Design of a Simulation Platform to Test the Suitability of Different PEM Electrolyzer Models to Implement Digital Replicas

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Abstract: Green hydrogen is produced from renewable energies, being a promising integration in the field of microgrids. For a proper utilization, hydrogen generators, known as electrolyzers, must be studied and handled with a deep knowledge about their complex and non-linear behavior. In this sense, digital replicas (DR) are mainly based on mathematical models and constitute a merging paradigm envisioned to accurately represent the operation of physical systems within a simulated framework. This paper presents the development and initial implementation of a platform to simulate different models of proton exchange membrane electrolyzers aiming at evaluating their fitness and performance. The suite Matlab/Simulink has been applied including a Graphical User Interface to facilitate the interaction with the user. This tool is envisioned to contribute scientists to select and develop DR of such challenging equipment for tasks like performance analyses, prognostics and control purposes. The main features of the platform as well as preliminary results are reported.

1 INTRODUCTION

Renewable energy sources (RES) like solar photovoltaic and wind generators require energy storage systems to handle in short and long-term energy flows. This fact achieves higher importance due to the variability of such RES, which gives place to situations of significant surplus of energy. The combined use of RES and hydrogen is a promising solution for the storage of such surplus energy (Atlam, 2011).

Hydrogen must be produced using equipment called electrolyzers or hydrogen generators by different technologies. Among these, electrolysis of water using RES seems to be one of the best options (Guilbert, 2020). This way, the surplus of energy from RES can be devoted to produce hydrogen through water electrolysis, acting as long-term energy storage means (Ogawa, 2018).

Proton exchange membrane (PEM) electrolyzers (PEMEL) are considered as a viable alternative for generation of hydrogen from RES (Abe, 2019). In fact, hydrogen generated from RES is commonly referred to as renewable hydrogen or, even, green hydrogen (Noussan, 2021).

In this sense, a microgrid can be defined as an integrated power system made up of several power generation systems, energy storage means, and electrical loads. In general, it can consist of a single autonomous grid or it can be connected to the general distribution grid. The development of microgrid technology is of great significance to adjust the energy structure, protect the environment, solve the problem of energy consumption in rural and remote areas, and the transition from the traditional power grid to a smart grid (Wu, 2020).

The main goal of autonomous microgrids that include RES and hydrogen is to optimize electricity production, trying to adapt the production of electrical energy to the energy demanded, avoiding energy gaps at all times. In this context, PEMEL are becoming one of the most useful technologies to

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produce green hydrogen though RES in microgrids. The integration of PEMEL in microgrids has shown interesting advantages to improve microgrid performance and promote the use of hydrogen energy (Li, 2019).

PEMEL are composed of a number of individual cells stacked into a stack to get the desirable production of hydrogen at a given voltage. The objective of this approach is to adjust hydrogen production to the available surplus energy. Hence, a supervisory and control system must implement an energy management strategy (EMS) to handle the activation of the PEMEL (González, 2021).

Figure 1 shows the block diagram of the microgrid that is being developed in our laboratories. This one consists of a photovoltaic (PV) array, a lithium battery, and a combination of electrolyzer, fuel cell and hydrogen tank.

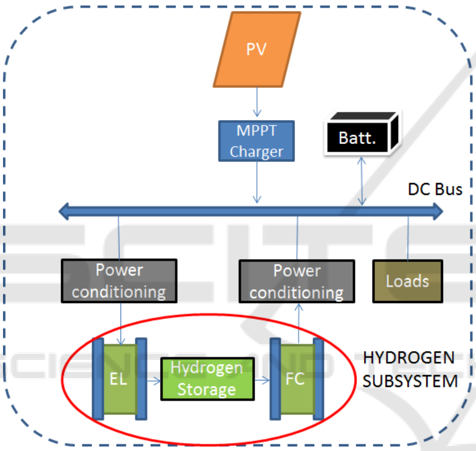

Figure 1: Schematic diagram of the stand-alone microgrid with hydrogen subsystem.

