Sustainability analysis and simulation of a Polymer Electrolyte Membrane (PEM) electrolyser for green hydrogen production

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Abstract

In recent years, green hydrogen has emerged as an important energy carrier for future sustainable development. Due to the possibility of not emitting CO_2 during its generation and use, hydrogen is considered a perfect substitute for current fossil fuels. However, a major drawback of hydrogen production by water electrolysis, supplied by renewable electricity, is its limited economic competitiveness compared to conventional energy sources. Therefore, this work focuses on analyzing the sustainability of a green hydrogen production plant, not only considering its environmental parameters, as well as its economic, energy and efficiency parameters. The polymer electrolyte membrane (PEM) is selected as the most promising method of green hydrogen production in the medium and long term. Subsequently, a small-scale production plant is simulated using chemical process simulation software to obtain key data for computing a set of sustainability indicators. The selected indicators are based on the Gauging Reaction Effectiveness for the Environmental Sustainability of Chemistries with a Multi-Objective Process Evaluator (GREENSCOPE) methodology and are used to compare the sustainability of the simulated PEM plant with alkaline water electrolysis (AWE) plant. Finally, the process is scaled-up to analyze the feasibility of the simulated PEM system and validated against data to determine the operation of the electrolyser at a large production scale.

1 Introduction

Green hydrogen is typically obtained via water electrolysis that uses renewable power source to generate hydrogen from water. This method allows for the production of hydrogen without any CO_2 emissions (Younas et al., 2022). The key element of water electrolysis is electrolyser, a device where direct electric current is applied resulting in two chemical reactions: one at the cathode that produces hydrogen, Equation (1), and the other at the anode, Equation (2), that generates oxygen (Noussan et al., 2021). The polymer membrane-based electrolyser, also known as PEM, is the most suitable choice for handling power variations due to its ability to quickly adapt to changes within seconds, unlike other types of electrolysers based on alkaline water electrolytes (AWE) that require minutes. In addition, PEM can operate at higher pressures than other electrolysers, reducing the sub-sequence compression stages (Wang et al., 2022).

Cathode reaction:

$$2H^+ + 2e^- \rightarrow H_2(g) \tag{1}$$

Anode reaction:

$$H_2O(l) \rightarrow \frac{1}{2}O_2(g) + 2H^+ + 2e^- \tag{2}$$

Despite the fact that green hydrogen offers an environmentally cleaner solution to reduce society's dependence on fossil fuels, the reality remains that most of the world's hydrogen production, approximately 96% in 2021, still comes from methods that emit greenhouse gases, commonly known as grey and brown hydrogen (IRENA, 2021). The reason for the present scenario is that current green methods, such as PEM or AWE water electrolysis supplied by renewable power, are not economical, which makes them less competitive than those based on fossil fuels (Younas et al., 2022). This article therefore proposes a method for quantifying the sustainability assessment of the hydrogen production process, creating tools to evaluate of green hydrogen production methods. In addition, it is considered important to explore cost reduction measures during sustainability analysis of the process. Therefore, the advancement of process simulation is seen as a viable approach to minimise design costs. However, a challenge arises due to the limited availability of larger scale simulation models. To address this limitation, the simulated process is scaled-up to evaluate the performance of the electrolyser in large-scale production scenarios.

2 Sustainability

By examining existing literature, this analysis assesses the present state of green hydrogen in terms of its environmental impact, efficiency, economic viability, and energy performance.

Environmental

Green hydrogen is considered as an environmentally friendly, carbon-neutral energy carrier. The contribution to climate change is minimal, as only oxygen is emitted during the production process. However, the environmental impact of hydrogen is not zero, the type of renewable energy source used, the origin of the water for the electrolysis process and the residues generated after the usage of the production equipment must be taken into account (Baykara, 2018).

Efficiency

The efficiency of a PEM electrolyser varies depending on the quality of the materials used, the design of the electrolyser, the operating temperature, the pressure, and the concentration of the electrolytes. In general, a typical Low Heating Value (LHV) efficiency of PEM electrolyser can range from 67% to 82%. To improve efficiency, efforts should focus on optimising the geometry of the electrolytic cell, using more efficient catalysts and optimising the operating conditions of the electrolyser (Wang et al., 2022).

