

Advanced Electrolyzer Modelisation for Green Hydrogen Production

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Abstract – In this work, we designed an advanced electrolyzer using Matlab Simscape. The main goal is to connect this component with a renewable energy source such as photovoltaic energy, wind energy, or a hybrid between them. And finding new technologies to control energy conversion in order to establish an integrated and much optimised system for the production of green hydrogen.

Keywords – green hydrogen, electrolyzer, photovoltaic, wind, control, optimise

I. INTRODUCTION

Currently, among various alternatives for hydrogen production, renewable electrolysis has the potential to overcome the incontinence limitations encountered in typical renewable energy power plants such as wind farms. Electrolyzers convert electricity from renewable sources into chemical energy, and when combined with fuel cells, hydrogen can be converted back to electricity. The system should lead to efficient storage and rapid delivery of power to the domestic grid.

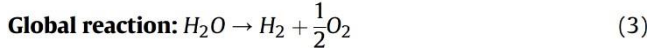
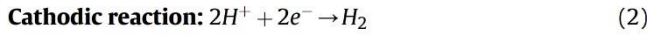
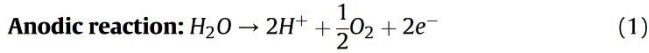
There are more or less complex models in the literature. The analytical model simulates fairly accurate polarization curves using simplified reasoning and is a sufficient tool to see the effects of key variables on electrolyte performance. Empirical/semi-empirical models allow prediction of electrolyser performance under operating conditions (pressure, temperature, etc.) using simple empirical formulas. The main drawback is that the application of this type of model is generally limited to the specific construction of this electrolyser and the operating conditions studied. Mechanical models are derived from the electrochemical phenomena occurring in electrolyzers using differential and algebraic equations and are numerically solved using a variety of methods. These models contain extensive calculations that accurately predict the polarization curves, flow rates and concentrations

of many species in the electrolyser. However, this increases the simulation time, which is considered too long for real-time applications.

II. BASIC RULES

As shown in Figure 1, the electrolyzer is an electrochemical energy converter that uses electricity to oxidize water, producing oxygen and protons at the anode. When oxygen is generated, it leaves the device as protons pass through the membrane and electrons pass through the outer circuit. On the cathode side, the electrons deprotonate, producing hydrogen. In the Fuel Cell, the opposite happens, with hydrogen and oxygen generating DC current, water and heat. The basic design of the electrolyzer consists of two half-cells with a thin, proton-conducting, insulating PEM in the center of the cell. Coming out of the two sides of the membrane, on each side of the membrane is a layer of porous catalyst, where the reactions take place. The PEM and the catalyst bilayer form the membrane electrode assembly (MEA). The encapsulated MEA is a current collector that physically and electrically connects the catalyst layer to the dipole plate. Even so, the bipolar plate is a structure that provides physical integrity to the cell, provides pathways for products and reactants, and separates one cell from another in a stack.

The reactions (anodic, cathodic, overall) that occur in an electrolyser are shown below.



Equations (1) and (2) are commonly referred to as the oxygen evolution reaction and hydrogen evolution reaction, respectively. Equation (3) is the total reaction resulting from the sum of the two halves of the electrochemical reaction occurring at the electrode in acidic medium and requires a DC power supply. A DC power supply is connected to the electrodes, and water decomposition begins when a DC voltage exceeding the reversible thermodynamic potential is applied. The water supply can be on the anode side or the cathode side. Since water is consumed on the anode side, most electrolyzers operate with feed water at the anode. Under reversible conditions (no leakage), the potential difference between the anode and cathode electrodes, called the reversible cell potential E_{rev}^0 , reaches a value that, in the presence of the required thermal energy, splits water to meet the under-thermodynamic criterion. Under the conditions ($P = 1 \text{ atm}$ and $T = 298.15 \text{ K}$), the Gibbs free energy (3) for the overall reaction is 236.483 kJ/mol (this positive value is due to the water removal reaction).