Such microgrid is framed in an on-going R&D Project that deals with the digital transformation in the field of RES and microgrids. Essentially, this project consists of the design and development of a digital representation or Digital Replica (DR) of the described microgrid.

The concept of DR, also known as digital twin, receives important research efforts from academicians and practitioners. There is a lack of a generalized concept of DR, so the definition proposed in (Calderón, 2019) is considered in the present work, namely, a DR is a representation of a physical process/system which runs in a digital environment.

The objective of DR is beyond simulating the behavior of the physical counterpart in an off-line mode, it is expected to accurately emulate the dynamics of the physical facility running in a software environment in parallel. Moreover, it is envisioned to support decision taking in the EMS for enhanced performance and reduction of degradation of hydrogen equipment.

In general, DR acts as a powerful workbench on which to test, evaluate, analyse, etc., as if it were the real system, avoiding the limitations and technical-economic disadvantages of taking the physical system to certain states operatives (Calderón, 2019). In particular, for the energetic context some interesting applications are conducting preventive and predictive maintenance to increase the life time; decreasing downtimes and associated costs; study of behavior, detection of deviations and reaction to extreme situations; optimization of efficiency and operation from an economic and energy point of view; as well as making decisions based on data management, just to name a few (Calderón, 2019).

There is a large and increasing amount of papers dealing with digital replicas in industrial context; however, for energy-related frameworks, this topic has been scarcely treated (Calderón, 2019). For instance, in (Tao, 2018) DR of wind turbines are addressed; buildings are digitally mirrored in (O'Dwyer, 2019); and a cyber-model for power electronics in microgrids is presented in (Senthilnathan, 2019). An IoT-based digital twin is proposed in (Saad, 2020) focusing on communication aspects of Energy Cyber-Physical Systems. An algorithm to schedule the energy storage system of a microgrid is proposed in (Park, 2020) under the concept of digital twin.

When deploying a DR, the choice of the software suite is not a trivial task. There is no consensus about the software that must be applied, in fact, different approaches are found in previous literature. EnergyPlus, focused in energy-related facilities, is used in (O'Dwyer, 2019) to implement a DR. Black-box models or artificial intelligence tools like Neural Networks are applied in (Rahman, 2018) and (Park, 2020). LabVIEW, widely used for monitoring and virtual instrumentation, serves to deploy a DR in (Senthilnathan, 2019). Focused on mathematical representations, Matlab/Simulink is selected in (González-González, 2018).

In this latter regard, a brief literature survey shows that Matlab/Simulink provides a high degree of maturity and versatility to implement models and DR of electrolyzers. For example, the work in (Xiao, 2009) develops the model of a PEM fuel cell under the Matlab/Simulink environment. A dynamic model of a PEMEL based on Matlab/Simulink is presented in (Awasthi, 2011). A Simulink-based model of a PEMEL is reported in (Beainy, 2014). An alkaline electrolyzer is simulated in (Tijani, 2014) trough Matlab. In (Yigit, 2016) Simulink is used to model a high-pressure PEMEL. The model of a PEMEL powered by a solar panel is implemented in Matlab/Simulink in (Albarghot, 2016). Matlab is applied to simulate hydrogen production through a PEMEL from PV energy in (Ismail, 2019).

It must be noted that a lack that most of previous literature present is a user-friendly Graphical User Interface (GUI), which is an important aspect when handling models and DR. Only (Xiao, 2009) and (Tijani, 2014) report the development of a GUI. Indeed, in (Rocca, 2020) it is asserted that digital twins need a proper GUI to be more user friendly and support easier decision making.

