Viability study of the state-of-the-art hydrogen electrolyser technologies

Undergraduate thesis project

Bachelor's Degree in Industrial Technologies & Economic Analysis

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Abstract

This paper provides a comprehensive evaluation of four hydrogen electrolysis technologies: alkaline, PEM, SOEC, and AEM. The assessment of their economic viability, and technical capabilities lead to the following conclusions.

Alkaline electrolysis is identified as the most mature, cost optimal, and reliable technology among the four. It offers high durability and gas purity, and its implementation is straightforward.

PEM electrolysis is considered an upgrade over alkaline electrolysis, as it achieves higher current densities, leading to increased electrical efficiencies. It also produces a highly pure and compressed hydrogen output, to the cost of being more expensive.

SOEC electrolysis demonstrates even higher electrical efficiency than PEM electrolysis and allows for significant heat integration. However, it is still in the demonstration stage and faces challenges related to intermittent power supplies and high heat requirements.

AEM electrolysis' main advantage is the use of a non-noble metal catalyst, reducing costs compared to SOEC electrolysis. It also offers a compact format, high purity and pressure output, and relative scalability.

Alkaline and PEM are already reliable hydrogen producers and they can be chosen in function of the buyers priorities (profitability or sustainability, respectively). AEM and SOEC technologies are still at an early stage of development, but with the ongoing research that is being done they are expected to become more cost effective than their commercialized peers.

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Acronyms

PEM – Proton Exchange Membrane

SOEC – Solid Oxide Electrolyser Cell

AEM – Anion Exchange Membrane

DC – Direct Current

YSZ – Ytrium-Stabilized Zirconia

LSM - Lanthanum Strontium Manganate

P – Proportional

I – Integral

D - Derivative

CAPEX – Capital Expenditures

OPEX – Operational Expenditures

LCH (or LCOH) – Levelized Cost of Hydrogen

NPV – Net Present Value

IRR – Investment Rate of Return

CF – Cash Flow

Acknowledgements

This thesis project concludes my undergraduate studies in Industrial Technologies and Economic Analysis, a degree that gave me the chance to keep expanding my knowledge in science and technology while giving me the ability to think business-wise.

I am deeply grateful to my Thesis Director and System Dynamics teacher Dr. Maria Serra Prat for her constant dedication to my project. The sharp insights and on-point feedback she provided me on our weekly meetings are what motivated me to keep on working. She helped me through every step of the way and I will always be thankful to her for that.

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Although Hydrogen is a promising renewable energy to decarbonize the planet, there is no better fuel than love. Thank you to all of those who provided me with it!

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1. Introduction and definition of objectives

Green hydrogen is a promising solution to the problem of decarbonising the planet by 2050 knowing that the global energy demand is expected to increase between 25% and 30% by 2040. From providing motive power for any kind of transportation to generating electricity via fuel cells, hydrogen fuel has a wide range of applications. Consequently, the demand for hydrogen powered technologies is on the rise and the methods for obtaining it as well.

There are various hydrogen production methods that can be powered with renewable resources, such as Photo fermentation, Pyrolysis or Photolysis. Nonetheless, green hydrogen is mainly generated through electrolysis, which is defined as a "process by which electric current is passed through a substance to effect a chemical change" by the Encyclopaedia Britannica. In this case, the chemical change we want to accomplish is the separation of hydrogen from the molecules that contain it (e.g. water). To do so we will need electrolysers, which are the set-ups capable of carrying out this chemical process. Nonetheless there exist many types of electrolyser technologies, each of which have their own advantages and disadvantages.

The aim of this viability study is to provide the reader an accurate, practical, in-depth review of each type of electrolyser so that industrial leaders as well as energy communities can choose the electrolyser that best suits their needs.

This study will be divided into three main parts. The first one will be a generic overview of the technical aspects surrounding the four technologies. In the second part we will use the Simulink block diagram environment to design a system that simulates the performance of the electrolysers. All technologies will be placed in parallel to perform an effective comparison. Afterwards, we will focus on the economic viability of each type of electrolyser. A thorough economic analysis of the investment, operation and maintenance costs will be performed.

2. Description of the main electrolysis technologies

Today's market is essentially composed of 4 types of electrolysers: Alkaline, Proton Exchange Membrane (PEM), Solid Oxide Electrolyser Cell (SOEC), and AEM. We will go through the process description, advantages and drawbacks, parameters of interest and include a commercially available example for each type of electrolyser. This general approach will enable us to perform and understand the dynamic systems that will be discussed in the second part.

2.1. Alkaline electrolysers

2.1.1. Process description

The first electrolyser technology we will review is the Alkaline water electrolysis. Essentially, an alkaline electrolyser uses electric current to split the water molecules contained in the alkaline electrolyte solution into Hydrogen and Oxygen.

Let us explain this technology in a more detailed manner by breaking down the process into several steps. The figure below will allow us to have a more graphical approach to the description. It shows a general scheme of an alkaline electrolysis cell and the operations that occur inside of it.

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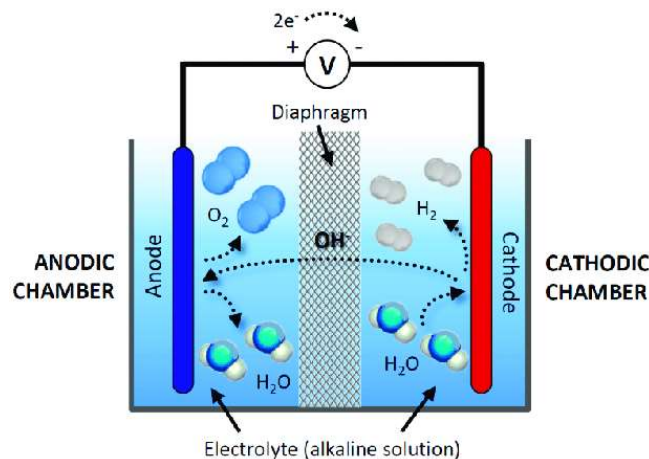
Figure 1 - General scheme and operation of an alkaline electrolysis cell

Note that this is a simplified scheme in which scales are not respected in order to better understand how it works. Commercially available electrolysers may not geometrically resemble the scheme below but do work in the same way.

0.ELEMENTS THAT CONSTITUTE THE TECHNOLOGY

Let's first describe the different elements of the set-up. To begin with, we can consider a recipient containing a liquid alkaline electrolyte solution, which is generally an aqueous solution of potassium hydroxide (KOH) or sodium hydroxide (NaOH). The main reason why we use aqueous solutions instead of water alone is that they can enhance reactions because they allow the presence of ions, while this may not happen in water alone.

This recipient is separated in two by a thin, porous foil with a thickness between 0.05 and 0.5 mm called diaphragm. This foil is a non-conductive to electrons, conductive to ions barrier. In this way, the ions needed for the desired chemical reactions can travel from the cathode to the anode while avoiding electrical shorts between the electrodes (which are likely to happen when both electrodes are relatively close). State-of-the-art diaphragms are made of a composite material of zirconia and Polysulfone.

To complete the set-up, we need to plunge two electrodes (an Anode and a Cathode) connected by a voltage source in the recipient while making sure that they are separated by the diaphragm. The side of the recipient containing the anode is called the anodic chamber and the side of the recipient containing the cathode is called the cathodic chamber. Note that we will talk about "green hydrogen production" whenever the voltage originated in the voltage source has been generated with renewable energies. The values of the voltage provided may vary depending on the quantity of solution in the recipient.

Electrodes are generally made of nickel-based metals. Such material has a good electrical conductivity, exhibits good resistance to corrosive solutions and is inexpensive. Also bear in mind that Ni is the least active non-noble metal when considering pure metals.

Nonetheless alkaline water electrolysis for industrial applications needs additional elements that allow it to obtain a larger scale production. The schematic flow corresponds to an industrial alkaline water electrolyser. The electrolyte is circulated through the electrolysis cell, where gas is produced. Gas separators are positioned next to the cell to separate the gas from the liquid phase. The liquid phase is then directed back to the electrolysis stack. Heat exchangers are used to maintain the appropriate temperature, and the final product gasses can be purified. Since all these additional elements are not essential to hydrogen production, we will not develop them in this part.

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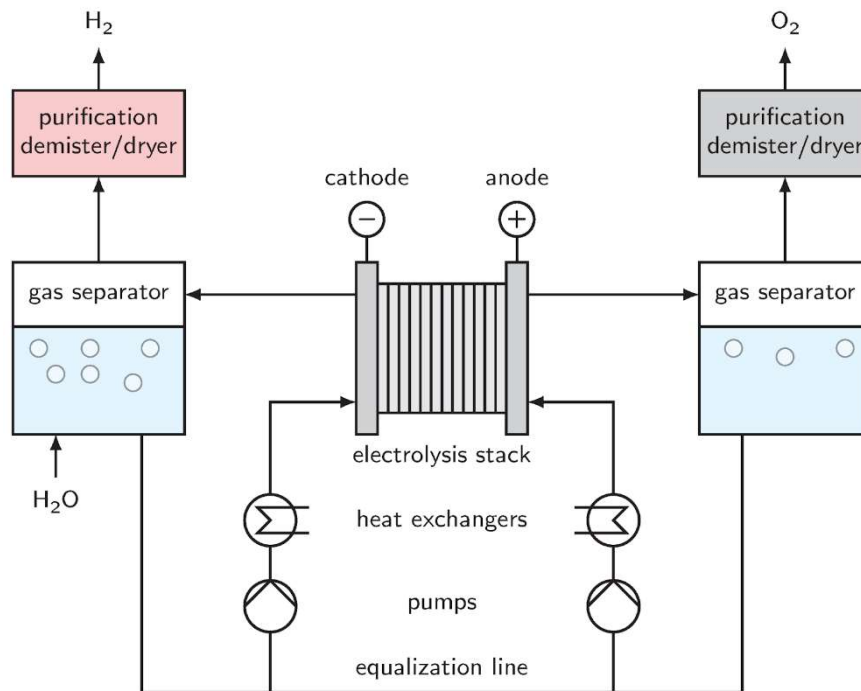
Figure 2 - Schematic flow of an industrial alkaline electrolysis set-up

Now that we have presented the elements that compose an electrolyser we will figure out how this technology is able to produce hydrogen.

1.CATHODE

We will start by focusing on the chemical reaction that occurs in the cathode side of the electrolysis cell. A pair of water molecules (in liquid state) will encounter two electrons coming from the anode side via the electric circuit that connects both sides. These electrons will split the two molecules into two $OH_{(aq)}^-$ anions and an $H_{2(g)}$ molecule, which is the product in which we are interested.

The chemical reaction that occurs is then:

$$\text{Cathode: } 2H_2O_{(l)} + 2 \cdot e^- \rightarrow H_{2(g)} + 2OH_{(aq)}^- \qquad \text{(Equation 3.1.1.1)}$$
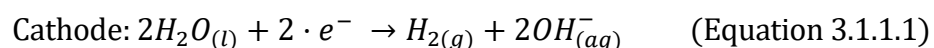
2.ANODE

On the anode side, a pair of $OH^-_{(aq)}$ anions produced in the cathode side enter in contact with the electrically charged anode, which leads to the formation of half an oxygen molecule (in gaseous state), a water molecule (in liquid state) and the two electrons we mentioned earlier.

The chemical reaction that occurs is then:

$$Anode: 2OH^-_{(aq)} \rightarrow 0.5 \cdot O_{2(g)} + H_2O_{(l)} + 2 \cdot e^- \qquad \text{(Equation 3.1.1.2)}$$
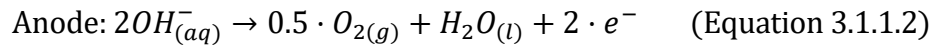
3.OVERALL REACTION

The sum of both chemical reactions leads to the chemical reaction below (after being simplified):

$$Overall\ reaction: H_2O_{(l)} \rightarrow H_{2(g)} + 0.5 \cdot O_{2(g)} \qquad \text{(Equation 3.1.1.3)}$$
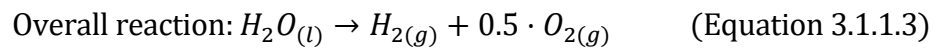
As we can observe, this equation describes the separation of a liquid water molecule into hydrogen and oxygen in gaseous state, which is the goal of this process. The hydrogen (and even oxygen in some cases since it has a medical application) climbs up the solution and is then stored in a new compartment being previously pressurized or not.

4.REQUIRED CELL VOLTAGE

Now that we know the chemical reactions that occur within the electrolyser, and consequently the moles of hydrogen that can be produced (at least in a theoretical level), we want to figure out the amount of electric current needed for the reactions to occur.