Economic

The current lack of extensive green hydrogen production is mainly due to poor economic competitiveness. Therefore, most of the hydrogen production is done using fossil fuels. The major costs of green hydrogen production are related with the cost of renewable electricity, the efficiency of the electrolysis process and the cost of the electrolysis equipment (Yue et al., 2021).

Energy

In the case of green hydrogen, it is estimated that the production of 1 kg requires 50-55 kWh of electricity, which is considered high energy consumption compared to some fossil fuels (Kurrer, 2020). This consumption depends on the efficiency of the electrolysis process (Antweiler, 2020).

3 Process simulation

The PEM electrolyser flowsheet considered in this study is simulated using Aspen HYSYS software. The PEM model is implemented using Aspen Customer Module (ACM) software. The schematic used in Aspen HYSYS for the simulation of the entire system is shown in Figure 1, clearly depicting the division between the cathode (C) and anode (A) sides.

3.1 Simulation model

Voltage model

The PEM electrolyser's voltage model is determined by Equation (3), which calculates the total voltage required for a single cell to perform the electrolysis process. This model consists of several components, including the ideal voltage and the minimum voltage required, different loses, and factors resulting from the activation of the reaction incurred throughout the process (Colbertaldo et al., 2017; AspenTech, 2021).

$$V_{\text{cell}} = V_{\text{id.}} + \Delta V_{\text{act.}} + \Delta V_{\text{ohm.}} + \Delta V_{\text{diff.}} + \Delta V_{\text{par.}} \quad (3)$$

The minimum voltage required to initiate an electrolysis process in a cell is known as the ideal voltage ($V_{\text{id.}}$), as described by Equation (4).

$$V_{\text{id.}} = \frac{1}{\text{nF}}(\Delta G + RT_{\text{op.}} ln(\frac{p_{H_2} + p_{O_2}^{0.5}}{a_{H_2O}})) \quad (4)$$

Where n is the number of electrons, F is the Faraday's constant, ΔG is the Gibbs free energy value, R is the gas constant, $T_{\text{op.}}$ is the operational temperature in the cell, p is the partial pressure for both elements H_2 and O_2 and a_{H2O} is the water activity value. For reactions to take place, an activation voltage ($\Delta V_{\text{act.}}$), Equation (5), is required, based on the Tafel equation and incorporating Butler-Volmer's simplification (García-Valverde et al., 2012).

$$\Delta V_{\text{act.}} = \Delta V_{act,cat.} + \Delta V_{act,an.} \quad (5)$$

Where $\Delta V_{\text{act,cat.}}$ is the activation voltage in the cathode side and $\Delta V_{\text{act,an.}}$ is the anode side voltage activation. These activation voltages have the same equation on both sides described in Equation (6).

$$\Delta V_{act.,x} = \frac{\text{RT}_{\text{op.}}}{\alpha_x \text{nF}} \ln\left(\frac{i_u}{i_{0,x}}\right) \quad (6)$$

Where x represents the anode or the cathode, R is the gas constant, $T_{\text{op.}}$ is the operational temperature in the cell, α_x is the charger transfer coefficient, n is the number of electrons, F is the Faraday's constant, i_u is the useful current density and $i_{0,x}$ is the exchange current density, which depends on the temperature associated with the Butler-Volmer's Equation (García-Valverde et al., 2012). According to Ohm's law, the electrical losses ($\Delta V_{\text{ohm.}}$) occurring in anode, cathode and membrane during the electrolysis process are represented by Equation (7).

$$\Delta V_{\text{Ohm.}} = (R_{\text{cat.}} + R_{\text{an.}} + R_{\text{mem.}})\ i_u A_{\text{cell}} \quad (7)$$

Where $R_{\text{cat.}}$ is the cathode side resistance and is calculated using Equation (8), $R_{\text{an.}}$ is the anode side resistance and is calculated using Equation (8), $R_{\text{mem.}}$ is