This paper presents a platform based on Matlab/Simulink to assess different models for PEMEL. The design and initial successful results are reported. The ultimate goal of the developed platform is to support the evaluation of different models available in previous literature in order to implement a DR. The user is able to choose the model among a variety and can also edit certain parameters. After that, the simulation of the selected replica is plotted and displayed. By using this tool, the suitability of the model can be analysed and evaluated for the hydrogen generator. A remarkable feature is that a GUI has been developed to provide an intuitive and easy-to-use interaction.

The structure of the rest of the manuscript is as follows. Section 2 reviews mathematical models widely validated in literature to be considered as DR. The organization of the developed platform is described in Section 3. The fourth section reports the preliminary implementation and results. Finally, the main conclusions of the work are addressed.

2 REVIEW OF THE SELECTED PEMEL MODELS

This section deals with the models, available in the literature, that have been considered for the development of the simulation platform. The goal of this platform is to corroborate the feasibility of each one of them to adapt itself to a certain real electrolyzer. Models based on electrical equivalents of the electrolyzer have been used, since the final objective is to obtain the relationship between the electrical energy consumed (input) and the flow of electrolytic hydrogen generated (output).

In this regard, having an accurate model of a real device is essential to reproduce its operation and the interactions with the rest of involved equipment.

The aim of this work is to obtain the input current-voltage characteristic for a single PEM electrolyzer cell under steady-state conditions. In these models, the reversible voltage is defined from Gibbs energy, whose calculation is based on the Nernst equation. The remaining voltages (activation overvoltage, ohmic potential and diffusion over-potential) are determined by applying the Taffel equation.

It is also possible to determine the electrolyzer operating efficiency from the H_2 generation ratio as a function of its operating point.

In this first proposal, the losses of the DC/DC converter have not been taken into account for the calculation of the performance of the electrolyzer stack.

All the considered models have been applied, tested and compared with the references used, obtaining results without significant errors.

2.1 Equivalent Electrical Model for a PEMEL under Steady-state Conditions

In this case, the equivalent electrical model developed in (Atlam, 2009; Atlam, 2011) for a PEMEL is simulated. This simulation is based on the equivalent circuit model that appears in Figure 2.

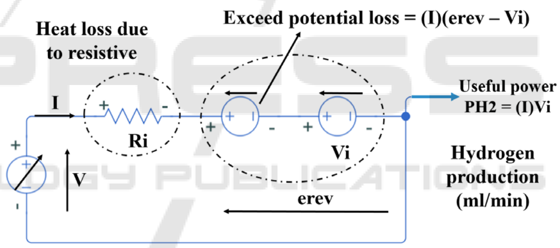

Figure 2: Equivalent circuit model for a single PEMEL.

As can be observed in Figure 2, the static behavior of the electrolyzer is represented by a reversible voltage in series with a resistance. The reversible potential is the voltage of the electrolyzer without losses. The higher heating value (HHV) for e_{rev} is considered a constant DC voltage source equal to 1.476V (T=20ºC, p=1atm).

The reversible potential consists of the ideal electrochemical potential, V_i, along with the activation over-potential.

The ohmic over potential during the operation are collected in R_i. For these conditions, the non-linear model used in this case responds to the equation,

$$V = 1.46760 - 1.4760e^{-\frac{5}{0.02}I} + 0.3264I \tag{1}$$

On the other hand, the ideal electrochemical potential, V_i, is defined for the electrolysis reaction and is obtained from the increase in Gibbs free energy according to the expression:

$$V_i = \frac{\Delta G}{2F} \tag{2}$$

Being:

$$\Delta G = 285{,}840 - 163.2(273 + T) \tag{3}$$

Under normal pressure and temperature conditions (20ºC and 1 atm), V_i=1.233V.