First of all we will want to obtain the reversible cell voltage U_{rev}, which is the voltage needed in the theoretical scenario where there are no irreversibilities involved (e.g. heat losses). This value can be determined using the following equation:

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$$U_{rev} = -\frac{\Delta_R G}{z \cdot F} \text{ (Equation 3.1.1.4)}$$

Where z is the number of electrons exchanged, which is two (see equation 3.1.1.3), F is the Faraday constant which is equal to 96,485 $C \cdot mol^{-1}$, and $\Delta_R G$ is the free reaction enthalpy. The latter is also known as the Gibbs free energy change and it can be obtained using equation 3.1.1.5:

$$\Delta_R G = \Delta_R H - T \cdot \Delta_R S \qquad \text{(Equation 3.1.1.5)}$$

Here, $\Delta_R H$ is the reaction enthalpy, $\Delta_R S$ is the reaction entropy and T is the temperature. That said, we must take into account the irreversibilities that take place in the reaction meaning that a voltage that is higher than U_{rev} will be required. Such voltage is the thermoneutral voltage U_{th} and can be determined using equation 3.1.1.6:

$$U_{th} = -\frac{\Delta_R H}{z \cdot F} \text{ (Equation 3.1.1.6)}$$

Notice that the above formula is very similar to the one in Equation 3.1.1.4. The only thing that really changes is that we have $\Delta_R H$ instead of $\Delta_R G$ because $\Delta_R H$ takes into account the irreversible thermal losses $T \cdot \Delta_R S$. Indeed, we can rewrite equation 3.1.1.6 in the following form:

$$U_{th} = U_{rev} - \frac{T \cdot \Delta_R S}{z \cdot F} \qquad \text{(Equation 3.1.1.7)}$$

Thus, we can obtain the numerical value of the voltage needed in standard conditions with the following values:

- $\Delta_R G = 237 \, kJ/mol$ at 25ºC and an ambient pressure of 1 bar (standard conditions)
- $\Delta_R H = 286 \, kJ/mol$ at 25ºC and an ambient pressure of 1 bar (standard conditions)
- $T = 25ºC$

Using Equation 3.1.1.4 we obtain $U_{re} = -1.23V$ and, finally, we can obtain the value of the voltage needed for the electrolyser to be functional using Equation 3.1.1.7: $U_{th} = -1.48V$. This means that assuming standard conditions, a direct current generated voltage of 1.48V will be required for the electrochemical reactions to occur.

2.1.2. Operating conditions and ranges

Each type of electrolyser is capable of producing hydrogen under certain specific conditions. These conditions can vary widely depending on the electrolyser. They will give us the necessary information to make a first comparison of the electrolysers focusing purely on technical aspects.

1.INPUTS

The inputs we will consider for our system are the liquid alkaline electrolyte solution and the voltage source. The solution used needs to have a reasonable concentration so that the wanted chemical reactions can take place. For instance, in the case of using a Potassium Hydroxide solution a 20-40 wt% of solute is needed. The usually used KOH and NaOH solutions are widely available and have a price of approximately 11€/L (30% KOH concentration) and 20€/L (1 mol/L NaOH concentration), respectively. Nonetheless, said solution does not have to be heated or pressurized to a certain temperature to enter the system. The amount of voltage needed is the one that allows the conduction of two electrons. This one is of -1.48V whenever the set-up is in standard conditions (25ºC and 1 bar).

2.THE ALKALINE ELECTROLYSIS CELL

The cell temperature oscillates between values going from 60 to 80 ºC and the maximum pressure it can bear is 30 bars. The system response is in the range of seconds while its cold-start time is less than an hour.

3.OUTPUT

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A table summarizing the operating conditions and ranges for the alkaline electrolyser can be found in the figure below.

Name of the parameter	Unit	Value(s)
Cell temperature	ºC	60-80
Stack pressure	bar	<30
Current density	A/cm^2	0.2 - 0.4
Cell voltage	V	1.8 - 2.4
Power density	W/cm^2	up to 1.0
Part-load range	Ø	20 - 40%
Specific energy consumption stack	kWh/Nm^3	4.2 - 5.9
Specific energy consumption system	kWh/Nm^3	4.5 - 7.0
Cell voltage efficiency	Ø	59 - 70%
System hydrogen production rate	m^3/h	<760
Lifetime stack	H	<90 000
Acceptable degradation rate	µV/h	<3
System lifetime	y	20-30

Table 1 - Table of state-of-the-art operating ranges of an alkaline electrolysis cell

To begin with, we can observe that the cell temperature and stack pressure are relatively close to the standard conditions which means that no extra amount of energy is required to make the setup work. On another hand, current density refers to the current flowing per cm^2 of membrane: it is an indicator of how well suited the material is for the exchange of electrons. The specific energy the stack consumes is smaller than the one the system consumes since the system often involves complementary machinery such as pumps, heat exchangers and driers.

Before commenting on the values of efficiency it is important to indicate how it is computed and which parts of the set up are in or out of scope. In the table above, the efficiency is based on the hydrogen yield. This efficiency is calculated as the ratio between the energy contained inside the produced hydrogen and the total electric energy consumed by the entire set-up, including pumps and gas separators as the ones we have seen before in Figure 2.

$$\eta = \frac{m_{H_2} \cdot LHV_{H_2}}{E_{elec}} \quad \text{(Equation 3.1.2.1)}$$

Where m_{H_2} is the mass of hydrogen produced, LHV_{H_2} is the lower heating value of hydrogen and E_{elec} is the total electric energy consumed. Note that we could have used the higher heating value of hydrogen to display more advantageous figures but the LHV is more realistic since it does not take into account the heat of vaporization of water (in fact, it is the HHV minus the heat of vaporization of water).

That said one may notice that the values are pretty similar compared to other hydrogen producing methods. For instance black and brown hydrogen, which is the hydrogen that is produced by burning coal and by burning lignite respectively, have an efficiency of approximately 55%.

2.1.3. Advantages, drawbacks and main features

In this part we will mainly focus on the practical aspects of the electrolyser to try to see for which applications each electrolyser is most well suited. The following table displays the advantages and disadvantages of an alkaline electrolyser with respect to its alternatives. We will comment on it afterwards so as to get a more detailed approach.

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PROS	CONS
• **Low cost** relative to the PEM alternative. • **Higher durability** due to an exchangeable electrolyte and lower dissolution of anodic catalyst, relative to the PEM. • **Higher gas purity** due to lower gas diffusivity in alkaline electrolyte, relative to the PEM. • It is the **simplest, most used** technology until now, which makes it **more reliable** than the others. • It is available for **large plant sizes** making it a good option for industrial applications.	• **Unable** to make an efficient use of intermittent power supplies. • Difficult to **stock** in an efficient manner. An additional **tank** or **compressor** may be needed since it is not produced at a sufficiently high pressure. • **Elevated** cold start time • **High maintenance cost** since the system is highly corrosive (electrodes should be changed regularly). • **Low current density** resulting in a relatively inefficient use of the voltage supplied.

Table 2 - Table showing the advantages and drawbacks of an Alkaline Electrolyser

Alkaline electrolysis has a long history in the chemical industry: it is the most used electrolysis until today to produce hydrogen. It is a reliable, cost-effective alternative for industrial applications since major improvements of the technology have been achieved through the years. The exchangeable electrolyte and lower dissolution of anodic catalyst in alkaline electrolysers make them more durable compared to other alternatives such as the PEM one. Additionally, due to the lower gas diffusivity in alkaline electrolyte, it has higher gas purity. However, this technology has an important drawback: it is unable to efficiently store and make use of intermittent power supplies. Another drawback is the elevated cold start time, which may impact its usability in certain conditions. Additionally, due to the highly corrosive nature of the system, the maintenance cost is high, and electrodes need to be regularly replaced. Lastly, there is a stocking problem due to the fact that the hydrogen is not produced at a sufficiently high pressure. The system may need an extra tank or even a compressor to solve this problem.

Despite these cons, alkaline electrolysers are a preferred choice for large plant sizes and are used extensively in the industry. More specifically alkaline electrolysis is well suited for any type of application that does not use a variable power profile such as the one provided by renewable energy sources or AC current sources. We may think about it for the needs of the chemical industry, such as the refining of petroleum, where hydrogen lowers the sulfur content of diesel fuel.

2.1.4. Commercially available electrolyser

Before presenting some examples that are present in the industry for each one of the electrolysers, it is important to highlight that their features vary significantly depending on the application of the hydrogen produced. For simplicity purposes, we will review a model that has relatively small dimensions (resulting in the production of hydrogen for non large-scale industrial purposes). Industrial-size electrolysers will be studied in chapters 3 and 4 of this paper.

As commented earlier, alkaline technology is by far the most popular technology nowadays, mainly because of its reliability. Therefore, many small-scale electrolysers of this kind are available in the market.

The example chosen is the "Alkaline Water Electrolyzer Stack - 30 Cell", which requires an electrolytic solution of 30 wt% KOH. Its diaphragm (also called membrane) is made of porous polymer (the polymer used is not specified) while the electrodes are nickel based. It has 30 cells (i.e. 30 pairs of electrically charged electrodes) and the electrolyser current density range (at 1.8 V/cell) of 300 to 500 mA/cm^2 depending on the operational temperature. Electrolyser current ranges (at 54V) vary between 60 and 100 A depending on the operational temperature and power ranges vary between 3.2 and 5.4 kW. The operating temperature range is 15 to 85ºC. Regarding the flow rates produced, the Hydrogen Flow Rate Range is [12.6; 21] L/min and the Oxygen Flow Rate Range [6.3;10.5] L/min

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The materials present in this set up are standard as well as the electrolytic solution needed. The current density is an interesting parameter to know, since it gives us an idea of how well the materials are suited to conduct electricity. The area where this parameter is evaluated is referred to as the active area, and in this case it is the membrane we are studying to see how well $OH^-_{(aq)}$ anions are being conducted from the cathode to the anode. Regarding current, this specification could have been replaced by V_{Stack}. The power mentioned in the last paragraph is the consumed power.

Then, the operating temperatures of this electrolysers are particularly low with respect to the other ones, which implies that less energy and/or thermally insulating material are needed. Indeed, that it is one of the main advantages of such technology.

Technical specification	Value(s) or name	Unit
Size	265*265*210	mm
Covering material	Fiber-reinforced plastic, Engineering plastic	$\emptyset$
Membrane material	Porous polymer	$\emptyset$
Electrode material	Nickel	$\emptyset$
Electrolyte	KOH	$\emptyset$
Electrolyte weight percentage	30	%
Number of cells	30	$\emptyset$
Operating Temperature Range	15 - 85	ºC
Electrolyser Current Density Range (at 1.8 V/cell)	300 to 500	mA/cm^2
Electrolyzer Current Range (at 54 V)	60~100	A

Technical specification	Value(s) or name	Unit
Electrolyzer Power Range	3.2 - 5.4	kW
Hydrogen Flow Rate Range	12.6 - 21	L/min
Oxygen Flow Rate Range	6.3 - 10.5	L/min

Table 3 - Technical specifications of the Alkaline Water Electrolyzer Stack - 30 Cell

In the table above, some data is given as a range rather than a specific number. For the case of current and current density, this is due to the operational temperature. The higher the temperature, the lower the current since heat acts as a disturbance for the conduction of electricity. This is illustrated in figure 4. For the case of power, the fact that there is a range is a direct consequence of the current variability (current is in the formula of power) and thus the production of hydrogen and oxygen come in the form of ranges as well.
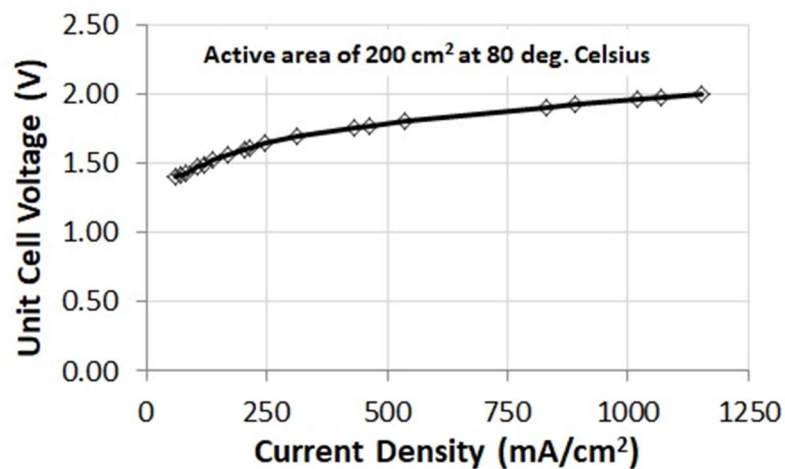
Figure 3 - Polarization Curve of an Individual Electrolyzer Cell (for an exemple performance)
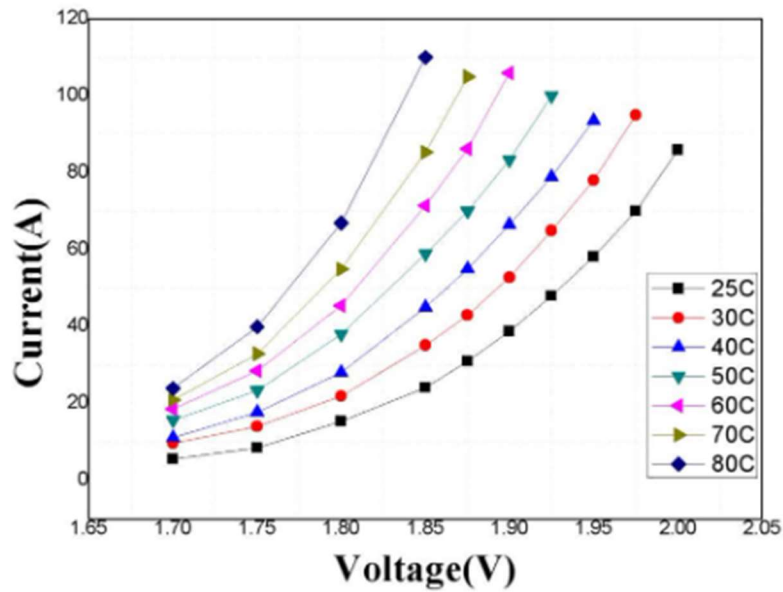
Figure 4 - Cell performance date for different operating temperatures

