Prediction of the thermodynamic behavior of SOFCs through Machine Learning

(Integrating of SOFCs with Machine Learning)

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SUMMARY

***Abstract* - This document examines advances in Fuel Cells and related technologies, concentrating on the manufacturing process through predictive formulations. The key objective is to integrate form and process, employing specialised tools to improve the outcome. A critical aspect of this approach is the systematic dissection of the final product into smaller components for thorough analysis. The manufacturing process is designed to incorporate the technology seamlessly, harnessing its capabilities to identify and capitalise on opportunities.**

Computing; Data Science; Process; Tools; Development; SOFCs

I. INTRODUCTION

Today's market is undergoing a significant transformation towards alternative sources of energy production with less environmental impact and lower CO2 emissions. CO2, one of the main contributors to climate change, is a major concern, not least because of its widespread use in large engines such as those on cargo ships. There are numerous ongoing studies dedicated to mitigating this impact and innovating new alternatives for the present and the future.

Several existing renewable energy technologies are proving effective in mitigating these environmental challenges. Solar and wind energy, integrated into the production matrix, combined with bioethanol (C2H5OH) and hydrogen (H2) in the fuel matrix, are emerging as promising solutions. These technologies play a key role in remodelling our energy landscape and solving the pressing problem of CO2 emissions.

The transition to cleaner and more sustainable energy sources reflects a collective commitment to combat climate change and promote a greener future. This change implies not only a reduction in dependence on traditional energy sources, but also the adoption of innovative and ecological alternatives to propel us into a more environmentally conscious era.

According to Zanin[1], with the arrival of the third generation of MS-SOFCs (Metal Supported Solid Oxide Fuel Cells) that use hydrogen, carbon, or biofuels in low temperature systems (around 600 °C), thus increasing efficiency and reducing emissions. In this way, the combination of these technologies would result in better electrification in many sectors, thus generating a major technological advance.

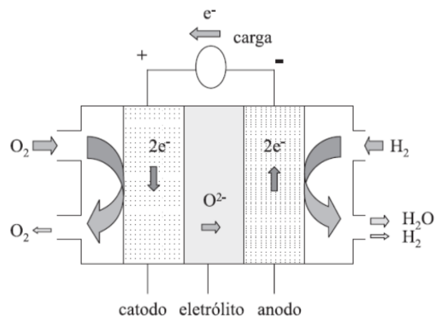

Figure 1 - Operating representation of SOFC (AMADO *et al.*, 2007)[2].

The SOFC system has greater possibilities for fuels in its matrix, such as natural gas, for example, which makes this model more attractive in essentially industrial applications, such as cogeneration systems, and because it has a solid electrolyte, it is more stable, unlike those with a liquid electrolyte, as it avoids problems associated with impregnation of the electrodes and wetting of the catalyst. One of its characteristics is its greater tolerance to contaminants in the fuel (DINCER, 2013)[4].

1. OBJETIVES

Primary Objectives

It is about finding the best production model through models already used in the manufacturing process, that is, using tables of previously tested results, inserting them into a database and then programming in Python, using tools available in the language to create a predictive model and thus obtain results in advance. Afterwards, by manipulating the table itself, we can change parameters such as diameter, density, weight, temperature, humidity, and other possible variables, so that we can observe the results through the predictive analysis that the script has brought to light.

Secondary Objective:

Finding the best way of cross-referencing information aligned with the SOFC development process, to create alternatives and seek the best energy index for the cells, thus achieving cells compatible with international standards or even seeking a new generation of cells.

2. STRATEGY AND METHODOLOGY

Basically, we need to understand what programming language is in a superficial way so that we can understand this vast world that is machine learning and data science, so that we can understand how we are going to act and develop this programme.

Firstly, Python, the most widely used language in the world of machine learning, comes from Java, which in turn is a widespread language used for a wide variety of applications, including applications for smartphones, computers, websites, among others.

Python, like other languages, has libraries, in this case libraries that are downloaded to the software terminal, which make it possible to automate the use of tables and, from these tables, generate automatic reports, reports that can predict behaviour.

According to DAS3, there are around 25 libraries for Data Science, where these tools facilitate the use of complex data and provide relevant results, and can be used to combine these libraries to arrive at a reliable predictive result.

In this way, we can understand that certain SOFC parameters can be grouped together to produce results that we can analyse and cross-reference with this information, hoping to find patterns that will help facilitate research and development into these variables.

