_{o,anode}$ and $J_{o,cathode}$ are the anodic and cathodic exchange current densities, respectively [A/m²].

The anodic and cathodic exchange current densities can also be modeled by Arrhenius's law based on experimental data (Yonekura et al. 2011a). There are several models for these parameters in the literature, as discussed by (Yonekura et al. 2011b). In this work, the models used by (Naouar et al. 2024) are adopted and represented in equations (11) and (12).

$$J_{o,anode} = Y_{anode} \left(\frac{P_{H_2}}{P_{ref}} \right)^a \left(\frac{P_{H_2O}}{P_{ref}} \right)^b e^{-\frac{E_{activation,anode}}{RT_{SOFC}}} \quad (11)$$

$$J_{o,cathode} = Y_{cathode} \left(\frac{P_{O_2}}{P_{ref}} \right)^c e^{-\frac{E_{activation,cathode}}{RT_{SOFC}}} \quad (12)$$

Where Y_{anode} and $Y_{cathode}$ are experimental coefficients for the anode and cathode [A/m²]; $E_{activation,anode}$ and $E_{activation,cathode}$ are the activation energies [J/mol]; a , b and c are theoretical or adjusted coefficients [-]; P_{ref} is the reference pressure; in this case, the atmospheric pressure [Pa] is used.

The ohmic overpotential is related to the Joule heating losses on the anode, cathode, and electrolyte. For this, experimental correlations are necessary to determine the electrical conductivity of these three components, as shown for each layer in equation (13) (Bossel 1992, Lisbona et al. 2007):

$$k_{layer} = A_{layer} e^{\frac{E_{ohm,layer}}{RT_{SOFC}}} \quad (13)$$

Where k_{layer} are the electrical conductivities for each SOFC component [ohm⁻¹ · m⁻¹]; A_{layer} is an experimental coefficient [ohm⁻¹ · m⁻¹]; $E_{ohm,layer}$ is the ohmic activation energy [J/mol].

The area-specific resistance computes the electrical resistance of all three components together in a unitary manner, as described in equation (14) (Lisbona et al. 2007):

$$ASR = \sum \frac{t_{layer}}{k_{layer}} \quad (14)$$

Where t_{layer} are the thicknesses for each SOFC component [m]; ASR is the area-specific resistance [ohm · m²].

It is possible to obtain an ASR for the entire cell as a function of temperature through experimental measurements. Therefore, equations (13) and (14) can be rewritten as only one in equation (15) (Leonide et al. 2009):

$$ASR = \frac{T_{SOFC}}{B_{cell}} e^{\frac{E_{act,ohm}}{RT_{SOFC}}} \quad (15)$$

Where B_{layer} is an experimental coefficient [$\text{ohm}^{-1} \cdot \text{m}^{-2} \cdot \text{K}$];

In this way, it relates the area-specific resistance with current and ohmic overpotential using the equation (16) (Lisbona et al. 2007):

$$\eta_{ohmic} = ASR \cdot J \quad (16)$$

Where η_{ohmic} is the ohmic overpotential [V].

The last overpotential to be discussed is related to the concentration; it is associated with the difficulty of chemical species to be available on the electrode surface, especially on the triple phase boundary (TPB) region. This region it is located where there is coexistence of gas phase, electrolyte and electrode (Tabish et al. 2020). The concentration overpotential is pronounced when mass transport effects prejudice the reaction on the electrode, that is, when the supply of reagent or removal of products by mass diffusion over the electrode is slower than the corresponding discharge current density. If the concentrations of the ions responsible for the charge transfer are low, the retardant of the entire electrochemical process occurs (Zhou et al. 2024).

First, it is necessary to calculate a binary diffusivity for each gas pair and effective diffusivity for each gas pair in the medium. The binary diffusivity $D_{binary, AB}$ can be determined using the Chapman-Enskog expression, as shown in equation (17) (Bird et al. 2006, Cussler 2009, Wang et al. 2020):

$$D_{binary, AB} = \frac{1.86 \times 10^{-3} \cdot T_{SOFC}^{3/2} \cdot \sqrt{\frac{1}{M_A} + \frac{1}{M_B}}}{P_{total} \cdot \sigma_{AB}^2 \cdot \Omega} \left(\frac{1}{10000} \left[\frac{\text{cm}^2/\text{s}}{\text{m}^2/\text{s}} \right] \right) \quad (17)$$

Where $D_{binary, AB}$ is the binary diffusivity [m^2/s]; M_A and M_B are the molar masses of each species [kg/kmol]; P_{total} is the total pressure, in this case, must be in [atm]; σ_{AB} mean collision diameter [$\text{\AA}$]; Ω collision integral [-].

The arithmetic mean of the collision diameter and the collision integral can be obtained from tabular data and equations (18) to (21) (Bird et al. 2006, Cussler 2009).

$$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2} \quad (18)$$

$$\epsilon_{AB} = \sqrt{\epsilon_A \epsilon_B} \quad (19)$$

$$T^* = \frac{K_{Boltzmann} T_{SOFC}}{\epsilon_{AB}} \quad (20)$$

$$\Omega = \frac{1.06036}{T^{*0.15610}} + \frac{0.19300}{e^{0.47635 \cdot T^*}} + \frac{1.03587}{e^{1.52996 \cdot T^*}} + \frac{1.76474}{e^{3.89411 \cdot T^*}} \quad (21)$$

Where σ_A and σ_B are the collision diameters for each species [$\text{\AA}$]; ϵ_A and ϵ_B are the Lennard-Jones potential parameters for each species [J]; T^* is the reduced temperature [-] (Neufeld et al. 1972).

For each species, it is also necessary to consider the Knudsen diffusivity, which depends on the electrode pore diameter, temperature, and molar mass. The Knudsen diffusivity is significant when gas molecules can collide more frequently against the pore wall than with other gas molecules in the mixture, and it can be calculated using equation (22) (Mills & Coimbra 2015, Naouar et al. 2024).

$$D_{Knudsen, i} = \left(\frac{d_{pore}}{3} \right) \sqrt{\frac{8RT_{sofc}}{\pi M_i}} \quad (22)$$

Where d_{pore} is the electrode pore diameter [m]; R is the universal gas constant and, in this equation, must be equal to 8314 [J/K.kmol]; M_i is the molar mass of each species [kg/kmol].