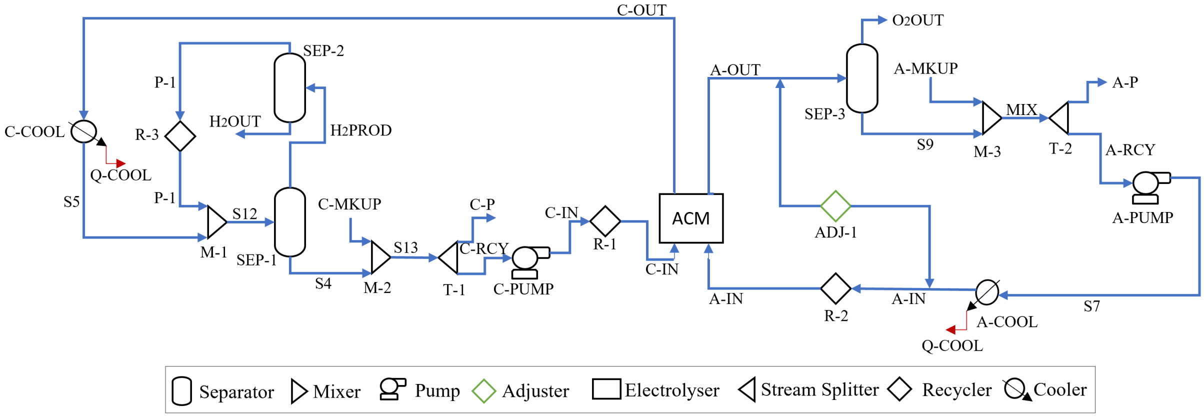

Figure 1. Process simulation schematic in Aspen HYSYS.

the membrane resistance and is calculated using Equation (9), i_u is the useful current density and A_{cell} is the active cell area.

$$R_x = \frac{t_x \rho_x}{A_x} \tag{8}$$

Where x represents the anode or the cathode, t_x is the electrode thickness, ρ_x is the resistivity and A_x is the active electrode area.

$$R_{mem.} = \frac{t_{mem}}{\sigma_{mem.} A_{mem.}} \tag{9}$$

Where $t_{mem.}$ is the membrane thickness, $\sigma_{mem.}$ is the conductivity based on the Springer model (Springer et al., 1991) and $A_{mem.}$ is the active membrane area. Diffusion voltage ($\Delta V_{diff.}$), Equation (10), represents the diffusion losses that occur when mass transport is hindered by the concentration gradient between the membrane surface and the main stream where the reaction takes place. These losses are the result of mass transport limitations due to the concentration gradient.

$$\Delta V_{diff.,x} = \frac{RT_{op.}}{\alpha_x nF} ln(\frac{i_L}{i_L - i_u}) \tag{10}$$

Where x represents the anode or the cathode, R is the gas constant, $T_{op.}$ is the operational temperature in the cell, α_x is the charger transfer coefficient, n is the number of electrons, F is the Faraday's constant, i_u is the useful current density and i_L is the limiting current density (assumed as 6 A/cm^2 the maximum current density). Parasitic losses (ΔVpar.), are typically expressed as a change in current rather than an increase in voltage. Essentially, the current efficiency is determined by the ratio of the input current to the useful current, Equation (11). This ratio is evaluated using the Faraday efficiency, which in the case of a PEM system, it is common to be close to 100%. Consequently, the Faraday efficiency used in the simulations is 99%.

$$\eta_{far.} = \frac{I_u}{I_{stack}} \tag{11}$$

Where I_u is the useful current calculated by multiplying the current density (i_u) by the active area of the cell (A_{cell}) and I_{stack} is the current in the cell.

Mass balance

The material balance evaluation in the electrolysis process is divided between the anode and cathode sides, and it is based on the assessment of the various flows involved. These flows include the water flow input, hydrogen production as described by Equation (12), oxygen production, electro-osmotic, diffusivity losses as described by Equations (13) and (14), respectively, and the pressure flow compensation as described by Equation (15).

$$\dot{N}_{H_2} = \frac{i_u A_{cell} N_{cells}}{nF} \tag{12}$$

Where i_u is the useful current density, A_{cell} is the active cell area, N_{cells} is the number of cells in the stack, n is the number of electrons and F is the Faraday's constant.

$$\dot{N}^{e-o}_{H_2O} = \frac{n_d i_u A_{cell} N_{cells}}{F} \tag{13}$$

Where n_d is the coefficient related with the humidification of the membrane extracted from (Colbertaldo et al., 2017), i_u is the useful current density, A_{cell} is the active cell area, N_{cells} is the number of cells in the stack and F is the Faraday's constant.

$$\dot{N}^{Diff.}_{H_2O} = \frac{D^{eff.}_{H_2O} \Delta C A_{cell} N_{cells}}{t_{mem}} \tag{14}$$