To assess the different properties of the cells, variables such as Temperature (K) and Membrane Thickness (L) were used, thus utilising the inputs expressed by Trindade, Sharaf and Azizi [5].

To formulate the programme to be used, we used the Jupyter programming platform in Python and installed libraries such as Scikit-learn[6], Pandas[7], Maplolib[8], in this way it was possible to carry out the study with Machine Learning combining two variables, temperature and the thickness of the edge where in the data prediction using a mass of data with 100 observations, with only one predictor variable, which will be the variable x and the target variable, which will be y. For this purpose, we use the parameters n_samples = 100 and n_characteristics = 1.

After entering the data, configuring, and predicting, the dispersion curve was created with the data before and after the prediction, thus being able to verify the dispersions found, which can be improved and worked on to reduce the dispersion curve according to the objective. In addition, few quantitative studies have been reported on the thermal behaviour of small SOFC systems. The aim of this article is to obtain information on the possibility of using small SOFC systems with fast and frequent starts and stops by analysing their thermal behaviour.

Observing the work of Shimada, Kato and Tanaka[9], there is a great deal of depth in the study where it is possible to visualise thermal points to be explored to achieve better results. It includes various phases and parameters, such as temperature, fuel flow rate, heat exchanger efficiency, SOFC stack height, fuel utilization, among others. As already mentioned, the aim of this work is to use these points of analysis to cross-check temperature information and find a parallel between them and other variables that have been explored in the future.

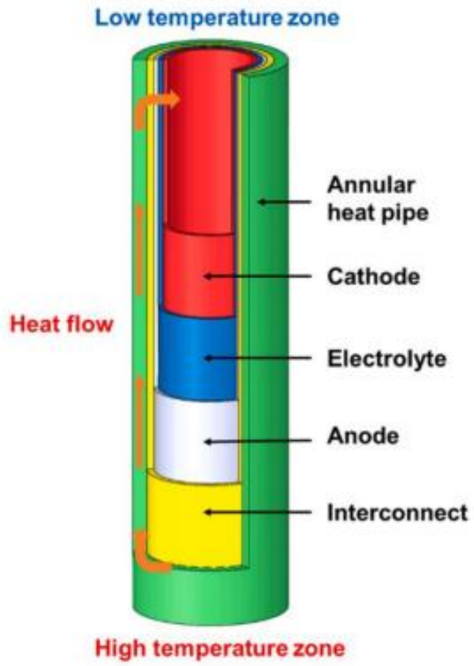

Figure 2 - SOFC Structure (ZEZHI, *et al.*, 2020)[10]

The text describes the development of small solid oxide fuel cell (SOFC) systems with a focus on rapid and frequent starts and stops. It emphasizes concerns about operating at high temperatures and the limited quantitative studies on the thermal behavior of these systems. A two-dimensional numerical model of a 1 kW cylindrical SOFC stack was used to study thermal behavior[9]. The text discusses energy generation efficiency under various operating conditions, model validation, and the dependence of start-up on structure and operating conditions. The conclusion is that under certain conditions, 1 kW SOFC systems may be suitable for rapid and frequent starts and stops, achieving an efficiency of approximately 60%.

The considered model consists of a cylindrical SOFC stack composed of single-disc cells, a pre-reformer in the stack, a heater, a gas exchanger, and a collector. In this configuration, we obtain two main formulas[9]:

CH4 + H2O = 3H2 + CO, H1300 = 227.5 kJ/mol – Endothermic.[9] (1)

CO + H2O = H2 + CO2, H1300 = approximately 31.8 kJ/mol - Weakly Exothermic.[9] (2)

In other words, methane and oxidizing air, considering reforming to combine the two components and provide fuel, where CH4 = 100%, and the O2 to N2 ratio in the air is 21:79, referring to the proportion of oxygen (O2) to nitrogen (N2) in the atmospheric air. In percentage terms, it indicates that approximately 21% is oxygen, and 79% is nitrogen in the composition of the air. This represents the relative concentration of these two essential components in the Earth's atmosphere.