To determine the hydrogen generation ratio according to the electrolyzer operation point, the Faraday law is used. The hydrogen production rate, v_H (ml min^{-1}) with respect to the input current I (A) can be calculated by expression,

$$v_H = v_M(l)\left(\frac{10^3\ ml}{l}\right)\left(\frac{60\ s}{min}\right)\left(\frac{I\left(\frac{C}{s}\right)}{2F(C)}\right) = v_M(10^3)(60)\frac{I}{2F} \tag{4}$$

The electrochemical power of hydrogen can be derived from V_i (i.e. useful power P_{H2}) through the expression,

$$P_{H2} = v_H\left(\frac{ml}{min}\right)\frac{\Delta G\left(\frac{l}{mol}\right)}{v_m\left(\frac{l}{mol}\right)\left(\frac{10^3\ ml}{l}\right)\left(\frac{60\ s}{min}\right)} = v_M(10^3)(60)\frac{I}{2F}\frac{2FV_i}{v_M(10^{3)}(60)} = IV_i \tag{5}$$

According to (Atlam, 2011) the input electrical power, P, of a cell is defined by Eq. (6):

$$P = VI = I^2 R_i + I e_{rev} = \left(v_H \frac{2F}{v_M 10^3(60)}\right)^2 R_i + \left(v_H \frac{2F}{v_M 10^3(60)}\right) e_{rev} \tag{6}$$

The PEMEL cell efficiency η_e is obtained from the ratio between the electrochemical power of hydrogen and the input power,

$$\eta_e = \frac{P_{H2}}{P} = \frac{V_i I}{VI} = \frac{V_i}{V} \tag{7}$$

The effect of pressure and temperature on the characteristic I-V curve of a PEMEL cell is investigated in this work. To do this, both R_i and e_{rev} have been modelled as functions of p and T.

$$R_i(T, p) = R_{io} + k\ ln\left(\frac{p}{p_o}\right) + dR_t(T - T_o) \tag{8}$$

$$e_{rev}(T, p) = e_{rev_o} + \frac{R(273 + T)}{2F}\ ln\left(\frac{p}{p_o}\right) \tag{9}$$

The I-V characteristic is obtained for a single PEMEL cell, with conditions of normal ambient temperature (20 ºC) and nominal atmospheric pressure (1 atm).

2.2 Modelling by Varying Temperature and Pressure

In the previous case, the reversible potential is considered a constant value of 1.476V. This is because both the ideal electrochemical potential, Vi, and the activation overpotential are calculated for nominal conditions of temperature and pressure (T=20 ºC, p=1 atm).

In this case, the effects of varying electrolyzer temperature and pressure on electrolyzer performance behavior and over-potentials are presented and analysed.

The developed model in (Awasthi, 2011) aims at determining the relationship between the cell current and cell voltage. This model is based on equation (9), but instead of considering $e_{rev,\ o}$ a constant value (1.229V), in this work a temperature dependant value is applied. The temperature dependant value or reversible cell voltage is given by:

$$E^0_{rev} = 1.229 - 0.9 \times 10^{-3}(T_{el} - 298) \tag{10}$$

The activation overpotential is calculated applying the Butler-Volmer equation for both anode and cathode, giving:

$$\eta_{act} = \frac{RT}{\alpha_{an}F} arc\sinh\left(\frac{i}{2i_{o,an}}\right) + \frac{RT}{\alpha_{cat}F} arc\sinh\left(\frac{i}{2i_{o,cat}}\right) \tag{11}$$

Ohmic over-voltages:

$$\eta_{ohm} = \frac{\delta_m I}{A\sigma_m} \tag{12}$$

2.3 Model According to Tafel's Law

According to Tafel's law, the cell voltage in this case is expressed as a function of the current density (Ismail, 2019):

$$V_e = a + b \times \log(I) + c \times I \tag{13}$$

The parameters a, b and c are defined according to the particular features of an electrolyzer cell (e.g., geometry, flow, material, pressure and temperature conditions)

Taking into account the ideal gas law, the hydrogen production rate is calculated by:

$$Q_{H_2} = \frac{N_{cell} \times R \times I_f \times T}{Z \times F \times P} = \frac{N_{cell} \times 8.32 \times I_f \times T}{2 \times 96500 \times 0.1013} \tag{14}$$

The efficiency of electrolyzer is given by the following equation:

$$\eta_{el} = \frac{1.23 \times s}{V_F} \tag{15}$$

2.4 Dynamic Emulation of a PEMEL

The objective of this case is to develop a dynamic model of a PEMEL. The equivalent circuit model considered is shown in Figure 3.