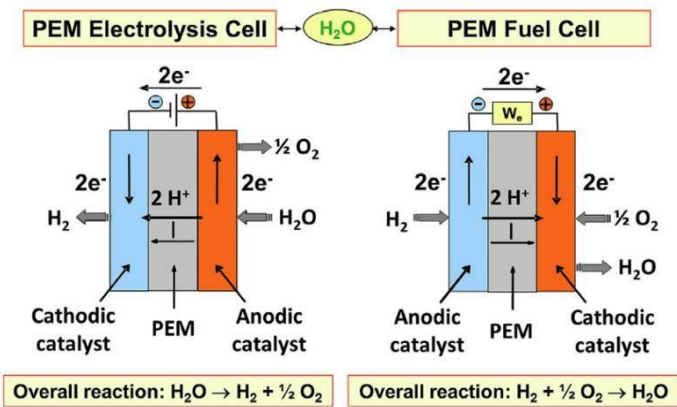


Fig. 1. Schematic representation of Electrolyzer and Fuel Cell (Lamy, 2016)

It requires an involuntary process, a source of energy. Knowing the values of the Gibbs reaction free energy (ΔG_R^0), the Faraday constant (F), and the number of moles of electrons transferred during the reaction (n), one can estimate E_{rev}^0 (Bessarabov, Wang et al., 2015):

$$E_{rev}^0 = \frac{\Delta G_R^0}{nF} = 1.229 \text{ V} \quad (4)$$

Since no external heat source is available, the total energy required for the reaction (ΔH_R^0) must be supplied by electrical energy. For the dehydration reaction (3), the ΔH_R^0 under standard conditions is 285.83 kJ/mol. Therefore, the stress required for the above reactions to proceed is greater than E_{rev}^0 and is called the thermoneutral stress in the standard state (E_{th}^0) (Bessarabov, Wang et al., 2015).

$$E_{th}^0 = \frac{\Delta H_R^0}{nF} = 1.481 \text{ V} \quad (5)$$

When a current is passed through the cell, the irreversible losses occurring in the cell make the actual voltage of the water splitting reaction higher than the reversible cell potential. These losses can be classified as Faraday losses (activation losses) and non-Faraday losses (ohmic losses and mass transfer or concentration losses). Activation loss is due to activation of the electrochemical reaction. There is a shift from thermodynamic equilibrium, which slows down the reaction rate occurring at the surfaces of the anodic and cathodic electrodes (Bessarabov, Wang et al., 2015). A change in charge storage requires that part of the cell's available thermodynamic potential be lost, which has a pronounced effect on the activation barrier. Activation loss (V_{act}) is the primary cause of efficiency loss when operating cells at high voltages and low current densities, and the amount of gas produced by the electrochemical process is proportional to the gas produced by the electrochemical process. Determined by Faraday's law that can be correlated with the amount of Charge consumed by the cell:

$$Q = nzF \quad (6)$$

Q is the charge in coulombs (C) and z is the number of charges. Considering equation (6) and the Arrhenius equation, we can derive the Butler-Volmer equation commonly used to describe the turn-on overvoltage, all considerations and equation extensions are very well explained and can be found in Bessarabov et al. (2015).

In the moderate operating range, the main losses are due to the resistance of the electrolytic cell (R_{cell}) generated by ionic and electronic conduction. Total resistive loss is determined by

applying Ohm's law. Due to the high electrical conductivity of commonly used materials (such as titanium), electron transport is likely much faster than proton transport, so only resistive losses due to proton transport through the PEM are considered. . At very high current densities, the largest loss (loss of concentration or diffusion over potential, V_{diff}) is due to mass transfer limitation. However, many authors argue that the "yes" cannot be explained by this limitation, since electrolyzers generally do not operate at high current densities. However, several studies (Hwang et al., 2009; Lebbal and Lecœuche; Kim et al., 2013) address these losses. At high current densities (greater than 2 A/cm²), the generated bubbles can block the active area, damage the electrode-electrolyte contact, and reduce catalyst utilization. Mass transfer losses are determined by the Nernst equation. This equation shows that as the product diversity increases due to transport limitation, so does the concentration at the reaction interface (Bessarabov, Wang et al, 2015).