2.2. PEM electrolysers

2.2.1. Process description

The acronym PEM can stand for Proton Exchange Membrane or Polymer Electrolyte Membrane. This type of electrolyser works in a very similar way to the Alkaline electrolyser, but with two key differences: the electrolyte is not an aqueous solution but a solid polymer and water alone is used as an input. We will see that this difference will allow us to overcome many of the issues the alkaline electrolysers have, which is why PEM electrolysers are considered to be an updated version of the Alkaline electrolysers.
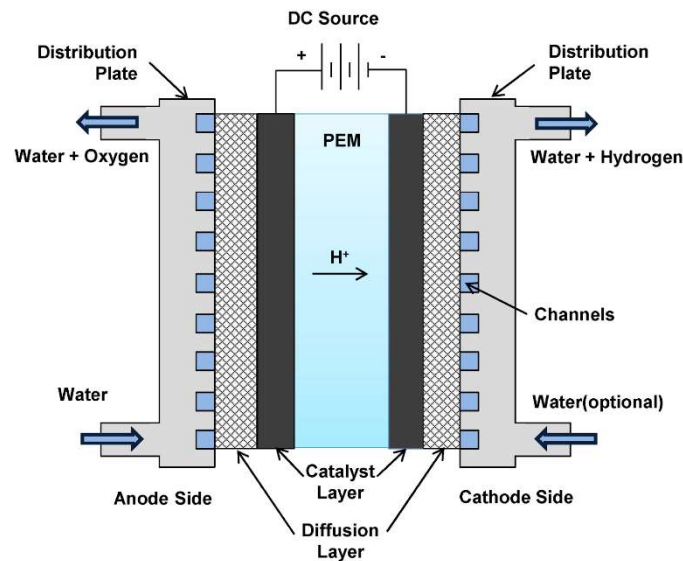
Figure 5 - General scheme and operation of a PEM electrolysis cell

The figure above is an overview of the PEM electrolysis cell. Notice that another main difference between this electrolysis and the Alkaline electrolysis is that the ion conducted through the membrane is H^+ instead of OH^-. Once again please note that commercially available electrolysers may not geometrically resemble the scheme below but do work in the same way.

0.ELEMENTS THAT CONSTITUTE THE TECHNOLOGY

Let us first start by identifying the elements that are common to both of the technologies studied so far. These are: the DC voltage source, the Anode side and the Cathode side. Even though the Anode and Cathode side have a different composition, their goal is the same: creating electrical current by means of a redox reaction.

Each electrode is composed of two layers: the diffusion layer and the catalyst layer. The first one, as its name implies, is in charge of conducting the incoming water molecules by means of diffusion to the next layer. Then, the catalyst layer accelerates the breakdown of water molecules into hydrogen and oxygen.

Apart from the two layers, each electrode has a distribution plate to conduct the inputs and the outputs of the cell. On the Anode side we have liquid water as an input and water and oxygen as an output. On the Cathode side, we have liquid water as an optional input and water and hydrogen as an output.

Finally, the membrane separating the electrodes is what characterizes this technology: the polymer exchange membrane. It is generally made of gold because it is an excellent conductor of electricity.

1.ANODE

Let's start with the Anode equation this time. Liquid water enters through the channels of the distribution plates. Then, water molecules travel through the diffusion layer all the way until the catalyst layer where the electrical current will split H_2O into 2 hydrogen cations, half an oxygen molecule and two electrons. This can be seen in the following equation.

$$\text{Anode: } H_2 \rightarrow 2H^+ + 0.5O_2 + 2 \cdot e^- \text{ (Equation 3.2.1.1)}$$
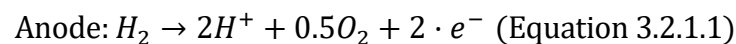
Note that the half oxygen molecule will be evacuated from the system since it is considered an output unlike the two electrons and the two cations. The two cations will traverse the PEM thanks to the conductor properties of it.

2.CATHODE

In this side, the two H^+ Cations who travelled through the PEM will encounter the two electrons coming from the anode side via the external circuit that connects both electrodes. This will form a molecule of hydrogen, which is the desired product.

$$\text{Cathode: } 2H^+ + 2 \cdot e^- \rightarrow H_2 \text{ (Equation 3.2.1.2)}$$
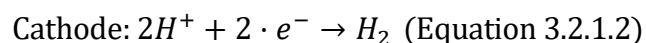
In figure 5, we see that water can also be inserted in the cathode side. Nonetheless, this water does not take part of the reaction at any moment and is only there to transport the hydrogen.

3.OVERALL REACTION

Finally we can sum both equations. they will lead to the following equation after simplification:

Overall reaction: $2H_2O \rightarrow H_2 + 0.5O_2$ \qquad (Equation 3.2.1.3)
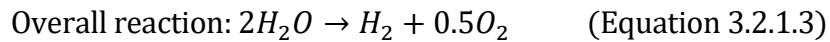
We can observe that the resulting equation is the same as the one for the Alkaline electrolyser (Equation 3.1.1.3).

4.REQUIRED CELL VOLTAGE

The reasoning to obtain the required cell voltage is exactly the same, as well as the numerical results obtained when both technologies are set to standard conditions. This makes sense because the overall reaction, which is the sum of all the previous reactions that have taken place, is the same in both cases. This implies that the energy required to split the water molecules, in identical conditions, should be the same. Using equations 3.1.1.4 and 3.1.1.5 in standard conditions, we obtain U_{rev} = 1.23 V and U_{th} = 1.48 V.

2.2.2. Operating conditions and ranges

1.INPUT

In this scenario the inputs we will consider are water and the voltage provided to the electrodes. Water alone (in liquid state) is enough since the voltage induced together with the density is sufficient for the anions to pass through the proton exchange membrane. The water does not have to be heated or pressurized at any specific temperature.

2.THE PEM ELECTROLYSIS CELL

For a PEM cell to work, the temperature of the system should be between 50 and 80ºC. The stack can reach a pressure of at most 200 bars which is approximately 200

times the atmospheric pressure. The system response and cold start time are smaller than for the Alkaline and for the SOEC.

3.OUTPUT

The hydrogen produced is particularly pure, reaching levels of 99.99%. The voltage efficiency of this electrolyser is similar to the one for the Alkaline ($\sim 75\%$)

Concerning the production rate, it can reach a maximum of 40 m3/h which is the same than for the SOEC. Regarding the capital cost, the value is ~ 2000 €/kWel. This price is partially explained by the high amounts of external energy required to achieve a high temperature as well as the expensive materials of the set-up.

Similarly to what was done for the first technology, we are going to review the essential parameters that characterize the PEM technology.

Name of the parameter	Unit	Value(s)
Cell temperature	ºC	50-80
Stack pressure	bar	<30
Current density	A/cm^2	0.6 - 10.0
Cell voltage	V	1.75 - 2.20
Power density	W/cm2	up to 4.4
Part-load range	Ø	0 - 10%
Specific energy consumption stack	kWh/Nm^3	4.2 - 5.6
Specific energy consumption system	kWh/Nm^3	4.5 - 7.5
Cell voltage efficiency	Ø	65 - 82%
System hydrogen production rate	m^3/h	30
Lifetime stack	H	<20 000
Acceptable degradation rate	µV/h	<14
System lifetime	A	10-20

Table 4 - Table summarizing the state-of-the-art operating ranges of a PEM
electrolysis cell

Overall, the values found in the table are very similar to the one for the alkaline electrolyser. For instance, both technologies have an almost identical cell temperature and stack pressure range: both require reasonable amounts of power to attain the needed Pressure-Temperature conditions of the cell. Other similar parameters may be the cell voltage, the specific energy consumption and the cell voltage efficiency.

The improvement with respect to the latter technology is its current density, which is up to ten times higher than for the Alkaline electrolyser. This is a very important accomplishment because significantly increasing the conduction of ions allows to take advantage of the sudden spikes of energy input. This last fact is

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particularly interesting for the use of renewable energies which provide intermittent (and unpredictable) power supplies. As a direct consequence, power density is also larger. Another advantage it has is its relatively high acceptable degradation rate. Most importantly, improving the current density has a direct, positive impact in the efficiency based on the hydrogen yield (the same criteria used for the Alkaline cell). On average efficiency has increased 9%.

2.2.3. Advantages, drawbacks and main features

The following table displays the advantages and disadvantages of a PEM electrolyser with respect to its alternatives. We will comment on it afterwards so as to get a more detailed approach.

PROS	CONS
• **Main advantage:** Can operate at a **high current density (dynamics)**. • **Compressed** hydrogen output. • **Thin membrane** is sufficient. • **Low** ohmic losses. • **Low gas crossover** due to solid membrane → **high gas purity** (which is important for safety). • **Low cold start time.** • **No corrosive substances.** • **High power densities** • **High pressure (> 100 bar)** which means it can be efficiently stocked without making use of compressors or large tanks.	• **High cost** relative to the Alkaline alternative. • **Expensive**. • **Fast** degradation.

Table 5 - Table showing the advantages and drawbacks of a PEM Electrolyser

What makes the PEM a cutting-edge technology is the high current density it can manage. This is an advantage since it enables the technology to take advantage of sudden spikes in energy input. This is particularly important when it comes to green

hydrogen, which usually deals with intermittent power supplies. Other advantages are the high gas purity it yields, its low cold start time and its high-pressure output, allowing a more space efficient stock of the gas. On the other hand, those advantages are followed by a higher cost of the cell and a faster degradation rate due to the high temperatures at which the materials are exposed.

2.2.4. Commercially available electrolyser

In this section we will comment a PEM electrolyser for educational purposes, similarly to what we did for the Alkaline.

The model to be analyzed is the E208 - 1-Cell Rebuildable PEM Electrolyzer. Its dimensions (98 x 80 x 78 mm) and the fact that the kit can be completely disassembled make it a good fit for research purposes: it can be easier to observe what parts of the cell degrade first for instance. The technical description is the following:

- Electrode Area: approximately 16 cm^2
- Electrical voltage input (with room temp. de-ionized water, 20-23 deg Celsius): 0 V to 2.0 V
- Electrical current input (with room temp. de-ionized water, 20-23 deg Celsius): 0 A to 4.0 A
- Current Density (with room temp. de-ionized water, 20-23 deg Celsius): approximately 0 mA/cm2 to 250 mA/cm2
- Electrical voltage input (with slightly warmed de-ionized water, 36-39 deg Celsius): 0 V to 2.0 V
- Electrical current input (with slightly warmed de-ionized water, 36-39 deg Celsius): 0 A to 5.0 A
- Current Density (with slightly warmed de-ionized water, 36-39 deg Celsius): approximately 0 mA/cm2 to 312 mA/cm2
- Requires Commercial distilled (deionized) water with a conductivity of < 2 µS/cm

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- Max. temperature for de-ionized water (or distilled water) for anode inlet: 60 deg Celsius

By only looking at the technical specifications we can already see that the cell's hydrogen production increases with temperature (since current density is better) but higher current input will be requested. Notice as well that the cell, in reality, uses distilled or de-ionized water.
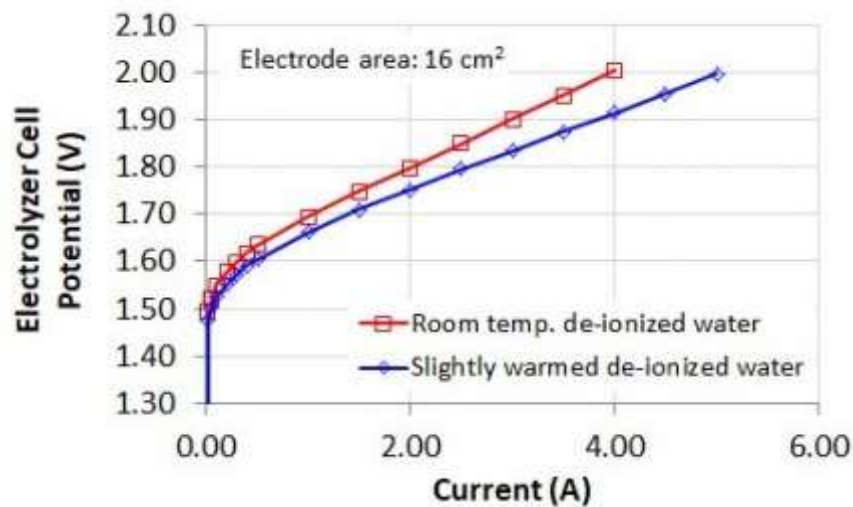
Figure 6 – Polarization curve of E208 - 1-Cell Rebuildable PEM electrolyser

The polarization curve of the electrolyser shows a quasilinear behaviour unlike for the Alkaline commercialized example, were we can see that the curve tends to a value of 2 V. This is due to the better conduction of electricity in the PEM, allowing to reach higher currents. Notice how the slightly warmed de-ionized water can reach higher values but at the cost of having a lower slope than for the room temperature.