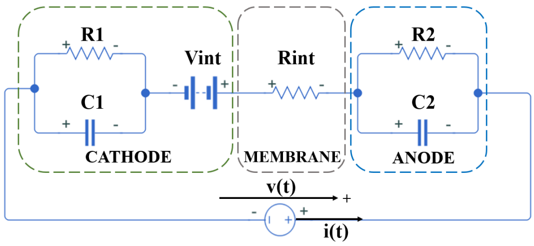

Figure 3: Equivalent circuit scheme of the PEMEL.

This model uses resistor-capacitances (RC) networks to represent the dynamic behavior of the electrolyzer in the cathode (R1C1) an in the anode (R2C2) respectively. As pointed in (Atlam, 2011), the V_{int} voltage reproduces the power converted into hydrogen, whereas the resistance R_{int} reproduces the losses in the membrane.

Although the two capacitances can be assumed equal, the resistors represent different effects: R_2 simulates Gibbs energy and the heat loss in the anode, and R_1 only just the heat loss in the cathode.

3 OPERATION AND STRUCTURE OF THE PLATFORM

The GUI serves as a centralized tool for the study of the behavior of the different electrolyzer models presented in the literature. The models selected for the interface have been (Atlam, 2011), (Awasthi, 2011), (Ismail, 2019) and (Guilbert, 2019).

The model (Atlam, 2011) has been taken as an example to explain the functioning and structure of the GUI.

In addition, the design of the GUI has been performed taking into account the guidelines reported in the ISA-101 standard.

The performance of the designed platform is based on the relationship between the block diagrams of the DR in Simulink, the Matlab workspace and the GUI. Fist, the user configures the values of the parameters used for a specific model of the electrolyzer. These values are loaded to the Matlab workspace from where they are read by Simulink in order to simulate the DR.

For the case of (Atlam, 2011), the block diagram in Figure 4 differentiates the voltage calculation for constant or pressure and temperature dependant values of e_{rev} and R_i.

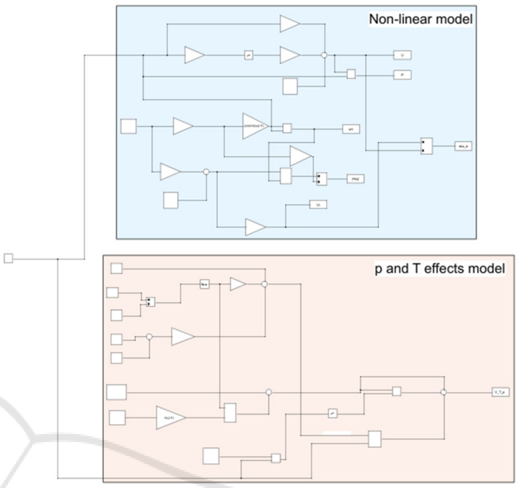

Figure 4: Block diagram of the model described in subsection 2.1.

To finish, the results are sent back to the workspace and read by the GUI to present the data to the user.

The flow of data and information during the execution of the GUI is represented in Figure 5.

The interconnection between environments allows the user to handle only the GUI without the need to interact directly with the models in Simulink or the Matlab workspace.

Data exchange between the platform and the experimental setup of the PEMEL will be handled by means of a middleware, namely using the interface OPC (Open Platform Communications).

This way, magnitudes gathered by the automation system of the microgrid will be shared with the GUI for real-time operation.