Where $D^{eff.}_{H_2O}$ is the diffusivity function based in (Aspen Technology, 2021), ΔC is the comparison water composition in the anode and cathode side, A_{cell} is the active cell area, N_{cells} is the number of cells in the stack and $t_{mem.}$ is the membrane thickness.

$$\dot{N}_{H_2O} = -\frac{K_{\text{Darcy}} A_{\text{cell}} \rho_{H_2O} \left(P_{\text{cat.}} - P_{\text{an.}}\right)}{\mu_{H_2O}} \quad (15)$$

Where K_{Darcy} is the membrane permeability, A_{cell} is the active cell area, ρ_{H2O} is the water density, $P_{\text{cat.}}$ and $P_{\text{an.}}$ are the pressure value in the cathode and anode side respectively and μ_{H2O} is the water viscosity.

Energy Balance

The energy balance is determined by comparing the energy inputs and outputs of the system equal to the total energy capacity. The inputs include the electrical power and the energy content of the inlet water flow, while the outputs encompass the heat losses (as described by Equation (16) as well as the outflow energy from both the anode and cathode sides.

$$Q_{\text{loss}} = h_{\text{free}} A_{\text{ext}} \left(T_{\text{op.}} - 10 - T_{\text{std.}}\right) \quad (16)$$

Where h_{free} is the heat transfer coefficient based in (AspenTech, 2021), $A_{\text{ext.}}$ is the exterior area (AspenTech, 2021), $T_{\text{op.}}$ is the operational temperature in the cell and $T_{\text{std.}}$ is the standard temperature.

3.2 Process validation

The simulated process is validated using simulated data, at an operating temperature of 55°C and an operating pressure of 30 bar, with the model presented in (Colbertaldo et al., 2017). The chosen operating conditions are based on the literature review performed during this study. Figure 2 illustrates the polarization curve demonstrating the relationship between the voltage cell and the current density. Furthermore, it provides insight into how various voltages incorporated in the model change as the current density increases. The specific comparison is made at a current density of 1,3 A/cm^2, where the voltage value for the simulated plant in this article is known to be 2,27 V. For the same data point in the reference article, the voltage is observed to fall between the values of 2,2 and 2,3 V. For the rest of the data points, the adjustment between the two models is carried out in a similar manner. Thus, a correlation can be drawn between the figure presented in this paper and the one found in the reference paper, validating the simulated model.

4 Sustainability analysis

The research on the application of the GREENSCOPE indicators to evaluate a PEM electrolysis process is scares. Following indicators are used to assess the sustainability of hydrogen production plants that utilize PEM technology.

4.1 GREENSCOPE methodology

Using the approach of sustainability and aiming to measure sustainability in any new or existing chemical process throughout its life cycle analysis, the United States Environmental Protection Agency (US EPA) created the GREENSCOPE tool (EPA, 2015). The methodology in this tool is based on a set of metrics, GREENSCOPE indicators, used to evaluate the environmental performance of chemical products and processes in four different principal areas: Environmental, Efficiency, Economic and Energy. For the normalisation of the GREENSCOPE indicators, Equation (17) is used, which compares the actual process scenario with the best-case scenario of 100% sustainability and the worst-case scenario of 0% sustainability. The GREENSCOPE tables provide a comprehensive set of indicators and their corresponding parameters for calculating both the best and worst case scenarios. This Equation allows the comparison between different process (Li et al., 2016; Lima et al., 2016).

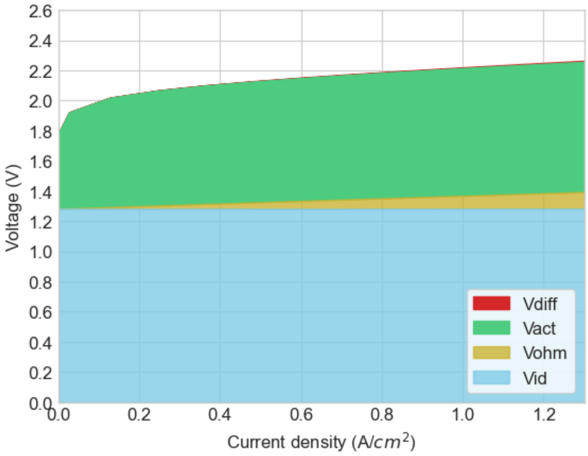

Figure 2. Polarization curve.