2.3. SOEC electrolysers

2.3.1. Process description

SOEC electrolyzers are no different from Alkaline and PEM technology. The

operation mode and elements constituting the technology are quasi-identical to the ones described in the previous models but with one key difference: the electrolyte is in solid state. Another remarkable difference is that the system not only processes water to produce Hydrogen but can also process (simultaneously or not) Carbon Dioxide to produce Carbon Monoxide (which has an important role in the fabrication of metal or some chemicals).
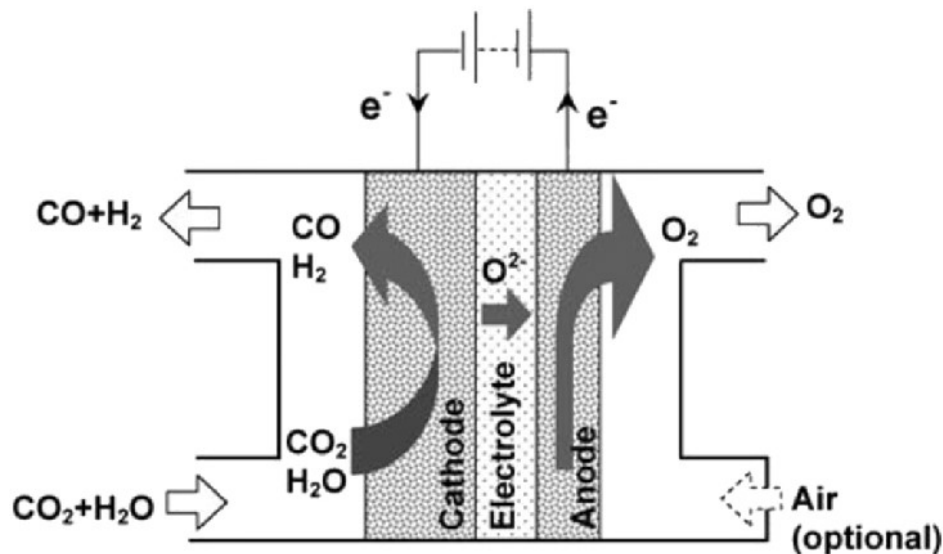
Figure 7 - General scheme and operation of a SOEC electrolysis cell

The figure above is an overview of the SOEC electrolysis cell. Notice that another main difference between this electrolysis and the previous ones is that the ion conducted through the membrane is O2- instead of OH- or H+. Once again please note that commercially available electrolysers may not geometrically resemble the scheme below but do work in the same way.

As it is the case for the other technologies, the SOEC cell is nothing more than a solid oxide cell that runs in regenerative mode (i.e. reverse mode). However the SOEC is the only technology discussed so far that can operate both as an electrolysis cell (to produce Hydrogen) and as a fuel cell (to produce electricity). This can be observed in the below figure.
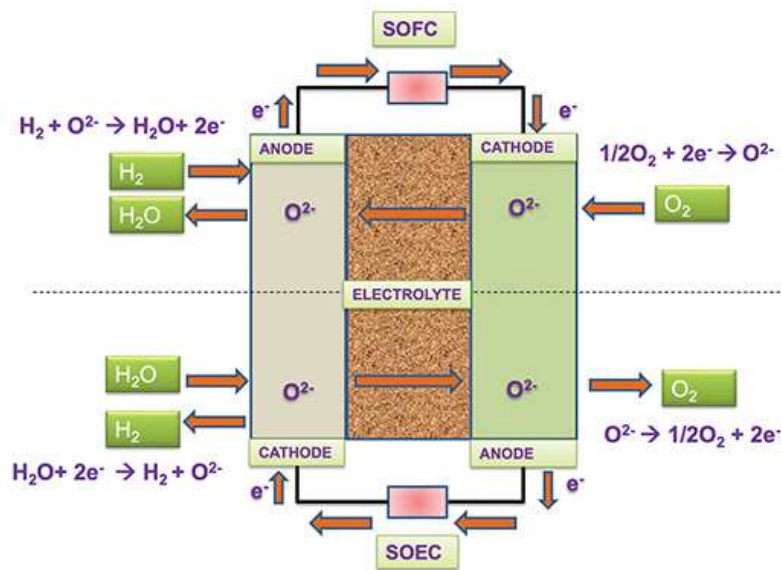
Figure 8 - General scheme and operation of a SOE and SOF (Solid Oxide Fuel Cell) cell

0.ELEMENTS THAT CONSTITUTE THE TECHNOLOGY

Similarly to what was done with the PEM electrolyzer we will start by identifying the elements that are common to all three technologies studied so far. These are: the DC voltage source, the Anode side and the Cathode side. Once again, we consider that the Anode and Cathode side are common elements because their function is the same. The Cathode (or Fuel Electrode) is most commonly a Ni doped YSZ (ytrium-stabilized zirconia) while the Anode (Oxygen Electrode) is most commonly Lanthanum strontium manganate (LSM) since it is highly performant under electrolysis conditions.

In between the two electrodes we find the solid oxide electrolyte, generally made of ZrO_2 doped with 8 %-mol Y_2O_3. This combination of materials provides everything that is needed to conduct ions in a solid environment. It has Zirconium dioxide, a strong material with high melting temperature (2 700ºC) and excellent corrosion resistance. Those properties are needed since electron conduction in a solid environment is only achieved with high temperatures. Additionally, it has

Yttrium(III) oxide (Y2O3) to stop the phase transition from the tetragonal to the monoclinic phase that can occur when the cooling is abrupt.

On the other hand, contrary to the Alkaline and the PEM, here there is no membrane separating the two electrodes. We can say that the solid oxide electrolyte acts as an electrolyte and membrane simultaneously since it conducts ions but does not allow anything else to flow through it.

Also note that end plates (where inputs and outputs enter and exit the system) usually have conduction channels to enhance the reactions as was the case for the PEM electrolyser. Nonetheless, the schematic drawing in Figure 11 does not show it.

1.CATHODE

Let's focus on the Cathode side. A water molecule will encounter two electrons coming from the anode side via the external circuit. These electrons will join the Oxygen molecule to form an anion while a Hydrogen molecule will be formed.

$$\text{Cathode: } H_2O + 2 \cdot e^- \rightarrow H_2 + O^{2-} \ (\textit{Equation 3.3.1.1})$$
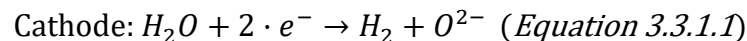
2.ANODE

Then, two anions of O2- will appear on the side of the anode. The electric current generated by the DC voltage source will provide the necessary energy to break the two anions in four electrons and an oxygen molecule.

$$\text{Anode: } 2O^{2-} \rightarrow O_2 + 4 \cdot e^- \ (\textit{Equation 3.3.1.2})$$
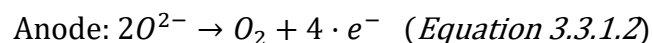
3.OVERALL REACTION

The net reaction that occurs in the electrolyser is then:

$$\text{Overall reaction: } 2H_2O \rightarrow 2H_2 + O_2 \ (\textit{Equation 3.3.1.3})$$

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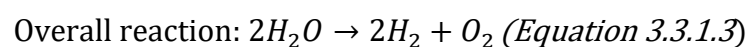
Notice that this equation is different from the ones obtained in the previous sections.

4.REQUIRED CELL VOLTAGE

The required cell voltage is the same than for the Alkaline, but at a different temperature. A typical SOEC cell works with a $U_{rev} = 1.48\ V$ at a temperature of 950 ºC (current density achieved in these conditions was -3.6 A/cm^2). The procedure to obtain said voltage is identical to the ones followed for the previous technologies.

2.3.2. Operating conditions and ranges

SOEC modules can work in three different operating modes: exothermic, endothermic and thermoneutral.

Exothermic mode has the advantage of preheating the inlet gas with the heat accumulation generated by the stack's increasing temperature. With this mode no external heat source is needed. The Endothermic mode has a lower electrical energy consumption but a higher heat energy consumption as its name indicates. As a direct consequence of the lower electricity consumption, current density decreases thus leading to a lower hydrogen production. The thermoneutral mode is the mode in which the heat generated through irreversible losses is equal to the heat required by the reaction. An external heat source is needed to compensate for the heat losses occurring during the reaction.

1. INPUT

Unlike for the other technologies, the input of the SOEC is in gaseous state whether it is for the production of Carbon Monoxide from Carbon Dioxide or of Hydrogen from water. For the case of Hydrogen, pure water in the form of steam

enters the fuel cell at a temperature between 500 and 850ºC. This range of temperatures is necessary to achieve high-temperature electrolysis.

2. THE SOEC ELECTROLYSIS CELL

For a SOEC cell to work, the temperature of the system should be between 650 and 1 000ºC.

The stack can reach a pressure of at most 25 bars which is approximately 25 times the atmospheric pressure. The system response and the cold start time of the technology are identical to the Alkaline, which is slower than the PEM.

3. OUTPUT

The hydrogen produced is particularly pure, reaching levels of 99.9%. Its pressure is close to atmospheric pressure. The efficiency of this electrolyser is surprisingly high compared to its peers. This is because of the criterion we chose to use: the efficiency based on hydrogen yield (or electrical efficiency). If we were to choose net efficiency, which takes into account the high amount of thermal energy involved in the process, efficiency would decrease to values as low as 50%.

Concerning the production rate, it can reach a maximum of 40 m^3/h which is the same than for the PEM. Stack energy is low (>3.2 kWh/m^3) while the system energy is bigger than 4.7 kWh/m^3 (when taking into account the electrical and thermal energy) which is a moderate value. Regarding the capital cost, the minimal value is of 2 000 €/kW$_{el}$ which is very expensive. This price is partially explained by the high amounts of external energy required to achieve a high temperature as well as the expensive materials of the set-up.

The below table summarizes the characteristics of the SOEC cell:

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Name of the parameter	Unit	Value(s)
Cell temperature	ºC	650-1000
Stack pressure	bar	<25
Current density	A/cm²	0.3-2.0
Cell voltage	V	0.7-1.5
Power density	W/cm²	1.3
Part-load range	Ø	0-10
Specific energy consumption stack	kWh/m³	>3.2
Specific energy consumption system	kWh/m³	>4.7
Cell voltage efficiency	Ø	90-100%
System hydrogen production rate	m³/h	<40
Lifetime stack	h	10000
Acceptable degradation rate	µV/h	<2.5
System lifetime	a	2.5

Table 6 - Table summarizing state-of-the-art operating ranges of a SOEC electrolysis cell

2.3.3. Advantages, drawbacks and main features

Solide Oxyde Electrolysis Cells are so far the most efficient technology in terms of electrical efficiency. It also bears the same great advantage the PEM has, which is a very pure output. Recall that certain levels of purity are needed for applications such as the automotive industry or even chemical industry. Another great advantage which exclusively applies to SOECs running in Exothermic mode is the integration of waste heat to the system, making it a relatively more sustainable and profitable alternative.

However, all these benefits bear a cost. The high operating temperature to which the cell is subjected to has as a consequence a high cold start time and a lower stack lifetime (the lowest among its peers). This combined with the high CAPEX requirements makes this option not very attractive to investors. Research is being performed in order to reduce CAPEX and increase stack life time.

PROS	CONS
Highest electrical **efficiency** among its peers **Integration of waste heat** possible - Suitable for **co-electrolysis:** direct synthesis gas generation - Hydrogen **purity** levels are **extremely high**	**Limited supply** and **capabilities** due to laboratory stage **Limited** long-term stability of the cells (relatively low life time) **Not suited** to fluctuating systems (renewable energies) **High** CAPEX **High** cold start time **High** operating temperature

Table 7 - Table showing the advantages and drawbacks of a SOEC Electrolysis cell

2.4. AEM electrolysers

2.4.1. General description

An AEM electrolysis solution combines the benefits of PEM and alkaline systems by allowing the use of non-noble catalysts while achieving energy densities and efficiencies comparable to PEM technology.

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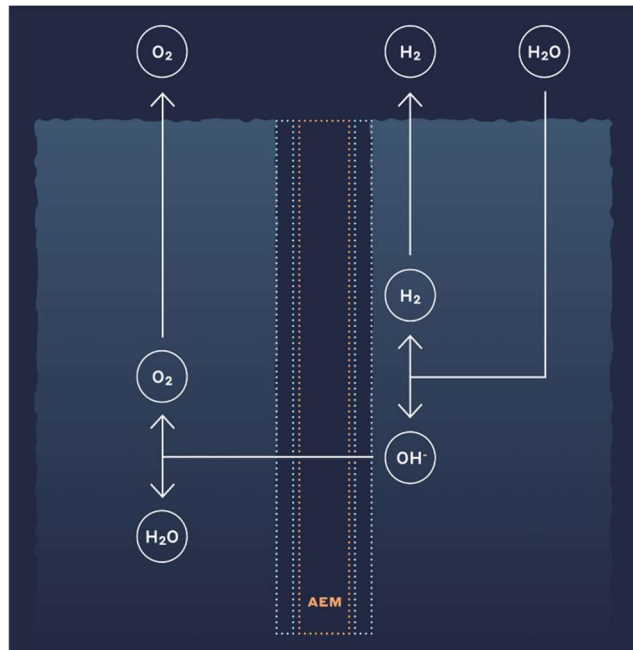
Figure 9 - Schematic flow of an AEM electrolysis set-up

As it can be seen in the schematic flow above, hydroxide anions travel through the AEM creating electrical current. Similarly to the PEM cell, in AEM electrolysers the membrane is the electrolyte as well. Typical non-noble catalysts used are based on Ni, Fe, Co, Mn, etc.