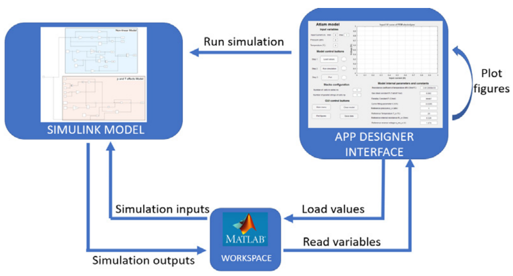

Figure 5: Data flow and operation scheme.

3.1 Structure of the GUI

The GUI has a structure composed of several tabs navigable between them by a series of buttons. The main tab "Electrolyzer model selector" allows the user to access the display and control tabs of each of the DR modelled on Simulink.

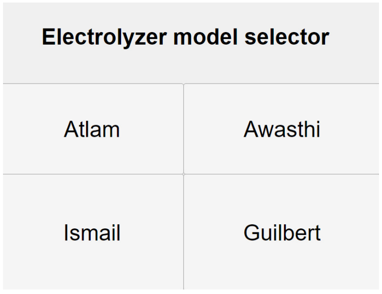

Figure 6: Main tab Electrolyzer model selector.

Inside the model tab (see Figure 7), the GUI shows a configuration zone of the parameter used in the DR, buttons ordered in a specific sequence to execute the Simulink simulation and represent the results, and a graph associated with the I-V curve characteristic of the electrolyzer.

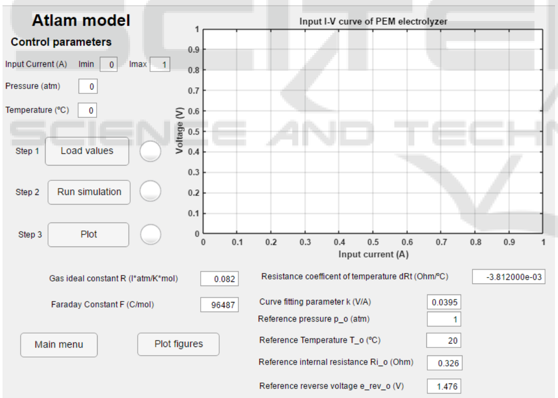

Figure 7: Atlam model tab.

The "Load values" button sends the values of the model parameters to the Matlab workspace to be read by Simulink in its simulation. The "Run simulation" button runs the simulation of the current Simulink model. At the end of the simulation, the results are stored in the Matlab workspace. The "plot" button reads the values stored in the workspace and generates the figures of the model's representative curves.

Each button is accompanied by a LED indicator that shows the state of the step. If the indicator is in red color it means that the step is running and if it is in green color, the step has finished, and the user can continue to run the next step.

The "Main menu" button returns the view to the main tab by saving the current status of the model tab. On the other hand, the "Plot figures" button changes the tab displayed to one centred on the representation on the remaining plots of the model, such as the curves I-vH, P-vH and P-ηe. (see Figure. 8)

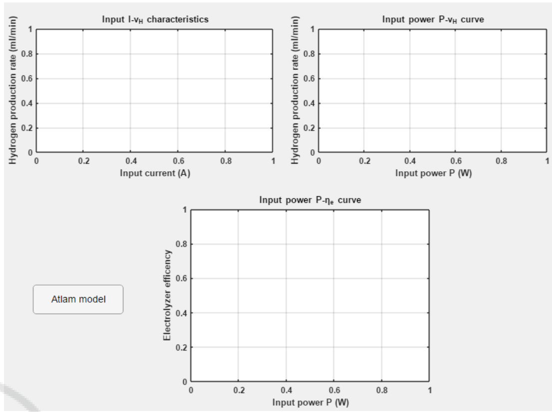

Figure 8: Plot figures tab.

4 IMPLEMENTATION AND RESULTS

In order to demonstrate the implementation of the developed platform, the model (Atlam, 2011) has been simulated under normal pressure and temperature conditions (T=20 ºC, p=1 atm) to compare the result of the DR with the model. The obtained results are seen in Figure 9.