III. MODELLING OF THE PROPOSED SYSTEM

In this study, we modelled an advanced electrolyte with the help of MATLAB Simulink software, the system consists of two sides: the anode side, which consists of fluid channels connected to a heat exchanger and a recirculation system to increase efficiency, and we will use a water tank as a source of water. On the other side, we find the cathode fluid channels connected to a dehumidifier to separate the water vapor from the produced hydrogen, and the latter is stored in a hydrogen tank. A cooling system is used to keep the system temperature stable as shown in fig. 3.

As an energy source we used three profiles: Solar power profile, Step current, Ramp current (fig. 2).

IV. SIMULATION RESULTS

As we can see on the resulting curves below. In the case of the solar configuration (fig.4), the percentage of hydrogen production increased with increasing light intensity, reaching a maximum of 0.52 g/s, then decreasing with decreasing light intensity. The same is true for energy, as it gradually increases with increasing light intensity to reach 100 KW, then decreases again, and since the energy is higher than the required energy, the gain converted to heat reaches a maximum of 22 KW. For the temperature of the electrolyzer, it also

continues to rise with the increase in hydrogen production, as it reaches 80 °C and stabilizes itself thanks to the cooling system, so the profit of the electrolyzer does not decrease due to excessive increase in temperature.

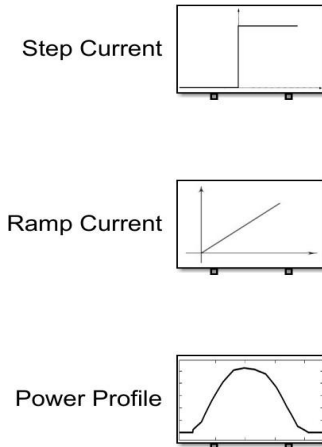


Fig. 2. Power Source Profiles

For the Step Profile (fig.5), the production rate is temporarily increased from 0 to 0.43 g/s, then it stabilizes in response to the power supply. The same applies to energy, as it jumps from 0 to 80 KW then stabilizes, and the liberated heat is constant at 20. While the cooling system manages to keep the temperature of the electrolyzer at 80 °C.

And in the Ramp Profile case (fig.6), the rate of hydrogen production gradually increased, reaching 0.45 g/s and continuing to increase. The same goes for power, as it reaches 80 KW, while the temperature reaches 80 °C and then stabilizes thanks to the cooling system.

As can be seen from the results, Due to various losses, the power is greater than the power required to produce hydrogen. The difference is in the amount of heat dissipated. The graph also shows the thermal efficiency of the electrolyser. It indicates the percentage of electrical energy used to produce hydrogen, based on the calorific value of hydrogen. This electrolytic cell is about 87%. The cooling system ensures that the system temperature does not exceed 80 °C.