$$IndicatorScore = \frac{Actual - Worst}{Best - Worst}\ x\ 100\ [\%] \quad (17)$$

4.2 GREENSCOPE indicators

To calculate the indicators selected for the PEM electrolyser, the operating point of the simulation is chosen corresponding to an electrical power of 6 kW, a temperature of 55 °C and a pressure of 30 bar. This particular operating point is chosen because it is of a similar magnitude to the operating point used in the AWE simulation available in literature, a more mature technology, is selected for the purpose of comparing the sustainability analyses (Sánchez et al., 2020; Hancke et al., 2022). The indicators selected for the sustainability analysis comparison of the simulated electrolyser are as follows: Global warming potential (GWP) – Environmental indicator, Mass Loss Index (MLI) – Efficiency indicator, Fractional Water Consumption (FWC) – Efficiency indicator, Specific Energy Costs ($C_{E,Spec.}$) – Economic indicator, Resource Energy Efficiency (η_E) – Energy indicator

(Ruiz-Mercado et al., 2014). Table 1 shows the data for the selected indicators. Note that for the $C_{E,Spec.}$ the energy and the product cost are calculated by using the model develop by (Jovan & Dolanc, 2020). This model requires estimation of the CAPEX of the simulated plants, that are calculated using the estimation model develop by (Reksten et al., 2022). For the other indicators, data is taken directly from the simulations.

Table 1. Data used for the GREENSCOPE indicators.

	PEM	AWE	Indicator
H_2 (kg/h)	0,101	0,220	GWP, MLI, FWC, η_E
O_2 (kg/h)	0,026	1,355	MLI
CO_2 (kg/h)	0,000	0,000	GWP
H_2O (kg/h)	0,002	0,002	FWC, η_E
$Prod._C$(\$/kg H_2)	7,170	6,249	$C_{E,Spec.}$
$En._C$(\$/kg H_2)	1,779	1,363	$C_{E,Spec.}$

5 Process scale-up

The linearisation method has been chosen to transform the data, making it suitable for the computation of regression models. This methodology is introduced to extrapolate the data, enabling a comparative analysis with commercially available electrolysers capable of generating greater quantities of hydrogen. The simulated data pertaining to the operating conditions of 30 bar pressure and 55°C temperature is used for scale-up purposes.

5.1 *Regression and linearization model*

The objective of data linearisation is to apply a regression model that initially do not have a linear dependence (James et al., 2021). In this study, simulated cell voltage cell (Vcell), specific work (Spc. work) and efficiency (η) data were taken and scaled-up as a function of current intensity. These parameters and ratios are typically the ones present in the reference article for the comparison of the simulated and scaled data of electrolysers present in the market (Buttler & Spliethoff, 2018). Table 2 presents the detailed explanation of the relationships of the variables for which regression models have been sought, including the data transformations performed and the variables to which it applies. The table also includes the regression models ultimately used, along with their corresponding R-squared values determining their suitability for use. Notably, all R-squared values are close to 1, indicating the high degree of fit and confirming the suitability of the generated regression models for the study's purposes. As an example, Figure 3 shows the application of a square root transformation to the abscissa results in the linearisation of the data, which is then modelled using a regression model.

Table 2. Data linearisation

X	Y	Reg. model	R-sq.
i_u	Vcell	$y = 0,39\sqrt{x} + 1,85$	0,96
i_u	Spc. work	$y = 0,42\log(x) + 5,27$	0,94
i_u	η	$y = -0,04\log(x) + 0,57$	0,99

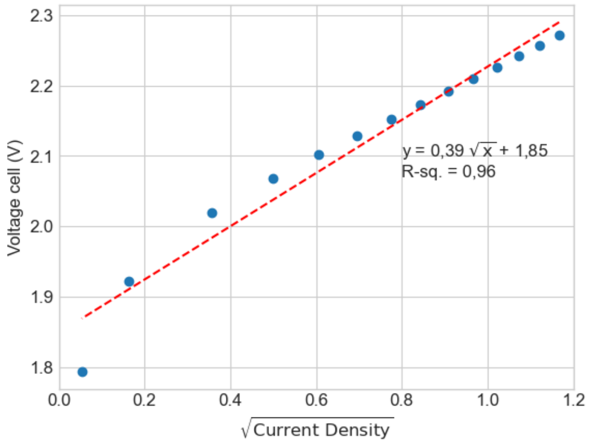

Figure 3. Plot of Vcell and Curr.Den linearisation

6 Results

The results of the Aspen HYSYS simulation, the sustainability analysis and the scaling-up process are presented below.