Combining the fundamental equations with predictive analysis of these variables, as demonstrated in the programming example, highlights the importance of using Machine Learning. This, along with the ability to analyze temperatures in the Reformer and/or Pre-Reformer, SOFC stack, Heat Exchanger, and Steam Generator, allows for a comprehensive examination of how each molar concentration derived from the thermal efficiency formula correlates with the other variables[9].

$$cc = \frac{P}{n\ddot{y}CH4, entrada \cdot \ddot{y}HCH4} \qquad (3)$$

Figura 3 - The thermal efficiency of the SOFC DC system (SHIMADA, *et al.*, 2007)[9]

Where P is the steady-state electrical output, nÿCH4 is the molar flow rate of methane at the inlet, and ÿHCH4 is the enthalpy change in the combustion of methane at 298 K in the Higher Heating Value (HHV)[9]. The HHV is considered the gross calorific value, where water vapor is condensed, and additional heat is recovered. Within this process, the interconnector has the function of utilizing this condensation to increase efficiency[11].

a. PYTHON PROGRAMMING

```
import sklearn as sk
import pandas as pd
import matplotlib.pyplot as plt
import array
>>> from sklearn.datasets import make_regression
>>> x, y = make_regression(n_samples=100, n_features=1, noise=20, random_state=100)
>>> x

#Temperature/K, Membrane Thickness/cm.

np.array([[343, 0.0178],# Trindade Model
          [353, 0.0254],# Sharaf Model
          [353, 0.0383],# Azizi Model
          [354, 0.0245],# Matozinhos test
          [356, 0.0246],
          [400, 0.0247],
          [430, 0.0248],
          [460, 0.0249],
          [490, 0.0250],
          [500, 0.0251],
          [550, 0.0252],
          [600, 0.0253],
          [650, 0.0254],
          [700, 0.0255],
          [750, 0.0256],
          [800, 0.0257],
          [850, 0.0258],
          [900, 0.0259],
          [950, 0.0260],
          [999, 0.0261]])# Matozinhos

>>> y
np.array([60, 70, 80, 90, 100])
# target with 60%,70%,80%,90%,100%
array([ 60,  70,  80,  90, 100])

from sklearn.linear_model import LinearRegression
modelo = LinearRegression()
modelo.fit(x,y)

#Output
 LinearRegression
 LinearRegression()
modelo.predict(x)
# Output Prediction Below
```

```
array([-1.60285561e+01, -4.97437661e+01, -7.23004616e+01,  3.96433566e+01,
       -7.05046022e+01, -4.56077192e-01,  5.79552854e-01,  5.06344477e+01,
       -6.76180675e+01, -2.45005910e+01, -8.34695572e+00,  3.13432004e+01,
        1.70233233e+00,  9.16919624e+00,  2.69942284e+01, -2.79943227e-01,
       -2.31131686e+01, -1.93537127e+01,  2.04974307e+01,  3.01800364e+01,
       -5.92834642e+01, -4.85944054e+00,  2.95963751e+01, -2.43051064e+01,
       -1.09039697e+01,  9.87243299e+00, -8.16325561e+00,  1.72570504e+01,
        3.88241967e+00,  2.75750087e+01,  6.98343285e+00,  5.52287287e+01,
       -7.16171853e+01, -3.70487413e+01, -5.10957111e+01,  1.40740387e+01,
       -3.45156726e+01, -2.28956400e+01, -3.51101478e+01,  2.45479408e+01,
       -2.88299430e+01,  6.57802802e+01, -3.15816953e+01, -4.33806181e+01,
       -2.23562778e+01, -3.69586505e+00, -4.17541208e-01,  3.29017842e+01,
        6.26087146e+01,  1.34662841e+01, -6.67183276e+01,  4.15124705e+01,
        3.65140020e+01, -4.44394991e+01, -6.47963251e+01, -6.98760324e+01,
        4.81813744e+01, -7.60477692e+01,  5.26952938e+01, -5.61768627e+01,
        8.28162673e+01,  8.53612442e+00, -2.57033520e+01, -1.41788889e+01,
        3.28856732e+01,  4.16276999e+01, -2.31528547e+01, -4.58527815e+01,
       -3.59213812e+01,  3.78300722e+01, -2.44199439e-02,  2.02347235e+01,
        2.77074599e+01,  1.45518119e+01, -1.85383906e+01, -3.67235738e+01,
        1.84229236e-01,  4.66817408e+01,  3.01803876e+01, -3.84292369e+00,
       -5.41517433e+01,  1.69729730e+01,  5.97029683e+01,  1.44259465e+01,
       -4.08844121e+01, -4.92751171e+01,  2.32172186e+01, -2.79672839e+01,
       -3.91110773e+01, -4.64182276e+01, -5.97354220e+01, -1.92684537e+01,
       -1.39518490e+01, -1.09267962e+01,  7.45090162e+01,  8.48612063e+00,
        7.63386453e+01, -1.02524996e+02,  2.93830340e+01,  3.88276898e+00])
```