The combined effects of binary and Knudsen diffusivities on molecular diffusivity are obtained using equation (23). (Xu et al. 2025):

$$D_{molecular, i} = \left(\frac{1}{D_{binary, AB}} + \frac{1}{D_{Knudsen, i}} \right)^{-1} \quad (23)$$

Finally, the effective diffusivity for each species is determined by applying the geometrical characteristics of each electrode, in this case, porosity and tortuosity, both determined by experimental procedures (Brus et al. 2014, Ye et al. 2014, Tan et al. 2024). The porosity is the void volume fraction on the electrode, and the tortuosity is the ratio between the shortest pathway through a porous structure to the shortest linear distance between two points, in this case, the electrode thickness (Tjaden et al. 2018, Martínez et al. 2009, Zhang et al. 2021). Hence, effective diffusivity is defined by equation (24) (Cussler 2009):

$$D_{eff, i} = \frac{\varepsilon_{p, electrode}}{\tau_{electrode}} D_{molecular, i} = \psi_{electrode} D_{molecular, i} \quad (24)$$

Where $\varepsilon_{p, electrode}$ is the porosity; $\tau_{electrode}$ is the tortuosity; $\psi_{electrode}$ is the inverse of MacMullin number (Martínez et al. 2009).

After finding the effective diffusivity for anode gases (H_2 - H_2O) and cathode gases (O_2 - N_2), it is possible to find the concentration overpotential. Equations for this overpotential can be deducted, linking the Nernst equation with Fick's law, so it depends on temperature, gas concentration, and effective diffusivity (O'Hayre et al. 2016, Primdahl & Mogensen 1999). The equations (25) and (26), for each electrode and its concentration overpotential, are described in a more general form: (Leonide et al. 2009, Wang et al. 2020):

$$\eta_{concentration, anode} = \frac{RT_{SOFC}}{n_{anode} F} \ln \left[\frac{\left(\frac{P_{H_2O, TPB}}{P_{ref}} \right) \left(\frac{P_{H_2}}{P_{ref}} \right)}{\left(\frac{P_{H_2O}}{P_{ref}} \right) \left(\frac{P_{H_2, TPB}}{P_{ref}} \right)} \right] \quad (25)$$

$$\eta_{concentration, cathode} = \frac{RT_{SOFC}}{n_{cathode} F} \ln \left[\frac{\left(\frac{P_{O_2}}{P_{ref}} \right)}{\left(\frac{P_{O_2, TPB}}{P_{ref}} \right)} \right] \quad (26)$$

Where $\eta_{concentration}$ is the concentration overpotential [V]; n is the number of electrons that participate in the reaction per mol of reagent, equal to 2 for the anode and equal to 4 for the cathode.

The partial pressures of each of the gases at the TPB region can be calculated by applying Fick's law, using the equations (27) to (29) (Leonide et al. 2009):

$$P_{H_2,TPB} = P_{H_2} - \left(\frac{RT_{SOFC} t_{anode}}{n_{anode} F D_{H_2}^{eff}} \right) J \quad (27)$$

$$P_{H_2O,TPB} = P_{H_2O} + \left(\frac{RT_{SOFC} t_{anode}}{n_{anode} F D_{H_2O}^{eff}} \right) J \quad (28)$$

$$P_{O_2,TPB} = P_{O_2} - \left(\frac{P_{total} - P_{O_2}}{P_{total}} \right) \left(\frac{RT_{SOFC} t_{cathode}}{n_{cathode} F D_{O_2}^{eff}} \right) J \quad (29)$$

A more sophisticated model with a cathode current collector and anode functional layer is discussed (Zhao & Virkar 2005, Zhu et al. 2015). Additionally, some authors prefer to simplify equations (25) and (26) to equation (30) (Lang et al. 2017):

$$\eta_{concentration} = \frac{RT_{SOFC}}{nF} \ln \left[\frac{J_{limit}}{J_{limit} - J} \right] \quad (30)$$

Where J_{limit} is the current density limit [A/m²].

The mass transfer process, pressure, and temperature affect the current limit density. Equation (30) has practical use when the V-J curve (as discussed in Figure 4 and Figure 5) is empirically available for different conditions, so J_{limit} can be found where the potential curve intercepts the abscissa. It is also possible to obtain J_{limit} for each electrode, as shown by (Wang et al. 2020, Yoon et al. 2009, 2007). However, in this work, equation (30) is not used; instead (25) and (26) are applied.

As the SOFC operates in constant current mode, the generated power is just the product between the potential and the current, hence:

$$P_{SOFC} = V \cdot I \quad (31)$$

where P_{SOFC} is the SOFC power [W].

Equation (31) is the objective function of this study. Inspection of equations (4), (5), (8), (9), (11), (12), (15), (17), (22), and (25) to (29) shows that the SOFC potential depends on the operating temperature, as well as on the partial pressure of gases and current density. The behavior of the potential and power with changes in partial pressure and current density are shown in Figure 4 and Figure 5 as a didactical example (Fryda et al. 2008).

Note in Figure 4 that the potential decreases with increasing current density; once in Figure 5, note that the power behavior is nonlinear with the total pressure and current limit.

In this work, the described model is validated using experimental data available in the literature (Leonide et al. 2009) for two temperatures (721 °C and 821 °C) and atmospheric pressure. All other parameters are defined in Table I, which summarizes all used parameters in order of use in the equations to facilitate the reader's comprehension.