ANODE COMPARTMENT

The anode compartment is located on the left side of the electrolyser if we look at the figure above. It is composed of anode flow field, which is where the reactant gas is introduced (air or oxygen). The next layer is the one charged to diffuse the reactant gas. It has to transport it to the surface while removing the excess water produced during the electrochemical reaction. The next layer is a thin, porous layer (called anode porous transport layer) who is in charge of the mass transport of the reactant gas as well but mainly the needed water. Finally we find the anode electrode, which is where the oxidation takes place.

ANODE EXCHANGE MEMBRANE

It is a selectively permeable membrane charged of only transporting negatively charged anions (hydroxide anions) while blocking positively charged ions (such as H⁺).

CATHODE COMPARTMENT

It is composed of four elements as it was the case for the anode compartment. The cathode electrode will receive the positively charged hydrogen ions to complete the reduction reaction. The reduction of H+ anions is what will allow the production of hydrogen gas. The cathode porous transport layer and cathode gas diffusion layer will play similar roles to their anode peers, their goal being to facilitate mass transport and diffuse gas. The cathode flow field is where the hydrogen gas will be liberated.

TECHNICAL SPECIFICATIONS

The technical specifications that will be discussed are the ones from the Enapter EL 4.0 model. We will analyse this specific model to study the features of an AEM electrolysis cell.
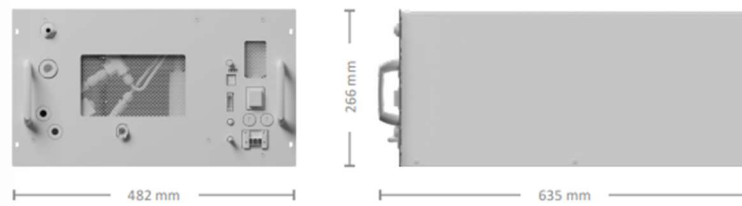
Figures 10 & 11 - Enapter EL 4.0 AEM electrolyser

This product yields extremely pure hydrogen with values oscillating between 98.8% and 99.9% of purity depending on pressure. Other remarkable features are its operative power consumption, which is of 2.4 kW/h producing 1.0785 kg of Hydrogen per day. The maximum water input conductivity of 20 μS/cm is a clear example of the high tolerance of water types that can be used for the electrolysis. The complete list of technical specifications can be checked in the figure below:

Production rate	Up to 500 NL/h, up to 1.0785 kg/24 h
Hydrogen output purity	35 barg: 99.9% (< 1,000 ppm H_2O and < 5 ppm O_2) at 25 °C 8 barg: 98,8% (< 12,000 ppm H_2O and < 5 ppm O_2) at 25 °C
Output pressure	Up to 35 barg
Nominal power consumption per Nm³ of H_2 produced	4.8 kWh/Nm³, beginning of life
Operative power consumption	2.4 kW, beginning of life
Peak power consumption	3 kW
Heat dissipation Max heat dissipation	0.6 kW, beginning of life 0.9 kW, end of life
Standby power consumption[1]	0.3 kW
Power supply	220 – 240 V (AC), 50/60 Hz
Maximum water input conductivity	20 μS/cm at 25 °C
Water consumption	~ 420 mL/h at 25 °C
Water input pressure range	1 – 4 barg
Ambient operative temperature range	5 °C – 45 °C
Ambient operative humidity range	Up to 90% humidity, non-condensing

Figure 12 - Technical specifications of the Enapter EL 4.0 AEM Electrolyser

2.4.2. Advantages and drawbacks

PROS	CONS
• Non-noble metal catalyst • Non corrosive electrolyte • Compact cell design • Low cost • Absence of leaking • High operating pressure • Flexibility in water quality • Scalability and system integration	• Limited supply and capabilities due to laboratory stage • Durability • Membrane degradation • Excessive catalyst loading • Potential formation of chlorine gas at anode

Table 8 - Table showing the advantages and drawbacks of an AEM Electrolysis cell

Let us comment some of the advantages and disadvantages. AEM technology uses non-noble metal catalysts, which can substantially reduce costs when scaling the production. Its absence of leaking as well as its non-corrosive electrolyte contribute to system durability (except for the membrane). Flexibility in water quality is also key: unlike PEM or Alkaline, the water (or alkaline water) requirements are not as demanding, allowing water recyclability. That being said, the fact that the product is still in a laboratory stage makes it very difficult to purchase today and may suppose additional costs. Membrane degradation is also a major issue that should not be overlooked.

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3. Dynamic modelling of the electrolysers

The aim of this section is to provide an accurate Matlab model allowing us to run some tests that will give essential information on the Alkaline and PEM technologies. SOEC and AEM technologies are out of scope for this chapter since they are still at an early stage of development, making it difficult to find updated data.

3.1. Description of the Simulink model

We will divide the description into the inputs, the blocks and the outputs of the system for each technology, separately. Nonetheless it should be noted that this model has some limitations which are:

- The model does not have the precision to take into account the thermal, ohmic and activation losses (it is a theoretical model).

- The electrolysers are not sensible to power input variations in the first part of the tests (technical performance evaluation).

- Temperature and Pressure inputs are assumed to be constant in our model. This means that the study will be performed in steady state conditions.

- Simulink does not tolerate very sudden spikes of input power (which can occur in real life scenarios). This limitation will be relevant for the second part of the tests (adaptability to intermittent power supplies).

An interesting test that could have been executed, but that cannot be done because of the reasons cited in bullet point 2, is one where we compare the efficiency of a technology for the same input power but with a different composition. In other words, we would compare the efficiency of an electrolysis with many cells and a small active area with an electrolysis having few cells and a

large active area in such a way that the same input power is consumed in both cases.

The Simulink models of this section are an adaptation of the ones found in the paper "Estudio comparativo de las tecnologías de electrólisis para la conversión de electricidad a hidrógeno a gran escala basada en fuentes renovables" by Juan David Gutiérrez Obando.
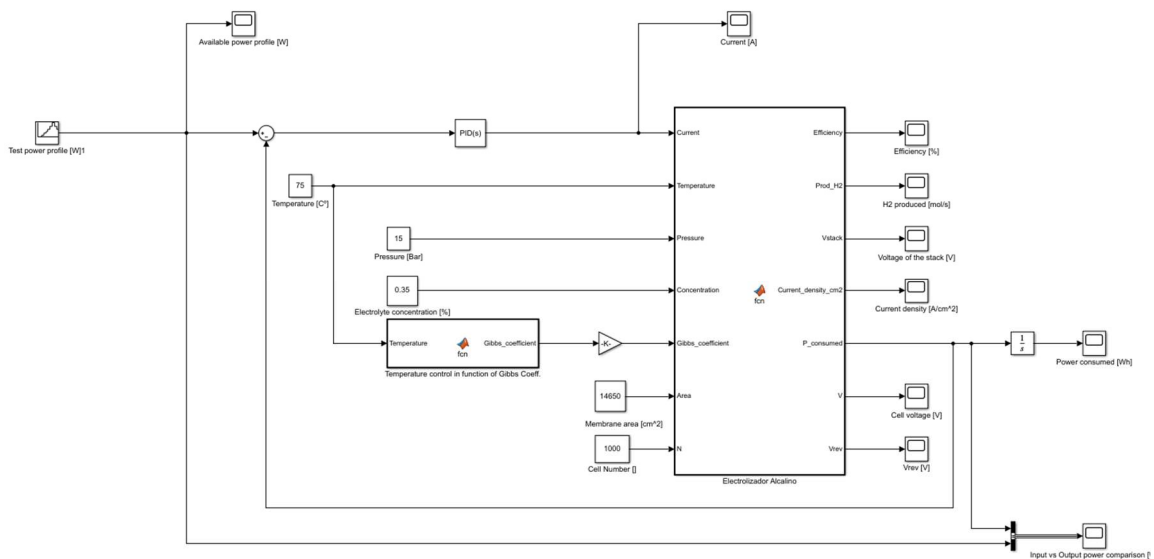
Figure 13 - Screenshot of the Simulink block environment corresponding to the Alkaline electrolysis

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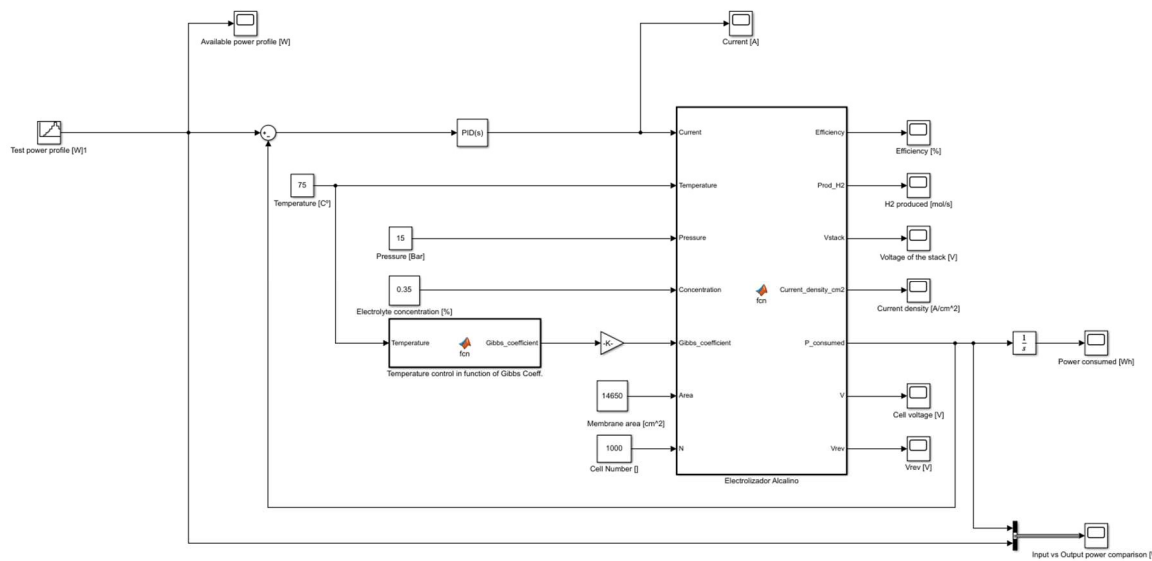
Figure 14 - Screenshot of the Simulink block environment corresponding to the PEM electrolysis

3.1.1. Alkaline electrolyser

We will start by describing the alkaline model which has seven inputs. The table below shows the name of the input variables in Simulink together with the units and a short description.

Input	Unit	Description
Current	[A]	Current provided by the power input
Temperature	[ºC]	Temperature of the electrolysis cell
Pressure	[bar]	Pressure of the electrolysis cell
Concentration	[%]	Concentration of the solution
Gibbs coefficient	[J]	The Gibbs coefficient is a Pressure and Temperature dependent value (G(P,T)) that determines the amount of energy needed for the necessary electrochemical

		reactions to occur.
Area	[cm²]	Area of the diaphragm, which is the area taken into account for the current density computation.
N	[]	Number of cells, which is the number of pairs of electrodes you have together with the DC voltage source and diaphragm within one electrolyser

Table 9 - Description table of the inputs of the Alkaline Electrolyser

Notice that there is no direct input of power into the electrolyser but an input of current instead. This current is generated by the voltage source of the circuit which is activated thanks to the input power. Physically speaking, this "transformation" corresponds to the job done by the voltage generator.

The system has seven outputs as well. As can be observed in Figure 9 they are all connected to a scope, which allows us to view the results.

Output	Unit	Description
Efficiency	[]	The efficiency is based on the enthalpies involved. This will be explained in more detail later on.
Prod H$_2$	[mol/s]	Hydrogen production
Vstack	[V]	Voltage of the stack. It is the total amount of voltage provided to the electrolyser (the one(s) provided by the voltage source(s)).
Current density (A/cm²)	[A/ cm²]	Current density is computed as the input current over the active area.
Electric Power	[W]	Total power consumed by the electrolyser.
V	[V]	Voltage provided to a single cell.
Vrev	[V]	Reversible voltage. Voltage needed in the theoretical scenario where there are no irreversibilities involved.

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Table 10 - Description table of the outputs of the Alkaline Electrolyser

After reviewing the inputs and outputs of the system, we will study the blocks that are in between them. We will distinguish between the electrolyser block (the one to which all inputs and outputs are connected) and the remaining blocks, which will be considered as complementary blocks for the electrolyser.

We will start by explaining the code of the electrolyser block (see Annex 1). The code has been divided into sections and each one of them is described in the table below.

Section of code	Description
%Input data	Shortening the name of the variables "Temperature", "Pressure" and "Concentration" Computing current density and converting it to A/m^2 for future computations.
%Model constants (found with non linear regression)	These parameters were found in the paper of Clemente, Sánchez and Rodriguez. They were determined experimentally, by means of a succession of non-linear regressions.
%Faraday's constant in Coulombs/mol	Self explanatory
%Reversible voltage	The formula to obtain V_rev corresponds to equation 3.1.1.4
%Equations of the model (found experimentally)	The equations of the model come from the paper of M. Clemente, M. Sanchez y L. Rodriguez and of O. Ulleber. Variables "r", "j" and "d" aim to model the dependence of ohmic losses on temperature, concentration and pressure of the model. The equations describing "s" and "t" aim to modelize the dependance of activation losses on temperature.
%Total voltage needed for the electrolysis to	The equations from the prior section are used to compute the total voltage V that is needed so that the electrolysis takes place. The equation can be simplified in the following form:

Section of code	Description
occur	V = V_rev + SUM(V_irr) The developed form is the following, taking into account that concentration losses are neglected: V = Vrev + (r+j+d)*Densidad_i+s*log10(t*Densidad_i+1) =V_rev + V_irr_ohmic + V_irr_activation
%Power consumed by the electrolyser	Self explanatory
%Production of H$_2$	This is the hydrogen produced by the electrolysis in one day. Supongo que aquí se trabaja bajo la assumption que toda el supplied current es utilizado para la prod. de hidrogeno (i.e. no losses)
%Efficiency	Hydrogen yield based efficiency.
%Vstack	Total voltage consumed by the electrolyser.