6.1 *Simulation results*

Figure 4 provides the correlation between voltage cell and current density, as well as the relationship between current density and efficiency. Where efficiency is defined as the ratio of energy extracted from the process in the form of hydrogen, using its LHV, and the amount of electrical energy input to the process. Solid lines are used to represent voltage cell, while dashed lines indicate the evolution of efficiency. For the various simulated points, the voltage of the cell is different for the same value of current densities. This is directly correlated with the amount of hydrogen produced. In other words, when less product is extracted, higher losses occur, resulting in a higher voltage for the cell. In terms of efficiency, a higher voltage increases hydrogen production and increases losses. Consequently, the simulation results represented by blue lines, corresponding to the highest pressure, has the worst performance.

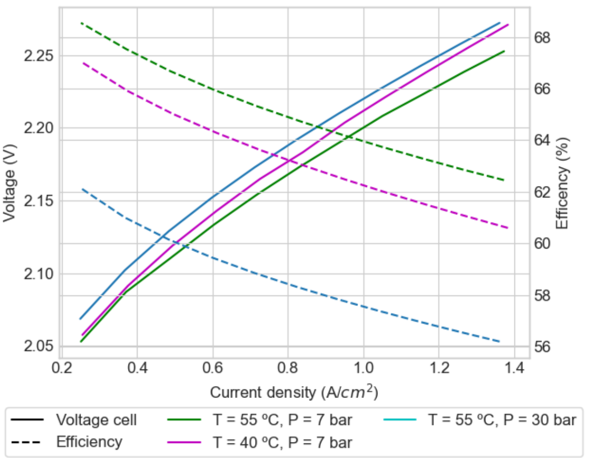

Figure 4. Plot of voltage cell and Efficiency of PEM electrolyser

6.2 *PEM sustainability*

The GWP indicator is employed as a precise and visually effective representation of the complete absence of gas or pollutant emissions in the production of green hydrogen when the energy used is from a renewable source. The score of this indicator is 100 % for both production methods, that evidence the zero emission of CO_2 pollutants during the process. The results of the MLI indicator shows that the PEM process achieves a normalization value of 99,74 %, whereas the AWE process yields a value of 93,84 %. This indicates that AWE processes are less efficient in terms of hydrogen production. In terms of the FWC indicator, the AWE process demonstrates superior efficiency in utilizing the required water resource for its operation compared to other processes, such as PEM. While the PEM normalization of the indicator reflects a level of 84,68 %, the AWE process achieves significantly higher levels, reaching close to 92,00 %. The normalized $C_{E,spec.}$ indicator value for the PEM process is 40,91 %, while for the AWE process it is 48,04 %, indicating that energy cost has a greater impact on both processes. It is possible to see how the more mature AWE technology has a better cost distribution, although the difference is not very large. The ηE indicators for hydrogen production using PEM technology and AWE are 77,50 % and 79,84 % respectively, indicating that AWE has slightly higher efficiency compared to PEM. Figure 5 displays the normalized values for all the indicators, along with the comparison between PEM and AWE technologies, depicted in blue and orange respectively. The variation in both electrolysers can be justified by method of operation and technology differences.