To establish a quantitative comparison between the model and literature results, it is used the relative error as described by equation (32):

$$relative\ error = \frac{V - V_{experimental}}{V_{experimental}} \times 100 \quad (32)$$

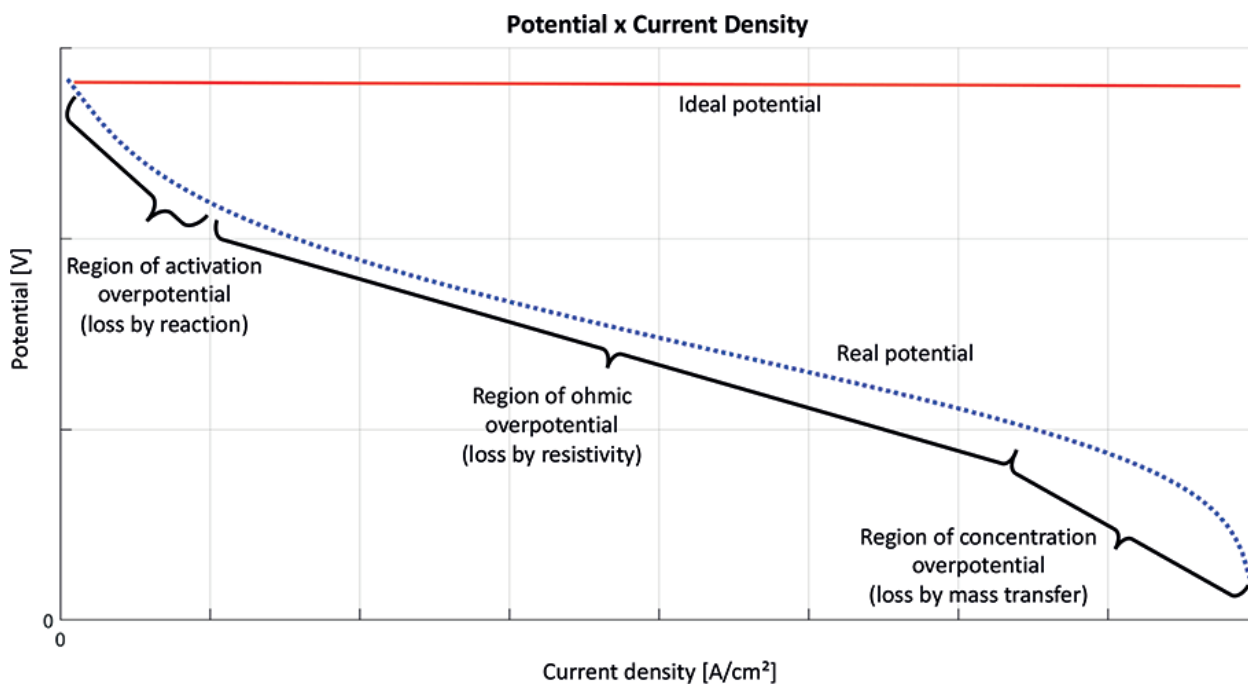


Figure 4. Behavior of the potential and overpotential for didactical purpose.

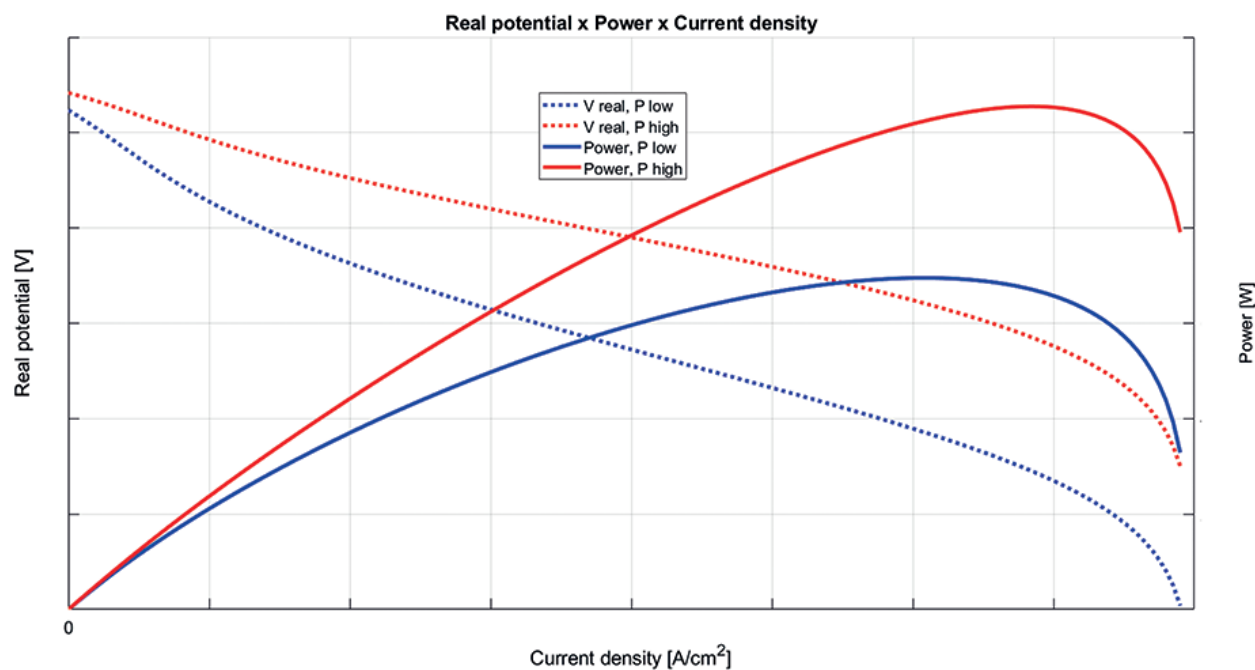


Figure 5. Behavior of the potential and power for didactical purpose.

Table I. Summary of parameters.