Table 1- Table Predict of Python Programmer

```
import matplotlib.pyplot as plt
plt.scatter(x,y)
plt.show()
```

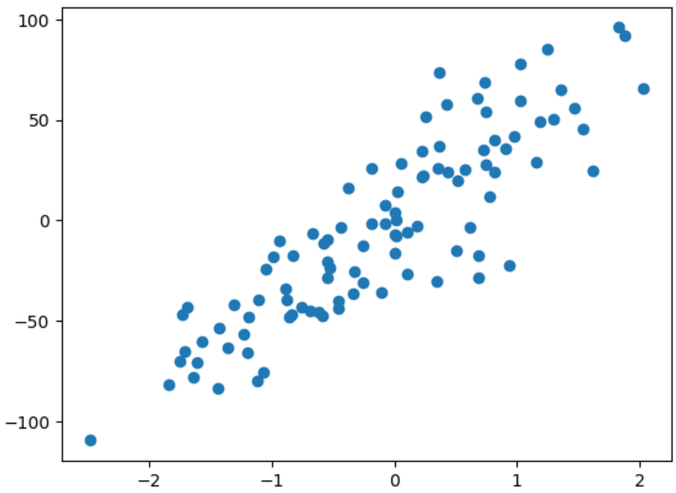

Figure 4 - Graphic Dispersion

#linewidth with 5 some target velour.

```
plt.scatter(x,y)
plt.plot(x, modelo.predict(x), color='red', linewidth=5)
plt.show()
```

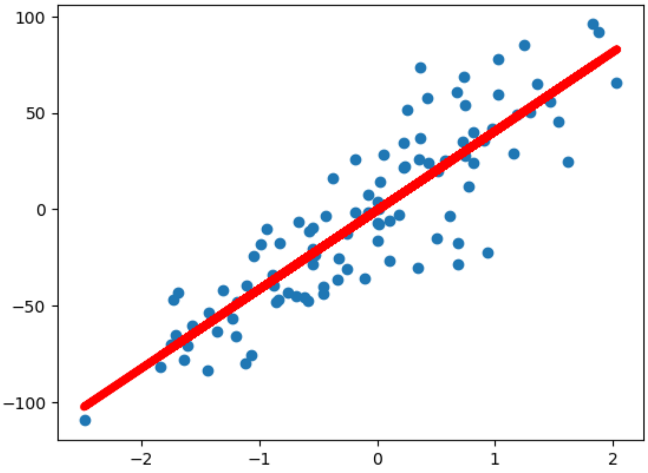

Figure 5 - Graphic Dispersion with target 60% to 100%

3. EXPECTED RESULTS

By analysing the scatter diagram, it is possible to see that after prediction the results are more closely grouped with the chosen target, knowing that this prediction was used, it is a simple prediction and can still be improved by adding more variables and also longer observation intervals for a more comprehensive analysis, seeking better results. Other tools can also be incorporated into the work; there is also the option of using the R language instead of the Python language as defined here. However, the Python language undergoes constant updates and significant improvements, making it possible to perfect models that contribute to the formation of more up-to-date SOFCs with higher yields.

A comparison was made between the temperatures possible with SOFCs in relation to cell membranes. These samples show that, out of a total of 100 observations, we obtained samples that represent better results, thus achieving values close to the expected target.

For future evaluation, other ambient temperatures, reference inlet, reference outlet, fuel cell inlet and outlet can be inserted. By measuring or predicting these temperatures, the efficiency can be analysed and important thermal losses can be checked, either due to direct loss due to flooding, or also due to loss by thermal conduction with the interconnection.

By empirically verifying through programming and cross-referencing this information with the literature reviews conducted, we can understand that thermal efficiency is composed of variables that can be modified to seek better results, and this can be achieved through Machine Learning. Comparing input temperatures and membrane data is just one step in a multitude of analyses that can be performed, thereby modifying the molar structure of the basic formulas (1), (2), (3). By cross-referencing data, one can stimulate the formulation of graphs for different models and, in this way, seek models that lead to advancements in the development of SOFCs.

Concluding the analysis of the presented work, it is evident that in the future, the study could be enhanced and serve as a foundation for new lines of thought, encouraging fresh research perspectives by combining information from various fields in collaboration with scientific and societal development. It is through science that significant advancements are achieved, and it is through ongoing scientific endeavors that these achievements will continue to unfold. There is a vast community of scientists and researchers who contribute to this progress.

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