Table 11 - Description table of the code that constitutes the Alkaline Electrolyser block

Let us give some precisions about the obtention of the parameters used in the voltage formula (see the "Model constants" row of the above table). Essentially, experimental data have been obtained from a test bank given some initial conditions. This data were values of current and voltage, which can allow us to plot a polarization curve. Then, using the data points obtained, non-linear regression enables us to find the parameters of the polynomial equations modelizing the polarization curve.

The rest of the blocks from the simulation complement the Alkaline Electrolyser block. We will start with the PID block, which can be regarded as a PI controller since it only has a proportional and an integral action. More precisely, the PID controller block has been set with P = 1 and I = 0.001. This combination allows a quick and precise regulation of the power consumed whenever there is a change in the power supply.
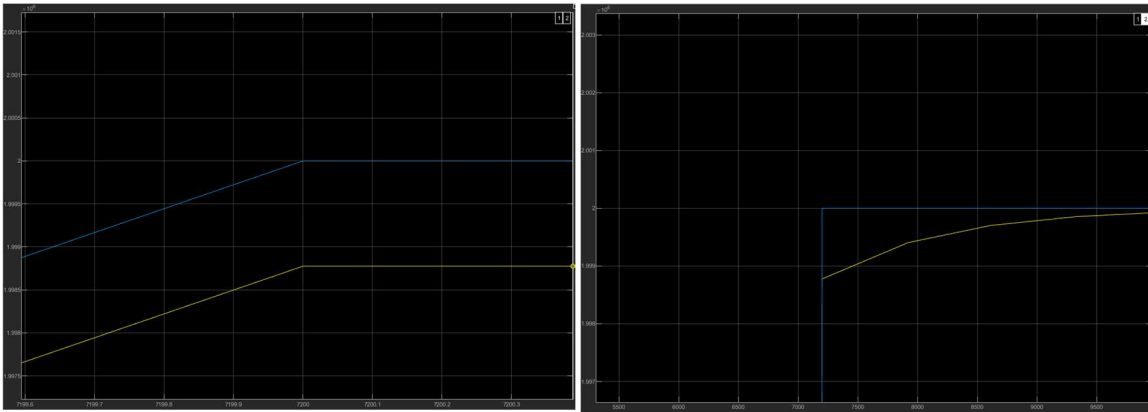
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Figure 15 - P adjustment to the desired value (left) vs PI adjustment to the desired

       value (right)

The figure below shows how PI action makes the system tend to the desired value while P action alone reaches a value that is 1200 W under the desired value. Note that the yellow line in both cases is the power consumed and the blue line is the input power (desired value).

Another complementary block is the "Temperature control in function of Gibbs Coefficient". It is an IF statement. If the temp is smaller or equal to 100ºC the Gibbs coefficient takes a value X(T). Else the Gibbs coefficient takes a value Y(T). The fact that the Gibbs coefficient only depends on Temperature is because pressure is a constant value in our model. This block is followed by a gain of 1 000.

Finally, an integrator is placed right after the power consumed output to determine the energy consumed by the electrolysis. The integrator does this by accumulating the power consumed values during the simulation.

3.1.2. PEM electrolyser

The PEM electrolyser was modelled in a similar way to the Alkaline electrolyser. For instance, we will only consider six inputs in this model since

concentration is not relevant anymore (there is no electrolytic solution involved here).

Input	Unit	Description
Current	[A]	Current provided by the power input
Temperature	[ºC]	Temperature of the electrolysis cell
Pressure	[bar]	Pressure of the electrolysis cell
Gibbs_coefficient	[J]	The Gibbs coefficient is a Pressure and Temperature dependent value (G(P,T)) that determines the amount of energy needed for the necessary electrochemical reactions to occur.
Area	[cm^2]	Area of the diaphragm, which is the area taken into account for the current density computation.
N	[]	Number of cells, which is the number of pairs of electrodes you have together with the DC voltage source and diaphragm within one electrolyser

Table 12 - Description table of the inputs of the Alkaline Electrolyser

Concerning the fact that we took out concentration from the inputs, one could argue that it should be replaced by a parameter that somehow characterizes the solid polymer acting as the electrolyte. We will see in the description of the code of the electrolyser that it is not necessary for our case.

The PEM Simulink model has five outputs. As can be observed in Figure 10 they are all connected to a scope, which allows us to view the results.

Output	Unit	Description
Efficiency	[]	The efficiency is based on the enthalpies involved. This will be explained in more detail later on.
Prod_H2	[mol/s]	Hydrogen production

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Output	Unit	Description
Vstack	[V]	Voltage of the stack. It is the total amount of voltage provided to the electrolyser (the one(s) provided by the voltage source(s)).
Current density (A/cm²)	[A/cm²]	Current density is computed as the input current over the active area.
Electric Power	[W]	Total power consumed by the electrolyser.

Table 13 - Description table of the inputs of the PEM Electrolyser

Similarly to what was done for the Alkaline, we will study the blocks that are in between them, starting with a description of the code from the PEM electrolyser block.

Section of code	Description
%Input data	Shortening the name of the variables "Temperature" and "Pressure" and converting temperature to K.
%Electrolyser data	Computing current density (warning: here the Area input has to be directly in m²)
%Faraday's constant in Coulombs/mol %Perfect gas constant	Self explanatory
%Reversible voltage	Formula to obtain V_rev, corresponds to equation 3.1.1.4
%Pressures	Dalton's law of partial pressures along with 4 assumptions on pressure allows us to compute PH2 and PO2. The expression of PH2O is just an empirical expression. Note that P_an = P_ca = P
%Cell paramters	Vstack, efficiency and electric power expressions are identical to the Alkaline model. Exclusive parameters of the PEM include: • ALFAan and ioan, which were found with numerical methods. • espesor_membrana which is Nafion 117 • Conductivity (we picked the upper value). • Rmenb indicates the resistance of the membrane

Section of code	Description
	• V is the voltage needed for the electrochemical reactions to occur

Table 14 - Description table of the code that constitutes the Alkaline PEM block

In the Cell Parameters row from the table above we mentioned the equation to compute V, the voltage needed for the electrochemical reactions to occur in the PEM cell. From the formula (see Annex) we can see that the voltage takes into account the open circuit voltage (sum of reversible voltage and Nernst equation), the voltage to overcome activation losses and the voltage to overcome ohmic losses. The Nernst equation is used for computing the reduction potential of an electrode whenever it is not in standard conditions. Even though an important part of losses are considered by this model, some of them are not and cannot be ignored as we will see in the next section.

The remaining blocks of the system are identical to the ones from the Alkaline. The PID block is a PI controller whose aim is to take advantage of the most power as possible, the Gibbs Coefficient is computed with a temperature dependent formula (together with a gain of 1000) and the integrator yields the energy consumed.

3.2. Tests performed on the dynamic models

The tests we will run are divided into two categories: technical performance and adaptability to intermittent power supplies. In the technical performance tests will compare the main parameters characterizing the Alkaline and PEM electrolysis. This will allow us to have detail on the advantages each technology has and under what conditions they are optimal. Finally we will assess how each technology responds to variations in the power supplies, which is key if we want to see which technology is more suitable for renewable energies. During the study we will

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systematically compare the results of our tests with the results of other papers as well as theoretical findings.

The table below summarizes all the tests that will be analyzed in this part.

Test #	Technologies compared	Test Category	Test description
1	Alkaline VS PEM	Technical performance evaluation	Hydrogen Production comparison
2	Alkaline VS PEM	Technical performance evaluation	Efficiency comparison
3	Alkaline VS PEM	Technical performance evaluation	Vtotal_consumed comparison
4	Alkaline VS PEM	Technical performance evaluation	Current density comparison
5	Alkaline VS PEM	Technical performance evaluation	Electric power consumed comparison
6	Alkaline	Adaptability to intermittent power supplies	Input power efficiency
7	PEM	Adaptability to intermittent power supplies	Input power efficiency

Table 15 - Summary table of the different test performed

3.2.1. Technical performance evaluation

In this section we will compare the performance of the Alkaline and the PEM electrolyser by putting the two technologies in parallel and feeding them with the same power source, which is the power profile given by a solar panel for ten hours. The figure below shows the Simulink block arrangement that will be executed.
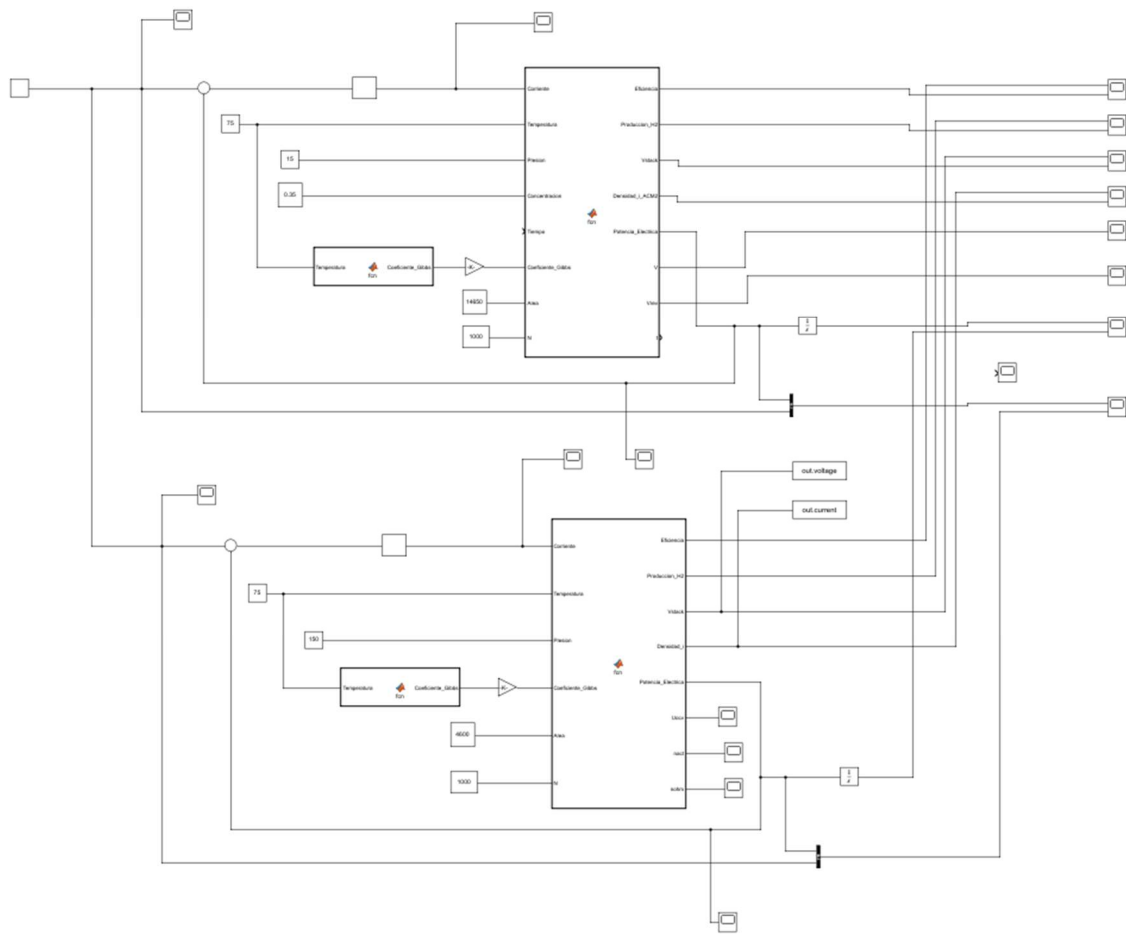
Figure 16 - Screenshot of the Simulink block environment corresponding to tests 1, 2, 3, 4, and 5

Technically speaking, only one test will be performed in this section, but we divided it into five subsections to analyse the results separately.

TEST CONDITIONS

To realize an effective comparison, not only the input power should be the same but the conditions for each electrolyser should be "relatively equal" as well. By relatively equal we mean that since each electrolyser has its own operation conditions delimited by ranges of values, we will pick the middle values of said

ranges so that all technologies behave "normally" in terms of hydrogen production, efficiency and stack voltage.

That said, Pressure and Temperature conditions for both technologies were obtained by doing the arithmetic mean of the lower and upper value of their ranges. For the Alkaline we obtained a pressure of 15 Bar, a temperature of 75ºC and we will set the concentration to 0.35%. For the PEM, since it works at a similar cell temperature but with a higher pressure, we will set the temperature to 75ºC as well, but the pressure will be ten times higher.

Current densities also need to be adjusted to obtain accurate results, which is why we need them to be within their specified range ([0.2; 0.4] A/cm^2 for the Alkaline and [0.6; 2] A/cm^2 for the PEM). Since current density is computed as the current entering the electrolyser divided by the active area, we will search for the adequate active areas to reach the wanted current densities on a try-error basis. The values found were 14 650 cm^2 for the Alkaline and 4 600 cm^2 for the PEM.