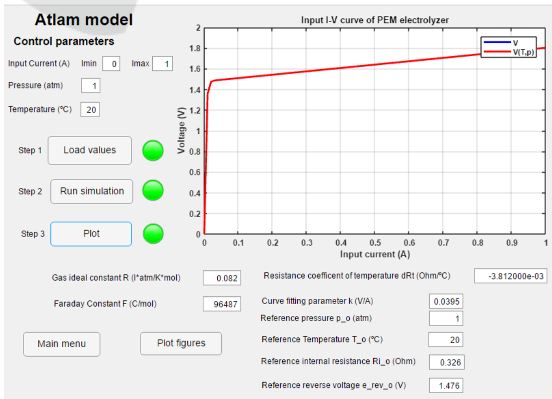

Figure 9: Input I-V curves at 20 ºC and 1 atm represented in the GUI.

The curves I-V and I-V(T,p) coincide because the simulated pressure and temperature conditions are equal to the reference pressure and temperature values (T=To=20 ºC, p=po=1 atm).

The LED indicators show that all steps have been successfully completed and all curves shown, including those in the “Atlam figures” tab, match the model curves (Atlam, 2011), as seen in Figure 10.

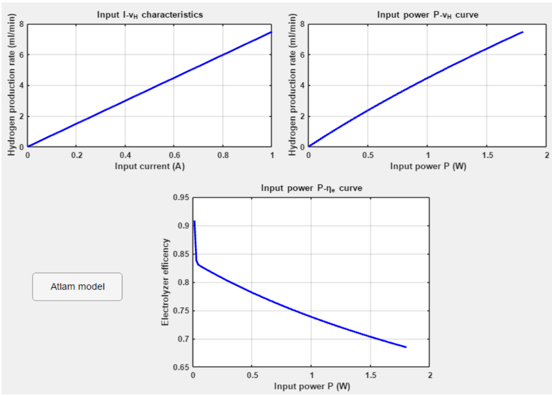

Figure 10: I-vH, P-vH and P-ηe curves simulated in the GUI.

By repeating the simulation under temperature condition 60 ºC and pressure 1 atm, the following I-V curves are obtained.

Figure 11 shows the effects of pressure and temperature variation on the voltage calculation, as well as the GUI response to interaction and parameter modification.

As in the previous simulation, the curves coincide with those of the model (Atlam, 2011), concluding that the behavior of the DR match with the model.

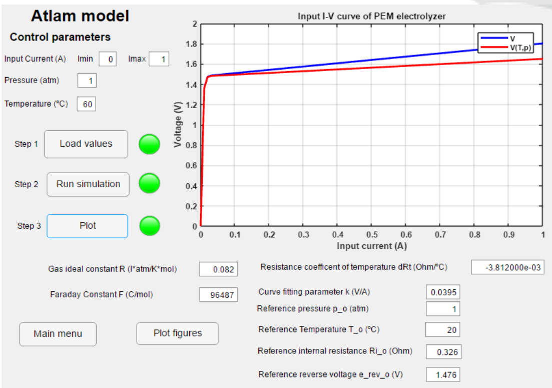

Figure 11: I-V curves at 60 ºC and 1 atm represented in the GUI.

5 CONCLUSIONS

This paper has presented a platform based on Matlab/Simulink to study models of PEMEL. A user-friendly GUI facilitates the visualization and interpretation of the simulated data, as well as the customization of certain parameters of the considered models. As a proof of concept, the results achieved for the well-known equivalent circuit model proposed in (Atlam, 2011) have been reported.

Further works will address the implementation of a DR through the comparison of experimental data of PEMEL stacks with the models using the developed platform. Moreover, the user-friendly features of the GUI are yet to be studied through usability tests in order to evaluate and improve its aspect and operation.

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