Parameter	Type	Original Value	Modified	Unit	Ref.
ΔS°	Theoretical	-22.38		J/mol-K	(Boles & Yunus A. Cengel 2014)
ΔH°	Theoretical	-241,820		J/mol	(Boles & Yunus A. Cengel 2014)
R	Theoretical	8.314		J/K-mol	(Boles & Yunus A. Cengel 2014)
F	Theoretical	96,485		C/mol	(Boles & Yunus A. Cengel 2014)
A	Arbitrary	$0.01 \cdot 0.01$	$0.04 \cdot 0.04$	m ²	(Leonide et al. 2009)
n anodic	Theoretical	2		-	(O'Hayre et al. 2016)
n cathodic	Theoretical	4		-	(O'Hayre et al. 2016)
α_{anode}	Experimental	0.59		-	(Leonide et al. 2009)
$\alpha_{cathode}$	Experimental	0.65		-	(Leonide et al. 2009)
γ_{anode}	Experimental	$1.82527 \cdot 10^8 T_{sofc}$		A/m ²	(Leonide et al. 2009)
$\gamma_{cathode}$	Experimental	$1.51556 \cdot 10^8 T_{sofc}$		A/m ²	(Leonide et al. 2009)
$E_{activation, anode}$	Experimental	$105.04 \cdot 10^3$	$115.04 \cdot 10^3$	J/mol	(Leonide et al. 2009)
$E_{activation, cathode}$	Experimental	$139.86 \cdot 10^3$		J/mol	(Leonide et al. 2009)
a	Experimental	-0.1		-	(Leonide et al. 2009)
b	Experimental	0.33		-	(Leonide et al. 2009)
c	Experimental	0.22		-	(Leonide et al. 2009)
$E_{Ohm, cell}$	Experimental	$90.31 \cdot 10^3$		J/mol	(Leonide et al. 2009)
B_{cell}	Experimental	$4.1879 \cdot 10^{12}$		S-K/m ²	(Leonide et al. 2009)
t_{anode}	Experimental	$1 \cdot 10^{-3}$		m	(Leonide et al. 2009)
$t_{cathode}$	Experimental	$30 \cdot 10^{-6}$		m	(Leonide et al. 2009)
$d_{pore, anode}$	Experimental	$1,200 \cdot 10^{-9}$	$800 \cdot 10^{-9}$	m	(Leonide et al. 2009)
$d_{pore, cathode}$	Experimental	$1,200 \cdot 10^{-9}$	$800 \cdot 10^{-9}$	m	(Leonide et al. 2009)
σ_{H_2}	Tabular	2.915			(Cussler 2009)
σ_{H_2O}	Tabular	2.641			(Cussler 2009)
σ_{O_2}	Tabular	3.467			(Cussler 2009)
σ_{N_2}	Tabular	3.789			(Cussler 2009)
ε_{H_2}	Tabular			K	(Cussler 2009)
ε_{H_2O}	Tabular			K	(Cussler 2009)
ε_{O_2}	Tabular			K	(Cussler 2009)
ε_{N_2}	Tabular			K	(Cussler 2009)
ψ_{anode}	Experimental	0.13	0.10	-	(Leonide et al. 2009)
$\psi_{cathode}$	Experimental	0.06		-	(Leonide et al. 2009)

Hence, it proposes to use a genetic algorithm, already implemented in MATLAB, to find the point for maximum power depending on operating temperature, partial pressure of gases, and current density. Therefore, this is a global optimization problem. This procedure must comply with the following practical ranges:

- T_{SOFC} - Operating temperature changes from 873 K to 1,273 K;
- P_{H_2} and P_{air} - Partial pressure on inlet changes from 1 Pa to P_{total} . Where P_{total} is equal to 101,325 Pa for the nonpressurized case and 500,000 Pa for the pressurized case;
- P_{H_2O} - Partial pressure on inlet changes from 1 Pa to $0.03 P_{total}$. This allows the hydrogen to be humidified at the inlet. Some studies report humidification percentages ranging from 3% to 4%. (Bae et al. 2005, Jang et al. 2018, Hagen et al. 2020);
- I - Current changes from 1 (0.062 A/cm²) to 128 A (8 A/cm²).

Also, there are two linear constraints to be satisfied. In the first constraint, the sum of partial pressures of hydrogen and water at the inlet must be equal to the pressure of the fuel system (anode side), as shown by equation (33):

$$P_{H_2} + P_{H_2O} = P_{total} \quad (33)$$

In the second constraint, the cathode side pressure must be equal to the sum of partial pressures of hydrogen and water at inlet, as shown by equation (34):

$$P_{air} = P_{H_2} + P_{H_2O} \quad (34)$$

Usually, the results related to current are expressed by the area unit, e.g., A/m² or A/cm². This is done because the effective area interferes directly with current and power. This work uses the absolute results to offer the reader a more didactic perspective and a proper notion of SOFC performance.

The SOFC reactions partially consume the oxygen in the atmospheric air. According to modeling studies and experimental tests, the airflow is usually significantly higher than the hydrogen flow. In an experiment with a unitary cell, the authors (Bae et al. 2005) used airflow up to four times higher than hydrogen flow. Others (Zhou et al. 2022) using a lumped model used airflow up to three times higher than hydrogen flow. The authors (Bahari et al. 2022) show that in a lumped model, the difference in the concentration between the admission and exhaust is just over 3%.

A molar balance obtains the water molar flow, as well as the hydrogen and oxygen molar flows and partial pressures at the outlet, through the Faraday law and the stoichiometric relations. Hence, equations (35) to (38) can be used:

$$\dot{n}_{H_2, outlet} = \dot{n}_{H_2, inlet} - \frac{I}{n_a \cdot A \cdot F} \quad (35)$$

$$\dot{n}_{H_2O, outlet} = \dot{n}_{H_2O, inlet} + \frac{I}{n_a \cdot A \cdot F} \quad (36)$$

$$\dot{n}_{O_2, outlet} = y_{O_2, inlet} \cdot \dot{n}_{air, inlet} - \frac{I}{n_c \cdot A \cdot F} \quad (37)$$

$$\dot{n}_{O_2, outlet} = y_{O_2, inlet} \cdot \dot{n}_{air, inlet} - \frac{I}{n_c \cdot A \cdot F} \quad (38)$$

Finally, through equation (39), which is obtained by the ideal gas law, the partial pressure of each species at the inlet and outlet is calculated.

$$P_i = \frac{\dot{n}_i R T_{soc}}{\dot{V}_i} \quad (39)$$

Where P_i is the partial pressure for each species; $y_{O_2, inlet}$ is the molar fraction of oxygen in atmospheric air and is equal to 0.21; $\dot{n}_i$ a $\dot{V}_i$ are the volumetric and molar flows for each species.