	Alkaline electrolysis	PEM electrolysis
Temperature	75 ºC	75 ºC
Pressure	15 bar	150 bar
Concentration	0.35 %	-
Number of cells (N)	1 000	1 000
Active area	14 650 cm^2	4 600 cm^2

Table 16 - Testing conditions for tests 1, 2, 3, 4, and 5

TEST 1 RESULTS

The results obtained after running the simulation for a time of 10 hours are the following.
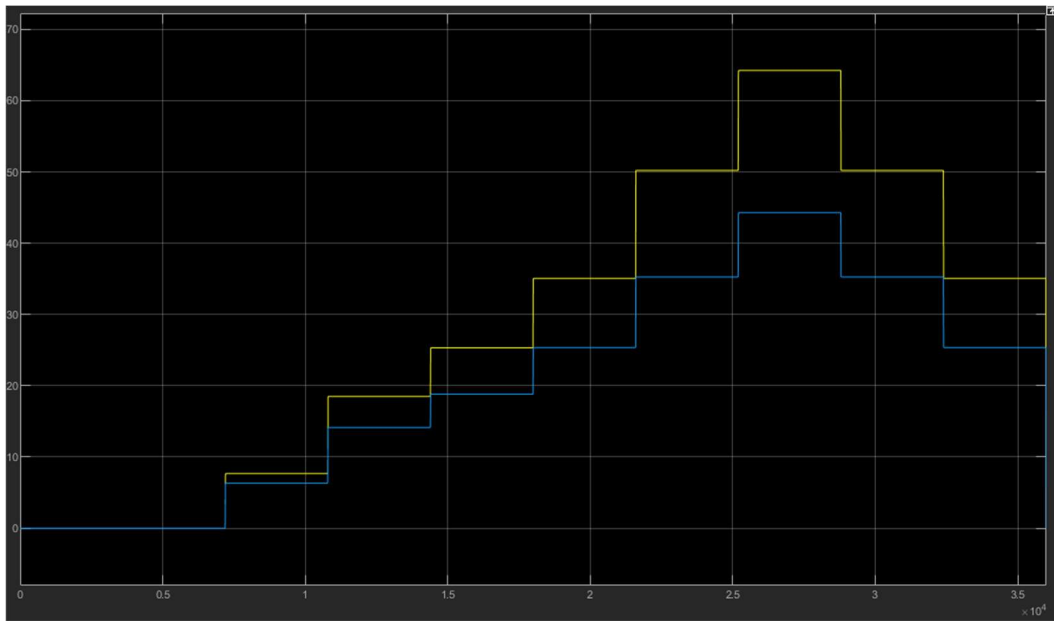
Figure 17 - Test 1 results: Evolution of hydrogen production in mol/s (simulation time = 10 hours)

The PEM electrolyser (yellow line) produces significantly more hydrogen than the Alkaline electrolyser (blue line) for the same input power and number of cells. In fact, the production of hydrogen in PEM is so good that it produces the same amount of hydrogen as Alkaline with way less power. Notice also that the greater the power, the greater the production gap between PEM and Alkaline.

This result coincides with the theoretical results found in literature: PEM produces more hydrogen than Alkaline given the same input power. Numerically, 18.82 mol/s of hydrogen are produced in the Alkaline model whereas 25.32 mol/s of hydrogen are produced by the PEM. Both values being realistic, we conclude that the PEM electrolyser is better than the Alkaline technically speaking.

TEST 2 RESULTS

The results obtained after running the simulation for a time of 10 hours are the following.
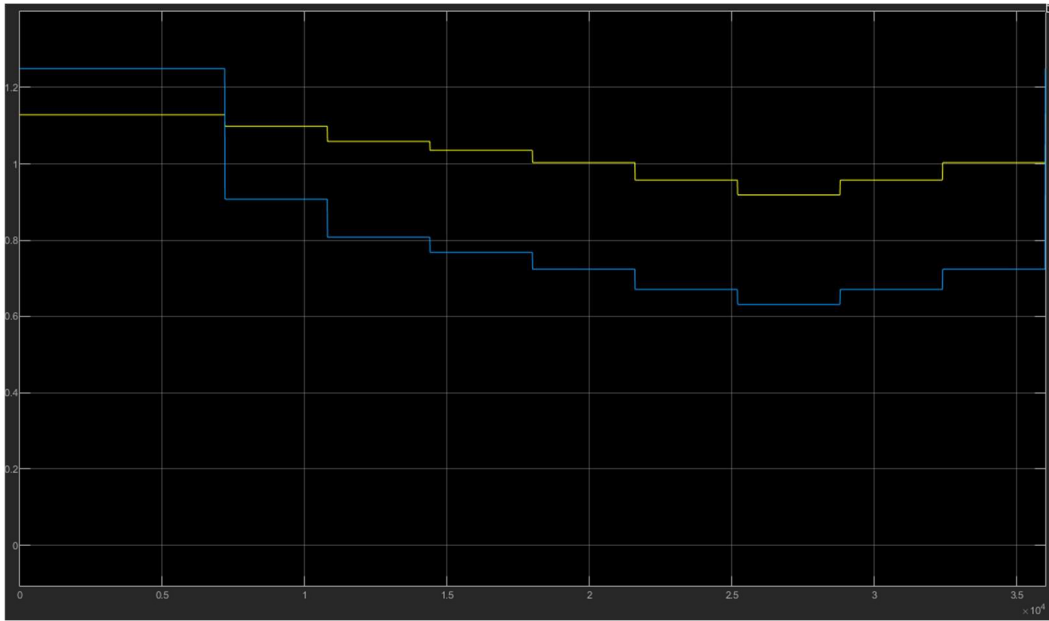
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Figure 18 - Test 2 results: Evolution of the efficiency (simulation time = 10 hours)

The above figure reveals three significant findings: values greater than 100% are observed for efficiency, the PEM technology (yellow line) demonstrates the highest overall efficiency, and both efficiencies decline with increasing input power.

Concerning the efficiencies having a value greater than one, this happens because of how the efficiency is defined in the model:

$$\eta = \frac{energy\ obtained\ in\ form\ of\ H_2}{electric\ energy\ supplied\ to\ the\ system} = \frac{2 \cdot F \cdot V_{rev} + T \cdot \Delta S}{2 \cdot F \cdot V} = \frac{286\ 000}{2 \cdot F \cdot V} \qquad \text{(Equation 3.2.1.1)}$$

The numerator is the high heating value of Hydrogen which can be decomposed into the electric energy ($2 \cdot F \cdot V_{rev}$) and the thermal energy ($T \cdot \Delta S$) that is necessary to obtain one mol of H_2 and the denominator is the electrical energy supplied to the system. That said, it makes sense that we obtain efficiencies that are higher than one since we are not adding the external heat needed to obtain H_2 in the denominator.

The reason why we are using this efficiency formula instead of one that considers the external heat in the denominator is because for some values of voltage the ohmic losses generate enough heat so as to not need an external heat source.

That said, under the assumption that ohmic losses compensate for the need of an external heat source, our efficiency model is valid but efficiencies with values greater than 100% should be ignored.

About the PEM technology being more efficient than the Alkaline one, this coincides with the theoretical findings claiming that higher current densities can be obtained for a same level of input power. This is also proven experimentally in TEST 4 RESULTS, since current densities are very tied to efficiencies.

Finally, from the observation that efficiencies decrease with increasing input power we can say that the disadvantage of producing Hydrogen at high flow rates is that the efficiency is lower. In other words, the price to pay if we want to produce at a high efficiency is that the flow rate will have to be lower.

TEST 3 RESULTS

The results obtained after running the simulation for a time of 10 hours are the following.
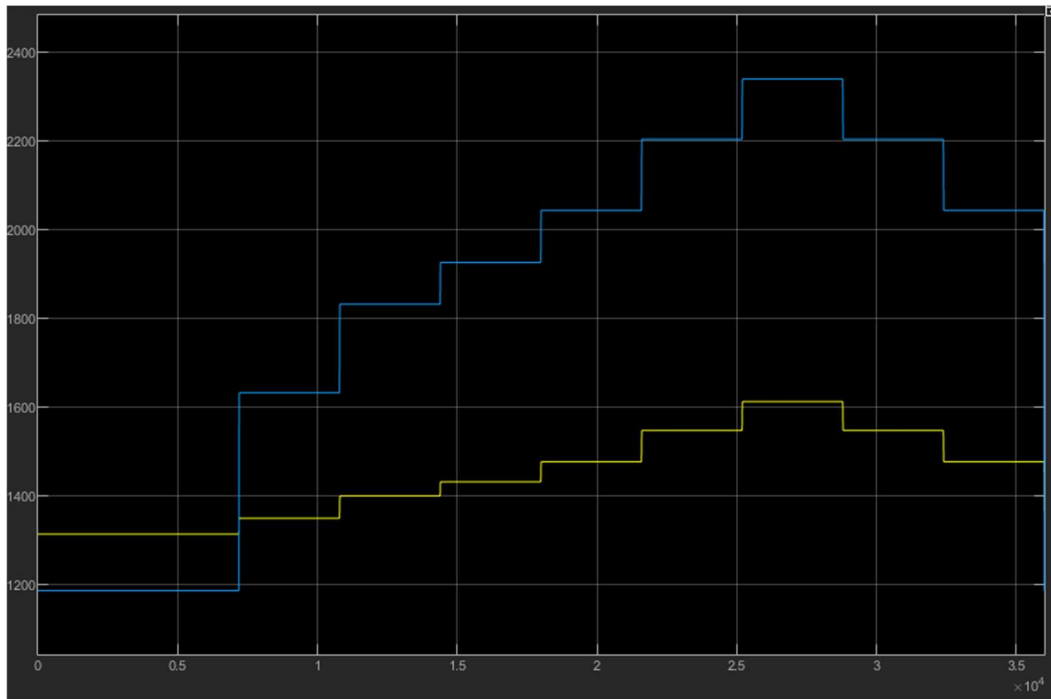
Figure 19 - Test 3 results: Evolution of the total voltage consumed by the stack in V (simulation time = 10 hours)

The voltage consumed by the Alkaline stack is significantly higher than the one consumed by the PEM. This makes sense if we analyze it from the perspective of the real power formula for a DC current voltage:

$$P_{total} = V_{stack} \cdot I \quad \text{(Equation 3.2.1.2)}$$

With P_{total} being the total power consumed, V_{stack} the total voltage consumed and I the current flowing through the closed circuit.

By looking at the power comparator which compares the input power and the power consumed by the stacks, we notice that nearly all the power provided is consumed for both technologies.

Thus, $P_{total\ Alk} = P_{total\ PEM}$ and therefore $V_{stack\ Alk} > V_{stack\ PEM} \Rightarrow I_{Alk} < I_{PEM}$. An implication of the last inequality is that the current density of the PEM technology is larger than for the Alkaline: this will be proven experimentally in TEST 4 RESULTS.

Furthermore, as the input power increases, the voltage difference between the two electrolysis also increases. This implies that the Alkaline technology demonstrates greater sensitivity to input power in terms of voltage. As a result, the Alkaline technology will experience a more rapid deterioration in current (and subsequently, current density), as indicated by the forthcoming test results.

TEST 4 RESULTS

The results obtained after running the simulation for a time of 10 hours are the following.
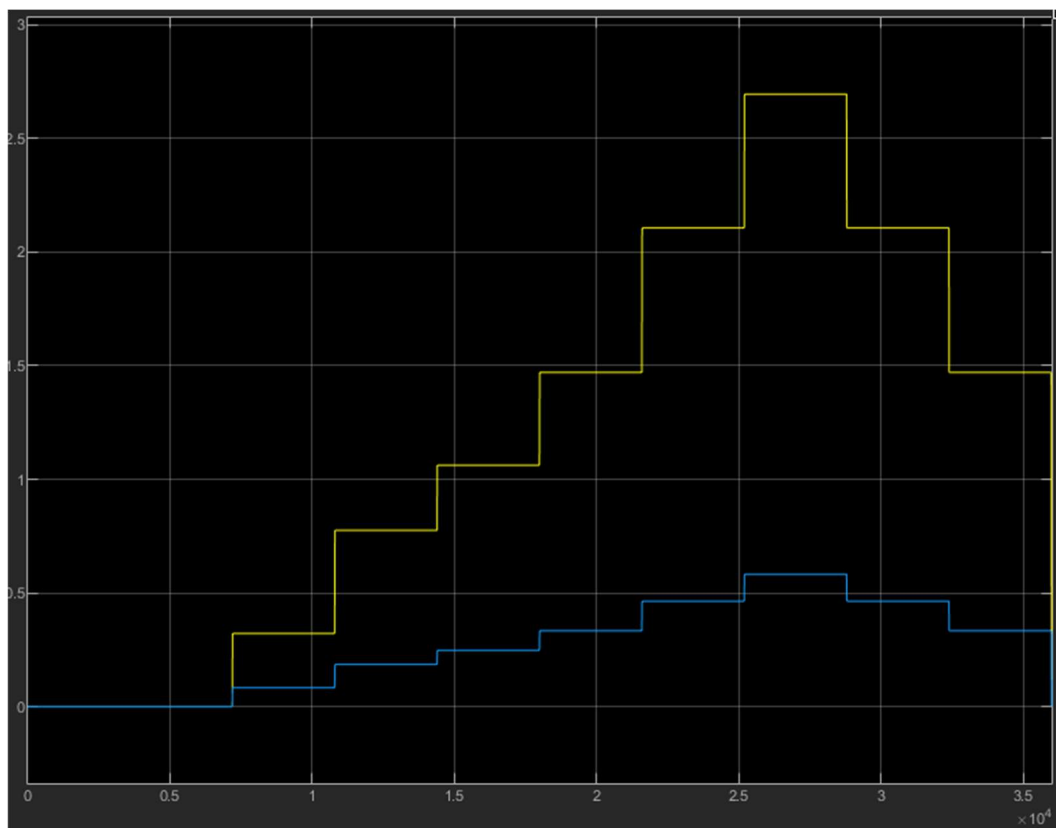

Figure 20 - Test 4 results: Evolution of the current density in A/cm^2 (simulation time = 10 hours)

Recall that we designed the simulation to obtain current densities within the ranges of operating conditions. It can be noticed that not all the values from

this simulation are inside the range, but this does not matter since the behaviour of the electrolysers analysed so far is aligned with the theoretical results.