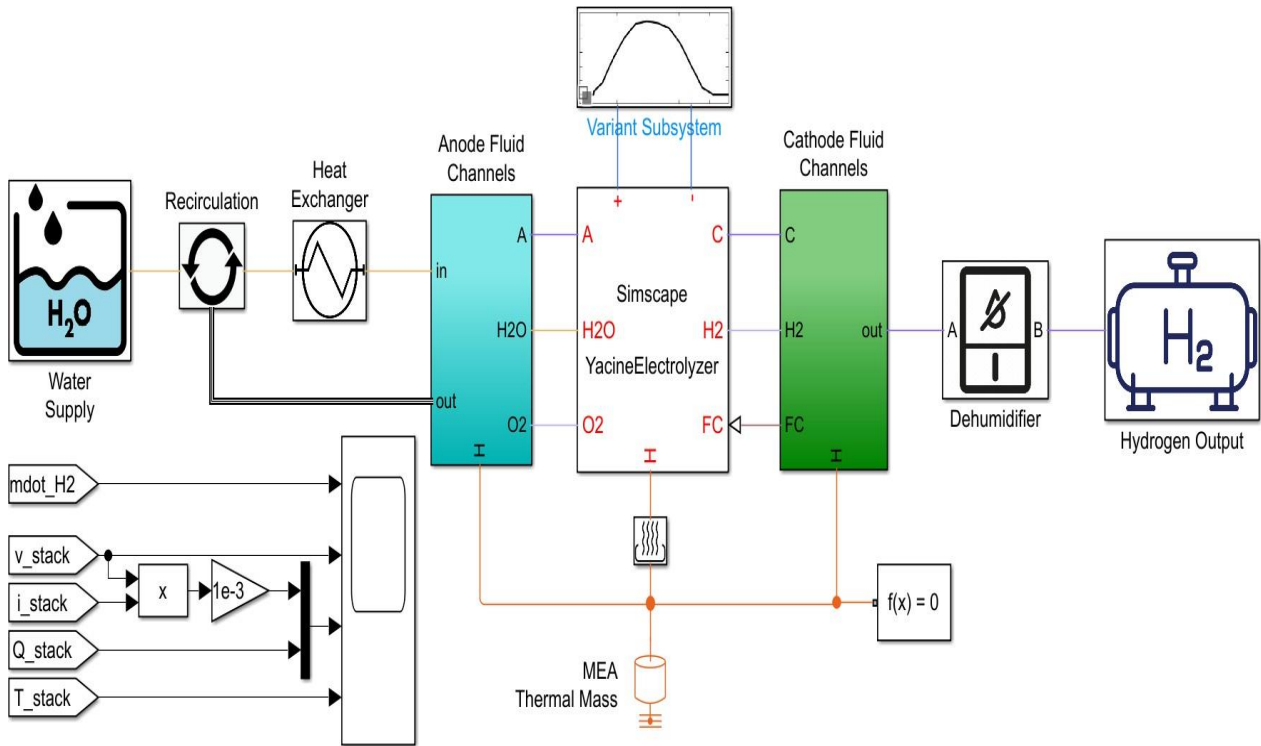


Fig. 3. Advanced Electrolyzer Simulation

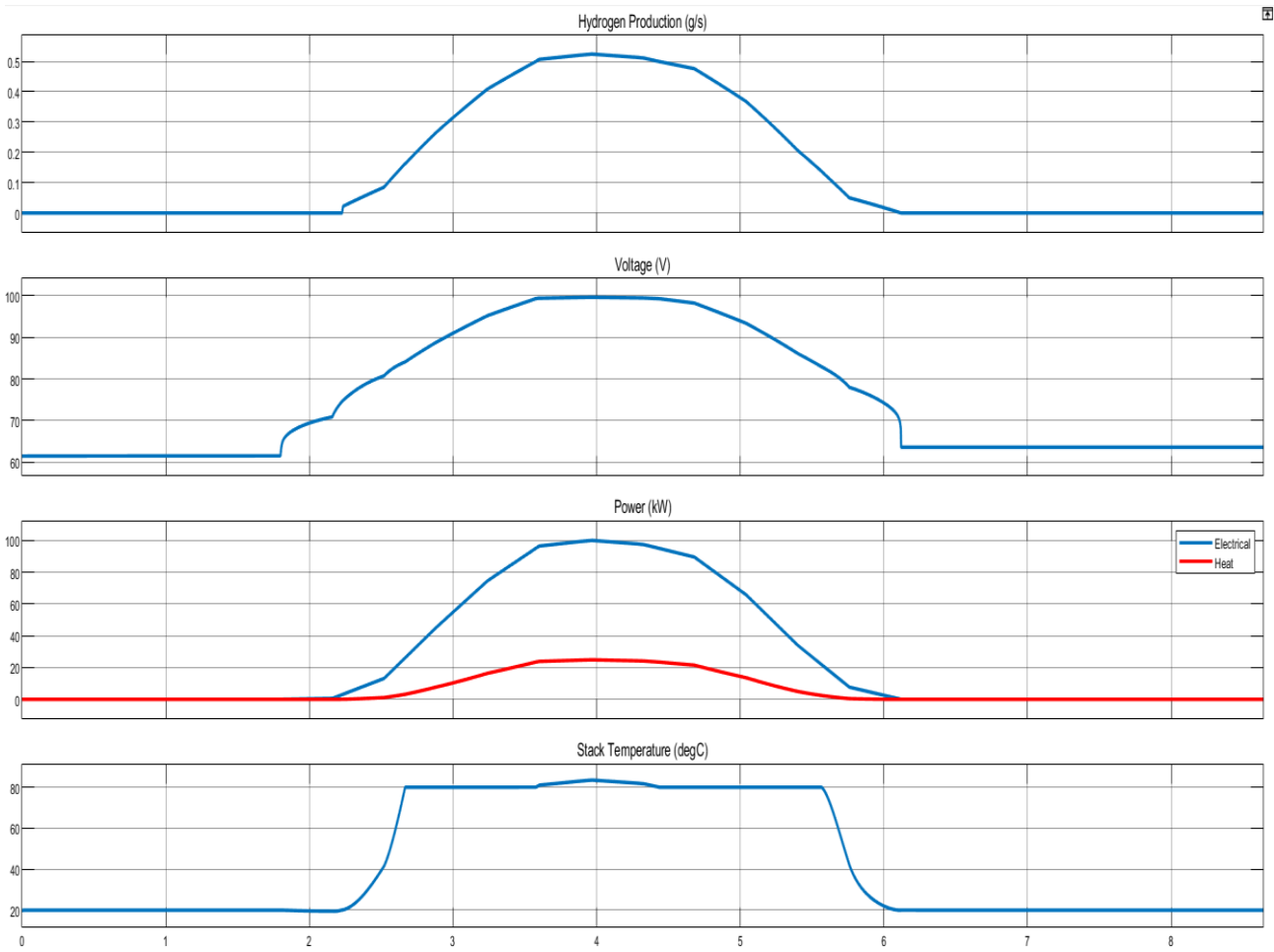


Fig. 4. Solar Power Profile graphs

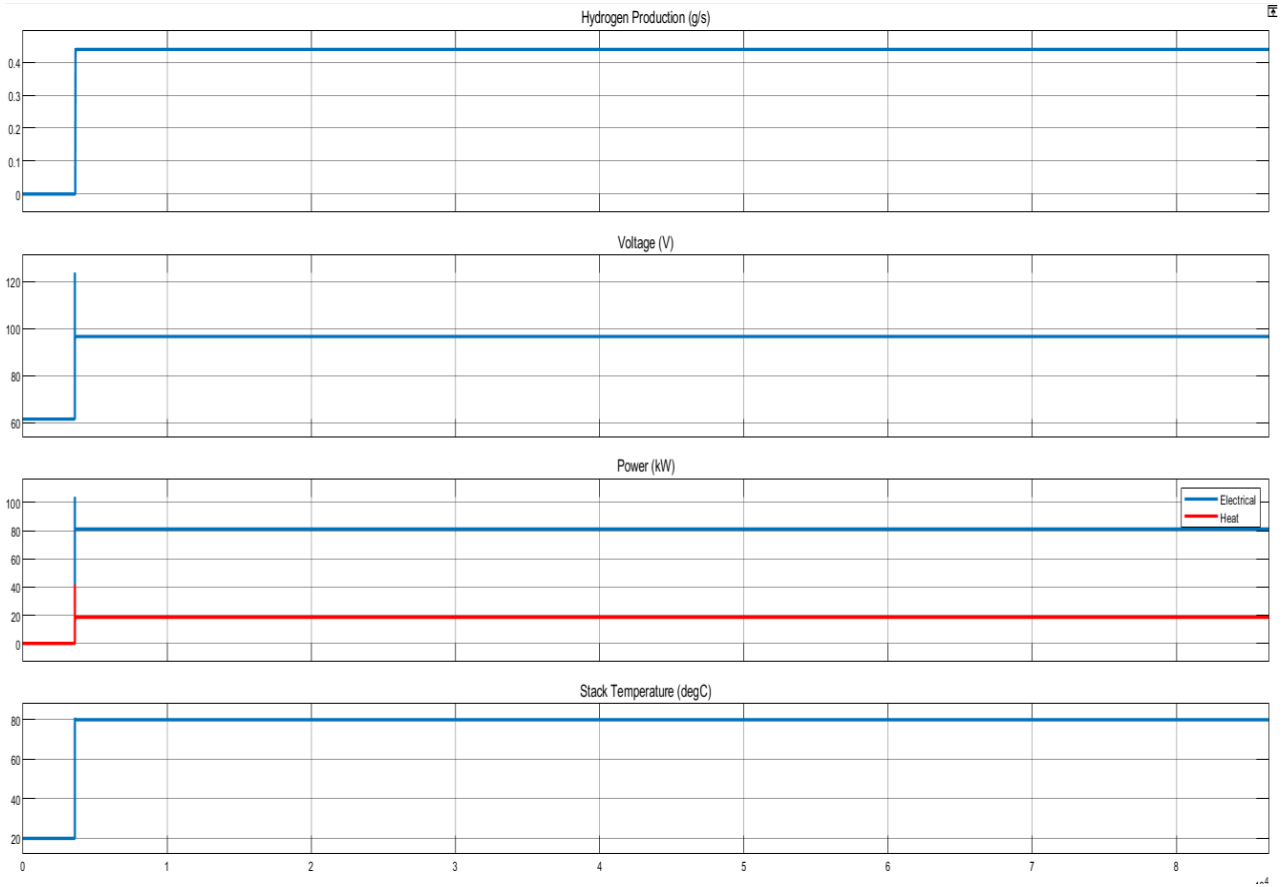


Fig. 5. Step Profile graphs

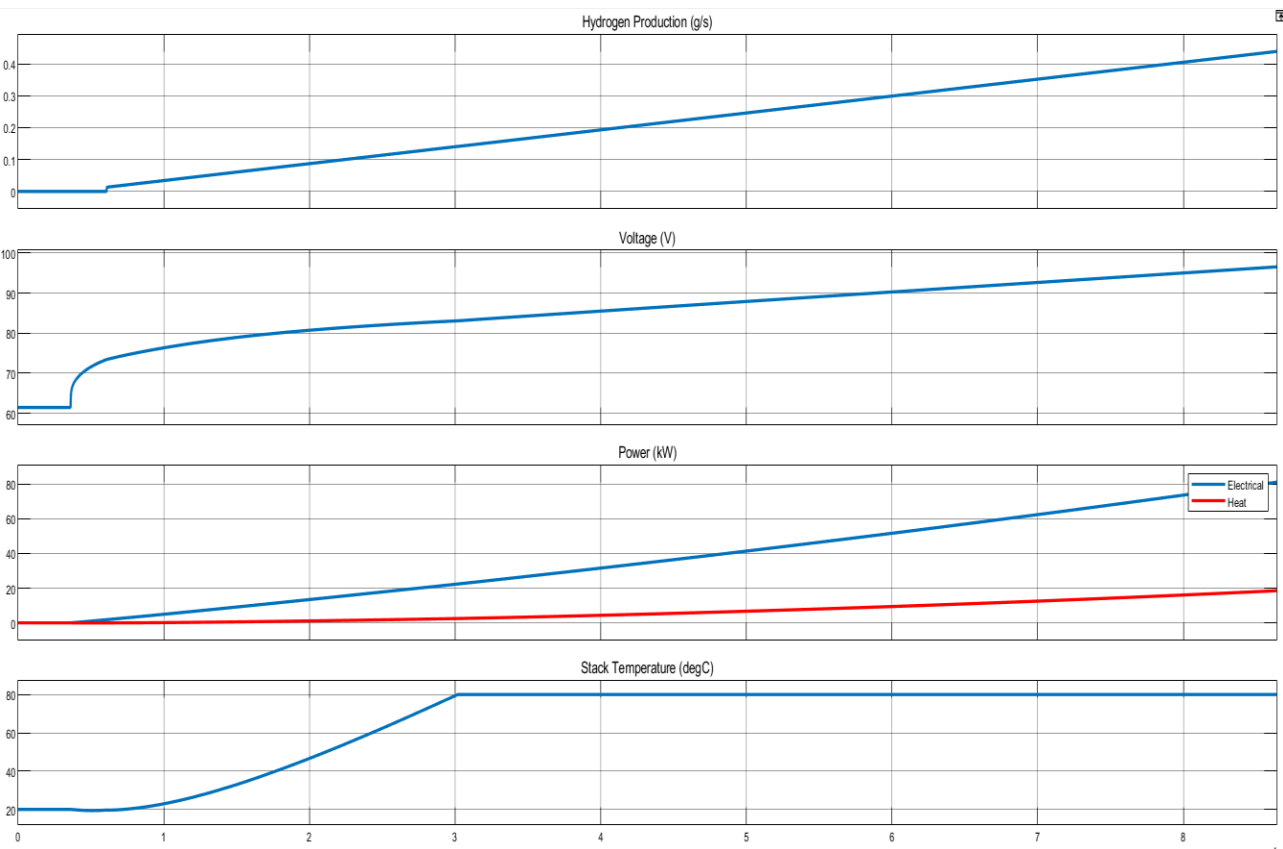


Fig. 6. Ramp Profile graphs

V. CONCLUSION

In this work, we used Matlab Simscape to design an advanced electrolyser. Productivity of the system remained stable at 87% yield, a