Equations 5, 11, 12, 25, and 29 use the mean partial pressure values between the cell's inlet and outlet for each species.

Moreover, the parameters ΔH° and ΔS° are determined through thermodynamic tables. The effective area and thickness of the anode, electrolyte, and cathode are arbitrary definitions associated with SOFC design.

For the described conditions, a genetic algorithm is used ten times using the settings described on Table II, which is capable to find the maximum on non-linear, discontinuous and nondifferentiable functions (Sivanandam & Deepa 2008, Conn et al. 1997).

This algorithm has a working logic based on natural evolution and can be used to solve many real engineering problems. Among them is the design problem of a fast-charging station based on fuel cells to supply electrical energy to electric cars (Domínguez-Navarro et al. 2019, Rahman et al. 2016).

Based on the evolution of living species, a genetic algorithm randomly creates a population of individuals (a set of optimization variables related to the objective function) (Edgar & Himmelblau 2001, Sivanandam & Deepa 2008). Individuals who offer the best solutions, i.e., present higher values

Table II. Summary MATLAB settings for genetic algorithms.

Group	Setting (MATLAB Terminology)	Value or option
Population	<i>PopulationSize</i>	<i>5 × optimization variables quantity</i>
	<i>InitialPopulationRange</i>	<i>practical ranges specified in this text</i>
	<i>PopulationType</i>	<i>doubleVector</i>
	<i>CreationFcn</i>	<i>gacreationlinearfeasible</i>
	<i>SelectionFcn</i>	<i>selectionstochunif</i>
Reproduction	<i>EliteCount</i>	<i>0.05* Population size</i>
	<i>Mutation function</i>	<i>mutationadaptfeasible</i>
	<i>CrossoverFcn</i>	<i>crossoverintermediate</i>
	<i>CrossoverFraction</i>	<i>0.8</i>
Stopping criteria	<i>MaxStallGenerations</i>	<i>50</i>
	<i>FunctionTolerance</i>	<i>1 • 10⁻¹⁰</i>
Migration	<i>MigrationDirection</i>	<i>forward</i>
	<i>MigrationFraction</i>	<i>0.2</i>
	<i>MigrationInterval</i>	<i>20</i>

for the objective solution, are more likely to be selected. Those selected individuals undergo a combination process called crossover so that new individuals emerge. In addition to crossover, there is also the probability that new individuals will undergo mutation, the result of which is not fully associated with the genes of two previously existing individuals. These new individuals, in turn, are a new population generation that allows new values to be found for the objective function (Edgar & Himmelblau 2001). This process continues until the difference between the maximum value obtained for the objective function between two generations is less than a tolerance, in this case equal to $1 \cdot 10^{-10}$. The default configuration was maintained for all other parameters of the genetic algorithm.

To ensure quality and avoid any biased influence over the results, the initial values for the optimization variables used in the genetic algorithm were random, with a well-dispersed population that satisfied all bounds and linear constraints previously described. Then, each set of optimized variables by the genetic algorithm is used as initial values in a deterministic multivariable nonlinear optimization algorithm, already implemented in MATLAB and called "fmincon." Hence, verifying the quality of the solution between the two techniques is possible. Moreover, in parallel and comparison, random values are used as initial values for "fmincon."

The following nonlinear constraint ensures that the optimization variables respect molar balance: the difference between the inlet molar flow rate and the outlet molar flow rate, for hydrogen and oxygen, must be greater than zero.

The computer used to run MATLAB has as a processor Intel(R) Core(TM) i7-8550U, 64 bits, 1.80 GHz, worked with 12 GB of memory.

RESULTS

Based on the equations described in the Methodology, the obtained results are discussed in this section. First, the comparison between experimental data and implemented model searching for validation is represented in Figure 6.

By inspection of Figure 6, it is noted that the error is below 9% for all experimental data available for both temperatures. Moreover, the mean of all error absolute values is equal to 5.3% for $T_{SOFC} = 721^\circ\text{C}$ and 3.5% for $T_{SOFC} = 821^\circ\text{C}$. Taking into account the results obtained by the model and based on Figure 6, the model is considered validated.

For illustrative purposes, the power behavior as a function of operating temperature and current is represented in two surface graphics in Figure 7. It is obtained for gas pressures with the following values: $P_{H_2} = 100,000\text{ Pa}$, $P_{O_2} = 21,278\text{ Pa}$ and $P_{H_2O} = 1,325\text{ Pa}$; that is, nonpressurized values. Additionally, for illustrative purposes, the following parameters were changed from Table I: $A = 0.04 \times 0.04\text{ m}^2$, $d_{pol} = 800 \cdot 10^{-9}\text{ m}$, and $\psi_{anode} = 0.10$.

It is noted in Figure 7 that the power has a range of values with nonlinear behavior as a function of current, as shown in Figure 5. Any cut view in Figure 7 on plane power versus current creates a similar graphic to the one shown in Figure 5. However, for sufficiently high current values, the voltage and power behavior become strongly nonlinear, especially at low temperatures and currents near the current limit (J_{limit}), which is the maximum current at which the cell can operate, that is when the potential is equal to zero. This last is related to the concentration overpotential, which is related to