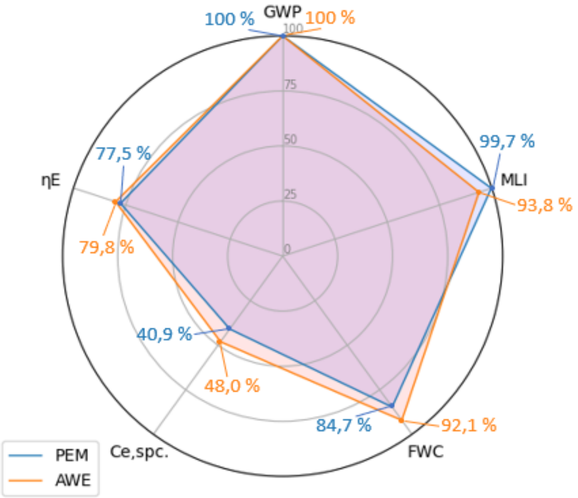

Figure 5. Plot of GREENSCOPE indicators for PEM and AWE

6.3 *Scale-up analysis*

To verify the suitability of the simulated installation for large-scale hydrogen production, the benchmarking study conducted by Buttler and Spliethoff is used as a referenced. This study includes graphical representations of the current market's PEM electrolysers (Buttler & Spliethoff, 2018). The figure 6 displays the current density against the voltage, specific work, and cell efficiency. The polarization line is shown in blue, while the efficiency using the lower heating value (LHV) as the reference value is displayed in grey dashed lines. Furthermore, a second y-axis is added, representing the specific work values. The minimum voltage is approximately 1,8 V. In commercial electrolysers, this value consistently remains below 1,75 V and approaches 1,5 V. This discrepancy arises because the results do not converge at lower power levels due to small scale nature of the simulated process. Nevertheless, the results for power levels of 1 kW and above are satisfactory and facilitated a comprehensive analysis. The specific work values adequately match those shown in the reference article. Therefore, it can be concluded that this variable can be compared with that of real electrolyzers. Additionally, efficiency values have been obtained that are realistic and, when compared to those shown in the article, indicate that the scaling of the simulation is satisfactory for the efficiency parameter. In summary, the initial attempt to scale-up the process has yielded favorable results. However, it must be acknowledged that certain challenges, exemplified by the encountered setback related to lower values, have surfaced. To further enhance these endeavors aimed at cost-effective design improvements, consideration should be given to exploring alternative scaling methodologies. One potential avenue involves the utilization of techniques such as Buckingham's π theorem (Polverino et al., 2019) or the incorporation of Artificial Neural Networks (ANN) strategies (Tian, 2020), both have demonstrated effectiveness in the context of enlarging hydrogen fuel cells. These approaches hold promise for facilitating significant advancements.

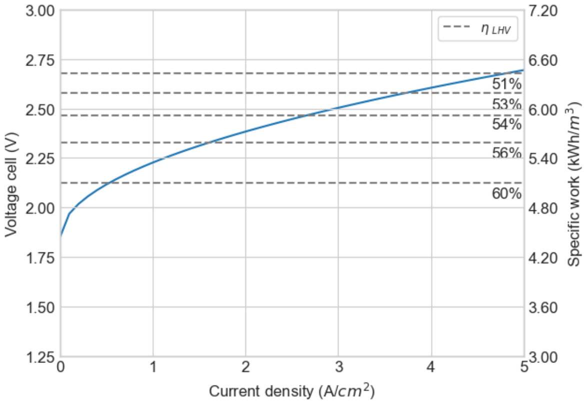

Figure 6. Plot of Scaled-up process variables of PEM electrolyser

7 Conclusions

The PEM simulation exhibited satisfactory performance when compared to the reference simulation. Specifically, the operating range of 1-6 kW was simulated successfully for subsequent analysis. The analysis shows that the higher temperature and electrical power levels increased hydrogen production, while pressure had an inversely proportional effect. This finding is consistent with observations made in various real and simulated PEM electrolysers documented in the literature. The sustainability analysis performed consisted of calculating indicator values according to the GREENSCOPE methodology, which was used for the first time in this paper to evaluate hydrogen production methods. In addition, a sustainability comparison was made between PEM and AWE technologies. The environmental indicator, GWP, was found to be 100 for both technologies as green hydrogen production with renewable energy sources does not generate CO_2 emissions. With regards to the efficiency indicators, the proportion of hydrogen produced, MLI, was found to be higher for PEM technology than for AWE, while water consumption, FWC, was better for AWE technology. These variations can be justified by technology differences present in both electrolysers. In terms of the economic indicator, $C_{E,spec.}$, it was observed that the weight of energy costs was higher in the case of PEM technology. Finally, the efficiency indicator showed that the energy efficiency, ηE, was slightly worse for PEM technology. The scaling-up process employed data linearisation and regression techniques. Through this approach, the simulation demonstrated satisfactory comparability with commercially available PEM electrolysers. While scaling-up processes for hydrogen fuel cells simulations using PEM technology are documented, methods such as Artificial Neural Networks (ANN) or Buckingham π theorem for electrolysers simulations are yet to be explored. The application of such methods holds promise for significant cost reductions in the production of commercialised electrolysers, further enhancing viability.

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