very encouraging result. The next step is to connect this component to a renewable energy source such as solar power, wind energy, or a hybrid of both. and exploring new technologies to control energy conversion to establish an integrated and highly optimized system for green hydrogen production. .

REFERENCES

- [1] Bessarabov, D., wang, H., Li, H., Zhao, N., 2015. PEM Electrolysis for Hydrogen Production: Principles and Applications.
- [2] Hwang, J.J., Lai, L.K., Wu, W., Chang, W.R., 2009. Dynamic modeling of a photovoltaic hydrogen fuel cell hybrid system. *Int. J. Hydrogen Energy* 34, 9531e9542. <https://doi.org/10.1016/j.ijhydene.2009.09.100>.
- [3] Lamy, C., 2016. From hydrogen production by water electrolysis to its utilization in a PEM fuel cell or in a SO fuel cell: some considerations on the energy efficiencies. *Int. J. Hydrogen Energy* 41, 15415e15425. <https://doi.org/10.1016/j.ijhydene.2016.04.173>.
- [4] Lebbal, M.E., Lecœuche, S., 2009. Identification and monitoring of a PEM electrolyser based on dynamical modelling. *Int. J. Hydrogen Energy* 34, 5992e5999. <https://doi.org/10.1016/j.ijhydene.2009.02.003>.
- [5] Kim, H., Park, M., Lee, K.S., 2013. One-dimensional dynamic modeling of a highpressure water electrolysis system for hydrogen production. *Int. J. Hydrogen Energy* 38, 2596e2609. <https://doi.org/10.1016/j.ijhydene.2012.12.006>.