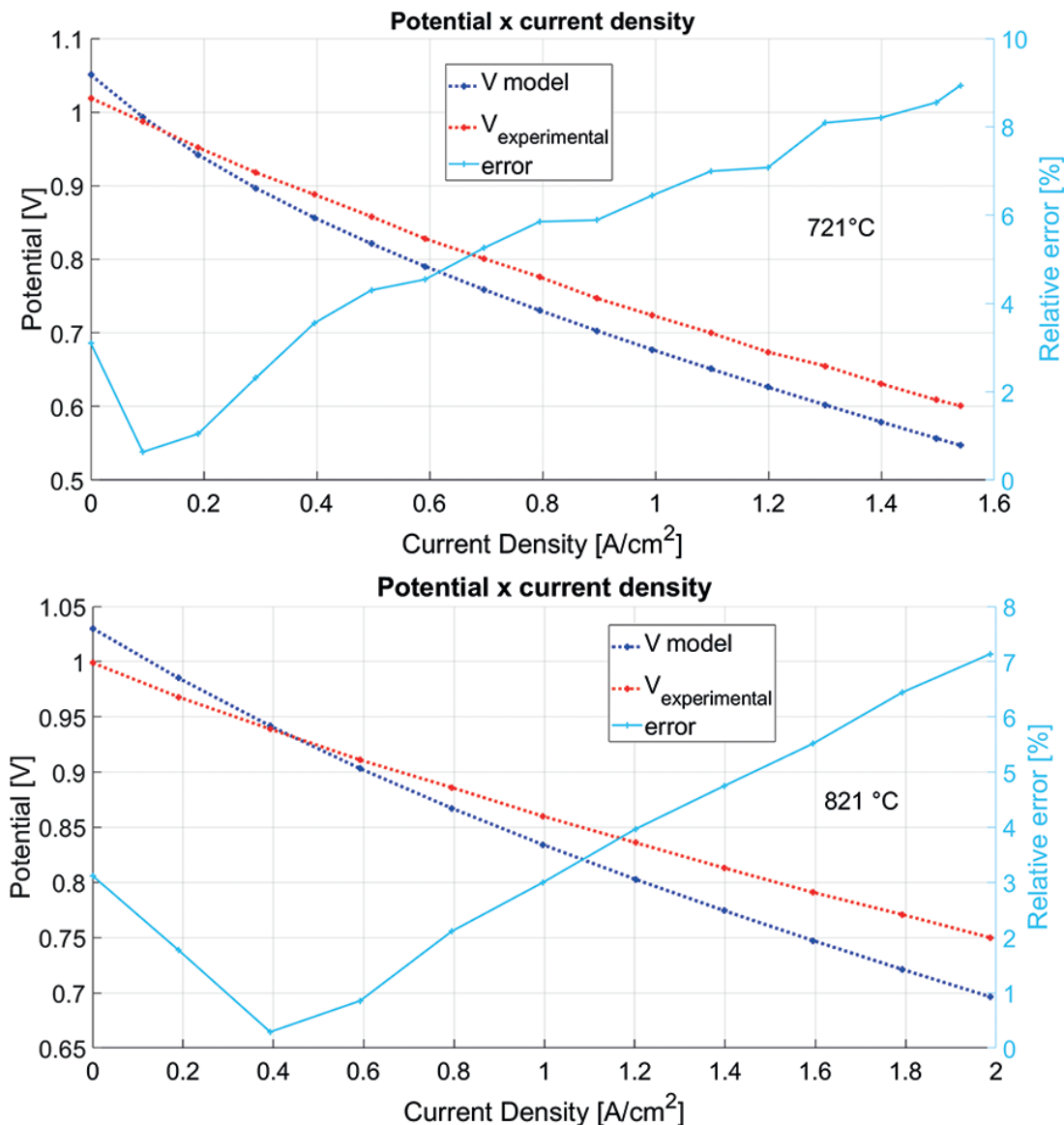


Figure 6. Comparison between experimental data and model results.

the mass transfer process on high currents, as can be seen in equations (25) to (27). As higher is the current density, lower will be the H_2 partial pressure and higher will be the H_2O partial pressure on TPB. So, in this way, the two partial pressures will let the concentration overpotential to higher values. It is also noted that there is nonlinearity with temperature variation but lower intensity than the current. Therefore, the region has a maximum power near 1400 K and 110 A.

Using initial values on a deterministic algorithm with random numbers or the results obtained by a genetic algorithm always leads to the same answer for power (objective function). The same occurred for the optimized and calculated variables. Hence, for all later results discussed in this study, the initial value for the deterministic algorithm equals the solution obtained by the genetic

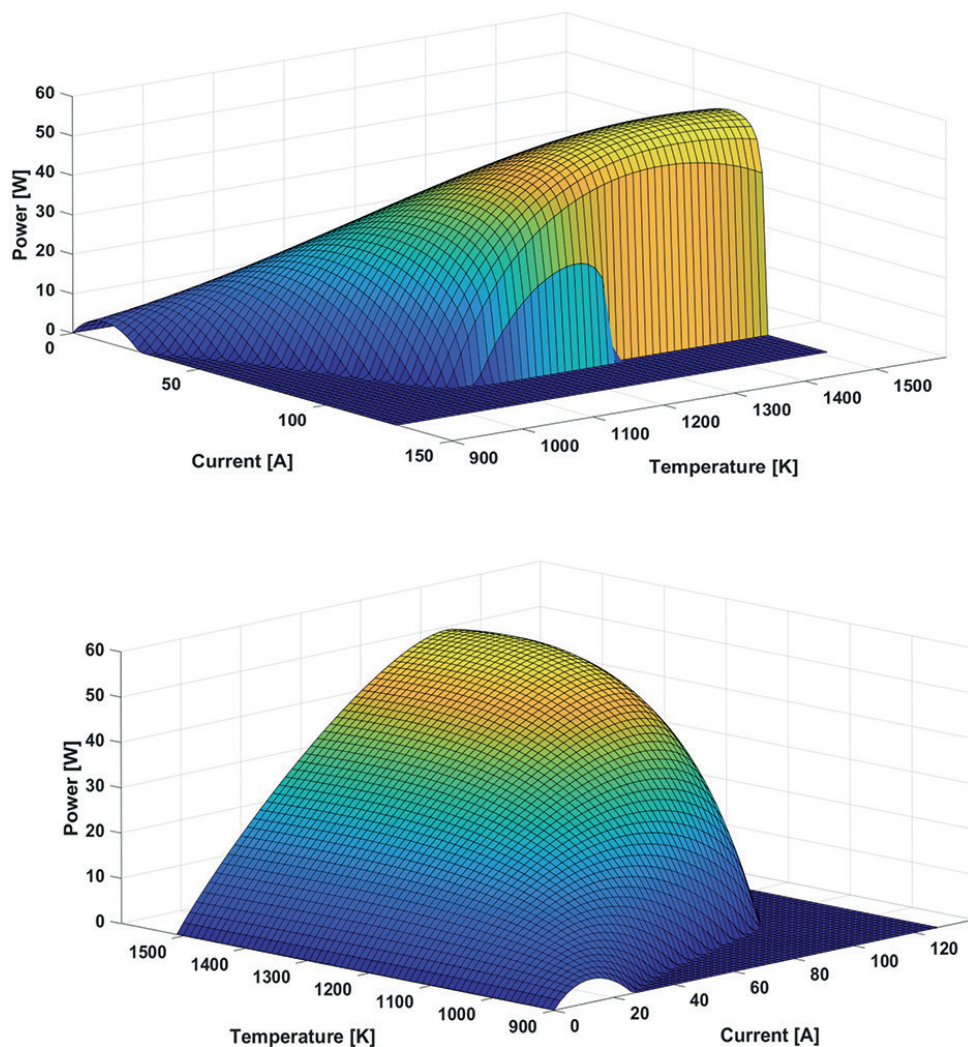


Figure 7. Surfaces representing the generated power as a function of operating temperature and current for the unpressurized case.

algorithm. Table III describes the results for ten runs obtained by the genetic algorithm for the unpressurized case. In the same way, Table 4 shows the results for a pressurized case.

It is noted that in Table III, the maximum global power was obtained on run n° 5, while in Table IV, it was found on run n° 4. These maximum values are not so near themselves, with a relative difference of 48%.

It is also noted that the mean values of power, temperature, and current are very close to those obtained in all ten runs, as shown in Table III and Table IV. This is easily perceptible by low standard deviation values in all runs, considering the range for each variable.

For the H_2 and H_2O pressures, in the first analysis, the values showed a variation more significant than the mean and those found in ten runs. However, the standard deviation of the maximum pressure (101,325 Pa and 500,000 Pa) is only 0.02% and 0.12|%, respectively. These deviations are of low significance from a practical engineering point of view.

Table III. Results for the unpressurized case.

Run	Heuristic - Genetic Algorithm						Deterministic	Relative Difference [%]
	Obj. Func.	Optimized Variables					Obj. Func.	
	Power [W]	Temperature [K]	H ₂ Pressure [Pa]	H ₂ O Pressure [Pa]	Air Pressure [Pa]	Current [A]	Power [W]	
1	38.64	1,171	100,407	918	101,325	63	57.84	-33.18
2	40.99	1,180	100,342	983	101,325	68		-29.13
3	35.97	1,170	100,740	585	101,325	56		-37.80
4	57.82	1,273	100,472	853	101,325	108		-0.12
5	57.84	1,273	100,647	678	101,325	108		-0.09
6	55.07	1,248	100,566	759	101,325	107		-4.87
7	35.17	1,168	100,428	897	101,325	54		-39.20
8	37.22	1,205	100,529	796	101,325	53		-35.65
9	57.83	1,273	100,524	801	101,325	108		-0.09
10	55.88	1,255	100,623	702	101,325	107		-3.46

mean	47.24	1,222	100,528	797	101,325	83
S.D.	10.3	46.8	121	121	0	26
max - min	22.7	104.9	398	398	0	55

Table IV. Results for the pressurized case.

Run	Heuristic - Genetic Algorithm						Deterministic	Relative Difference [%]
	Obj. Func.	Optimized Variables					Obj. Func.	
	Power [W]	Temperature [K]	H ₂ Pressure [Pa]	H ₂ O Pressure [Pa]	Air Pressure [Pa]	Current [A]	Power [W]	
1	83.61	1,269	496,227	3,773	500,000	128	85.62	-2.35
2	83.42	1,268	495,921	4,079	500,000	128		-2.58
3	77.12	1,233	496,302	3,698	500,000	128		-9.93
4	84.43	1,273	495,137	4,863	500,000	128		-1.40
5	78.93	1,243	496,349	3,651	500,000	128		-7.82
6	83.81	1,272	497,191	2,809	500,000	128		-2.12
7	51.66	1,180	495,276	4,724	500,000	75		-39.47
8	78.90	1,242	495,961	4,039	500,000	128		-7.85
9	84.42	1,273	495,141	4,859	500,000	128		-1.41
10	77	1,234	496,303	3,697	500,000	128		-9.71

mean	78.36	1,249	495,981	4,019	500,000	123
S.D.	9.8	29.4	648	648	0	17
max - min	32.8	93.2	2,053	2,053	0	53

Moreover, it perceives maximum power between the genetic and deterministic algorithms; the results have no significant difference in all variables. It can be seen, as expected, that from the theoretical perspective, the deterministic algorithm always found the same result for the maximum power. The genetic algorithm shows few standard deviations, where the maximum power obtained by it is 0.1% less than obtained by the deterministic algorithm for the unpressurized case. Hence, it showed the genetic algorithm's reliability in finding the SOFC maximum power point.

As expected and illustrated in Figure 5, the pressure rising on the SOFC also raises the potential and power. For a comparative effect, between the pressurized case (Table III – run n° 5) and the nonpressurized case (Table IV– run n° 4), the pressure increases of 493% allows the power to increase by 48%.

As shown in Table III and Table IV, the maximum power was obtained at the maximum value established inside the range for the temperature. Based on Figure 7 and even knowing that the typical maximum operating temperatures of the SOFC are 1273 K, the temperature range is expanded to 1500 K to find a maximum value that does not coincide with the range's limits. In this way, the following results are found in Table V.

It is noted in Table V that the maximum global power was obtained on run n° 9. For the unpressurized case, the results for power, temperature, and current are very close to the mean, as indicated by low standard deviation values. As illustrated by Figure 7, the increase in the temperature range demonstrated that, depending on the physical and chemical properties of the electrode materials, the continuous increase in temperature is not always accompanied by an increase in power.

Table V. Results for the unpressurized case and temperature interval from 900K to 1500K.

Run	Heuristic - Genetic Algorithm						Deterministic	Relative Difference [%]
	Obj. Func.	Optimized Variables					Obj. Func.	
	Power [W]	Temperature [K]	H ₂ Pressure [Pa]	H ₂ O Pressure [Pa]	Air Pressure [Pa]	Current [A]	Power [W]	
1	51.78	1,288	100,413	912	101,325	77	66.11	-21.68
2	61.54	1,317	100,632	693	101,325	111		-6.93
3	39.75	1,286	100,629	696	101,325	52		-39.85
4	61.63	1,318	100,776	549	101,325	111		-6.79
5	61.14	1,312	100,117	1,208	101,325	110		-7.53
6	52.80	1,280	100,369	956	101,325	81		-20.14
7	39.10	1,354	99,981	1,344	101,325	49		-40.85
8	51.87	1,280	100,251	1,074	101,325	78		-21.54
9	64.70	1,379	100,691	634	101,325	112		-2.14
10	62	1,329	100,718	607	101,325	111		-5.69

mean	54.67	1,314	100,458	867	101,325	89
S.D.	9.3	33.1	275	275	0	25
max - min	25.6	99.5	794	794	0	63

It stands out that the genetic optimization algorithm is high-speed even on a processor Intel^(R) Core^(TM) i7-8550U, 64 bits, 1.80 GHz with 12 GB of memory. Each run consumes 111 seconds and does not exceed 500 generations to satisfy the stop criteria; the relative difference between two generations is at least $1 \cdot 10^{-10}$, where Figure 8 illustrates this behavior.

It is relevant to note that the implemented model does not consider head loss and transport phenomena, which is hence simplified when compared to reality. For more reliable results, adding these phenomena for each electrode is necessary to allow the discovery of species composition locally. Differential models will be a good option for this kind of analysis. However, they significantly increase the computational effort. An intermediate method will use unidimensional models to calculate the pressure, reactions, and compositions along the flow over each electrode.

CONCLUSIONS

This work demonstrates that it is possible to use a genetic optimization algorithm to find the maximum global point for the power of an SOFC. A cell with an active area of $0.04 \cdot 0.04 \text{ m}^2$ obtained a maximum power of 57.84 W for the unpressurized case and 84.43W for a pressurized case. The respective temperatures, current, and species partial pressures are also determined. When comparing the genetic algorithm with the deterministic algorithm, the quality of the results is adequate for both unpressurized and pressurized systems. Based on these results and the analyses conducted, the proposed objectives have been successfully achieved.

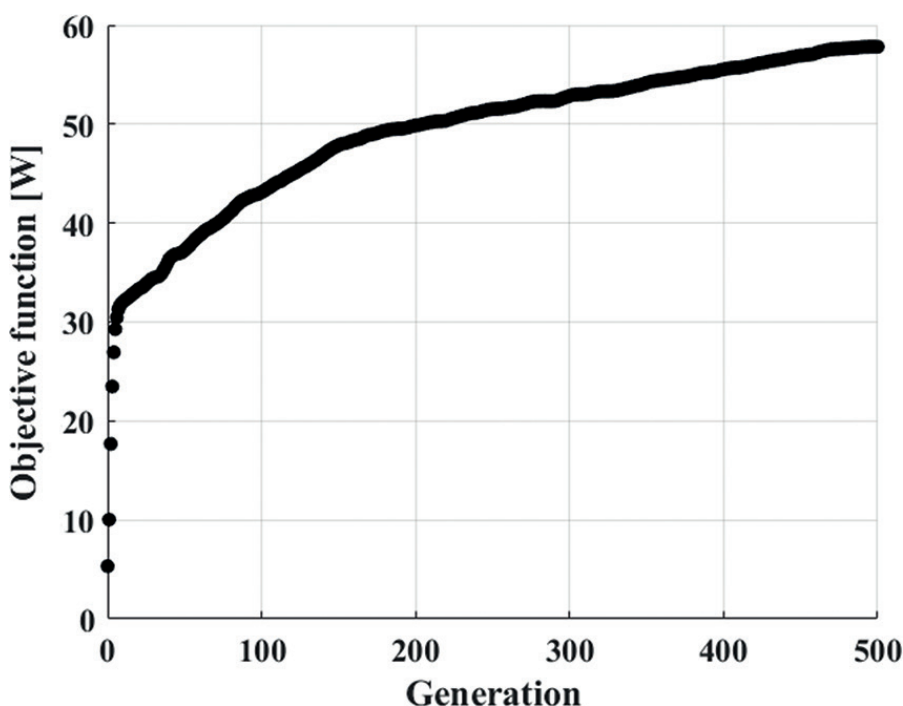


Figure 8. Results of the objective function for each generation on the genetic algorithm.

It is possible to develop more sophisticated models from the proposed model to calculate the pressure and reactions along the electrodes and elaborate a model that contains an SOFC stack. This is a challenge, as it requires significant computational resources and also requires solving the transport equations using the finite volume technique. For future work, validating the system using the solid oxide fuel cell produced at LaMPaC (Materials and Fuel Cells Laboratory) would be beneficial. Additionally, incorporating other energy generation and storage systems, along with a model for energy consumption, would enable the development of a system model applicable to practical applications, such as hybrid fast charging stations.

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Samuel Andrade established the numerical model and conducted simulations for the manuscript under the supervision of Esly Júnior, Tulio Matencio, and Rudolf Huebner. Also, Ingo Stadler, Rudolf Huebner and Rosana Zacarias gave their effort to analyze and discuss the detailed results, and they made useful comments on which the quality of study could be improved. Above all, Esly Júnior, Tulio Matencio, Ingo Stadler and Rudolf Huebner (equally contributed), have provided useful suggestions and have discussed research progress.