This diagram shows the main advantage of the PEM technology, which is its high current density which is, on top of being better than the Alkaline, more sensitive to input power. Recall that current density is one of the key indicators to determine the quality of an electrolysis.

TEST 5 RESULTS

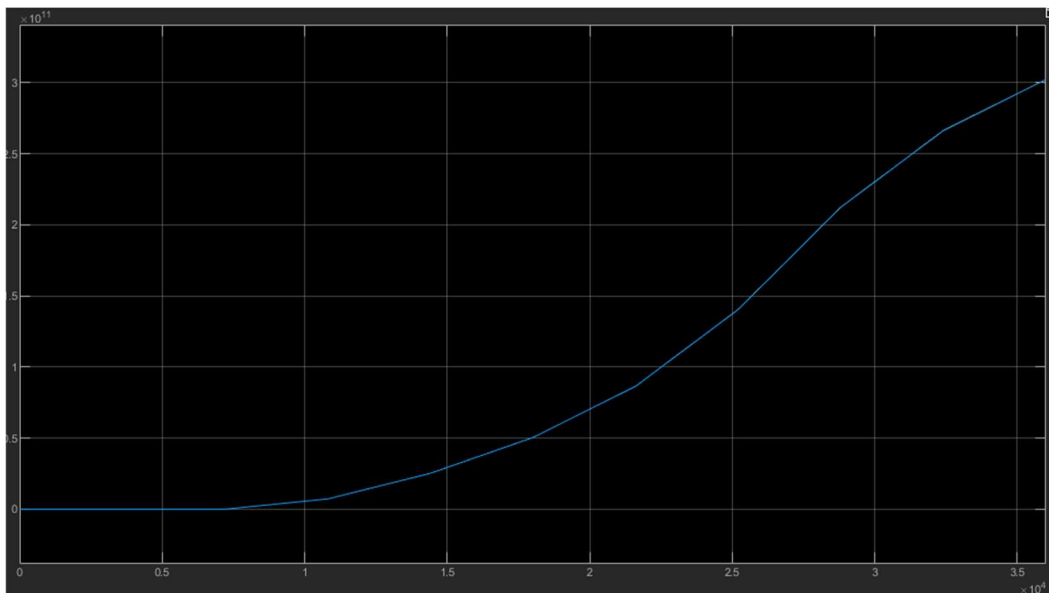The results obtained after running the simulation for a time of 10 hours are the following.

Figure 21 - Test 5 results: Evolution of the energy consumed by the cell in J
(simulation time = 10 hours)

The first thing we notice is the overlap of the two curves (the difference can be negligible). Indeed, both electrolysers consume all the energy supplied. This is important to know when performing the comparison because it could be the reason why a technology yields a better or worse efficiency. Knowing this we can

conclude that performance differences are due to physical concerns (such as thermodynamics, material science...) rather than control factors (feedback loop accuracy).

This assumption is very strong and in a certain way not very realistic since each technology has its own capacity to adapt to power fluctuations. We will discuss this topic in more detail in the adaptability to intermittent power supplies sections.

CONCLUSION

This simulation allowed us to confirm that the PEM technology is better than the Alkaline in terms of hydrogen production and hydrogen yield based efficiency. The total voltage consumption of the cell and the current densities are closely tied to the hydrogen production and efficiency, which is the reason why those results are in accordance with the previous ones. Note that characteristics such as profitability and viability were neglected in this section when they play a crucial role in determining which technology is best adapted to real world needs. Nonetheless this will be considered in the next chapter. Thus, we can safely say that PEM is better than Alkaline from a technical point of view.

3.2.2. Adaptability to intermittent power supplies

In this section we will study the adaptability of each of the electrolysers to intermittent power supplies. Here the power profile (still coming from a solar panel) used now will not be simplified, in the sense that it will have fluctuations (previously neglected) in between each hour.
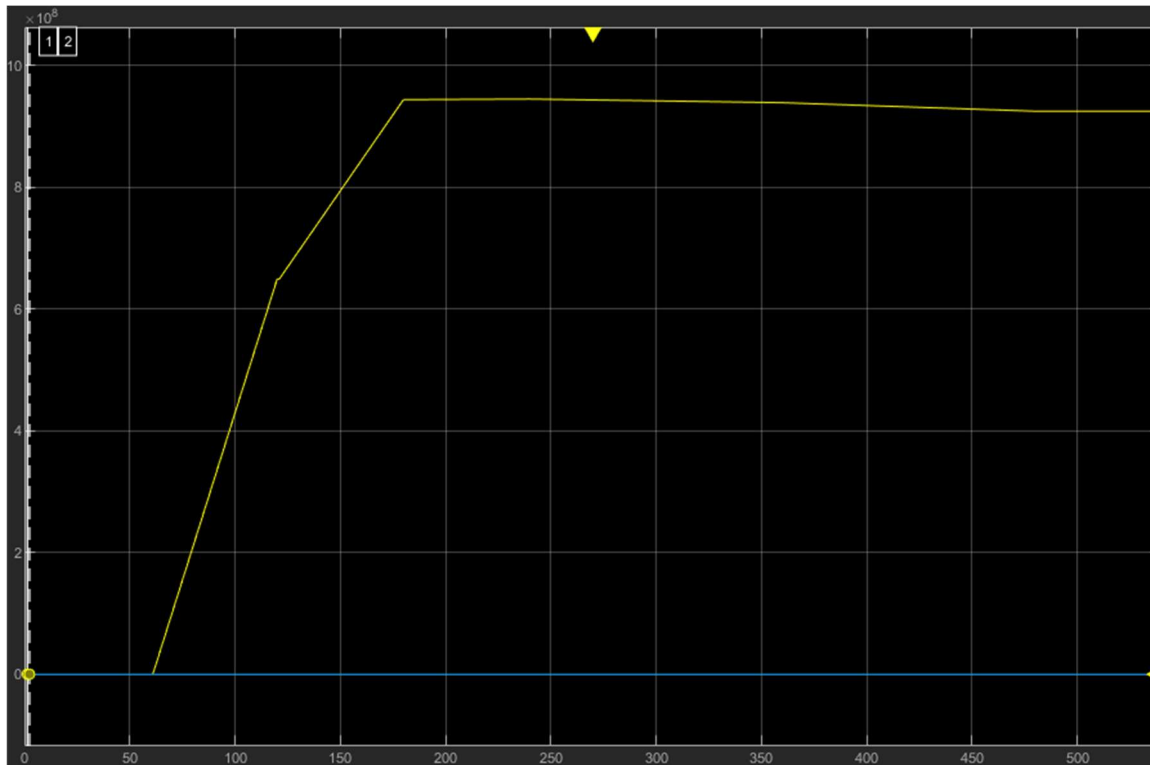
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Figure 22 - Screenshot of the power profile with variations

TEST CONDITIONS

Testing conditions will only involve the power input and the power filters, which simulate the capacity of an electrolyser to absorb the input power provided.

In [25] we have seen that a reasonable ramp rate for the Alkaline can be of 20%/s, meaning that the electrolyser will spend one second to adjust itself once there has been a change of 20% of the maximum power in the power supply.

In [26] we have seen that an electrolyser handling input powers of 20 MW can be seen as the sum of 20 electrolysers in parallel handling powers of 1 MW. Since each one of them has a ramp rate of 0.5 MW/s, the resulting ramp rate for our electrolyser would be 10 MW/s which is 50%/s.

Some assumptions have been made for the creation of these filters.

1. Both electrolysers have a linear response to setpoint changes. This can be observed by comparing figure 23 with figure 25 and figure 24 with 26. This is generally true and there are only a few exceptions (see [26]).

2. Ramp rates are the same for ramp up and ramp down i.e. ramp rates are the same whether there is a decrease or an increase in input power. Figures 25 and 26 below coming from paper [26] show that the small differences between ramp up and ramp down rates can be neglected without making rough estimations.

3. You will reach the maximum load from no matter what percentage you find yourself in with the same ramp rate. That is, to go from 20% to 100% of the electrolyser capacity you will need twice the time that was employed to go from 60% to 100%. This can be observed in figure 25 for instance, by seeing that the linear parts of the plot are all parallel between them (meaning they have the same slope).
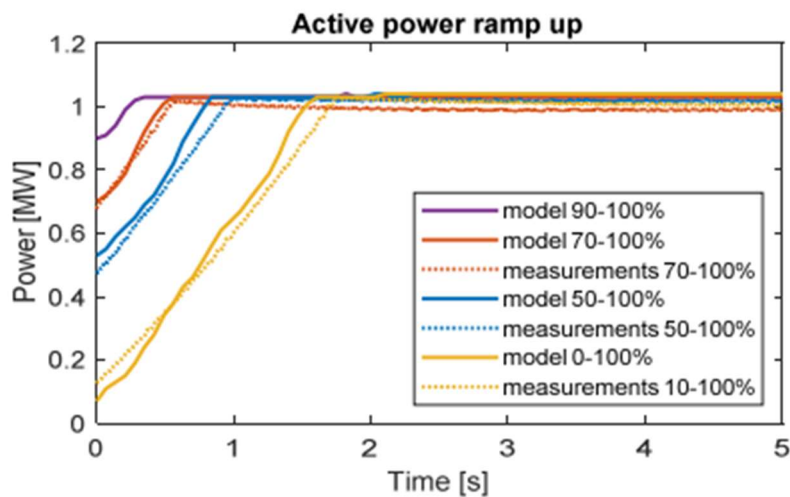

Figure 23 - Comparison between the detailed electrolyser model and the field measurements (ramp up)
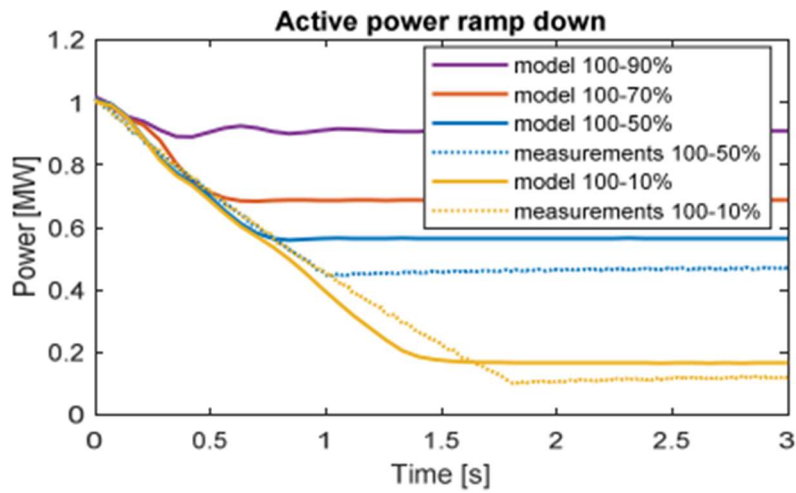
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Figure 24 - Comparison between the detailed electrolyser model and the field measurements (ramp up)
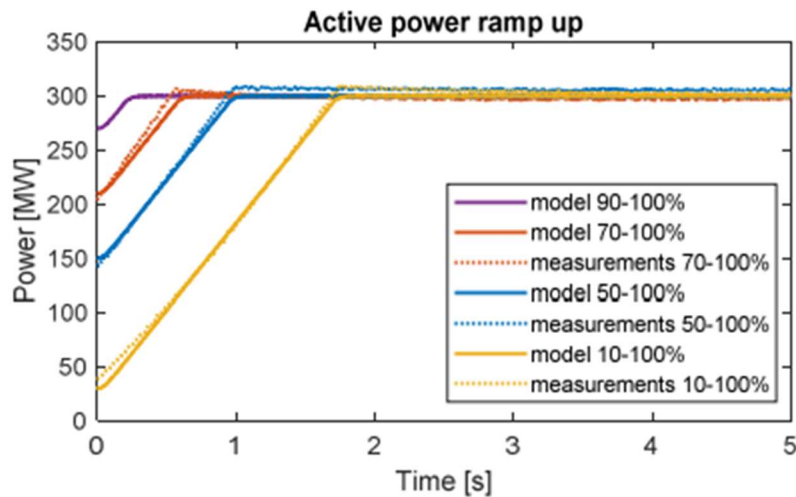

Figure 25 - Comparison between the simplified, scaled-up electrolyser model and the field measurements (ramp up)
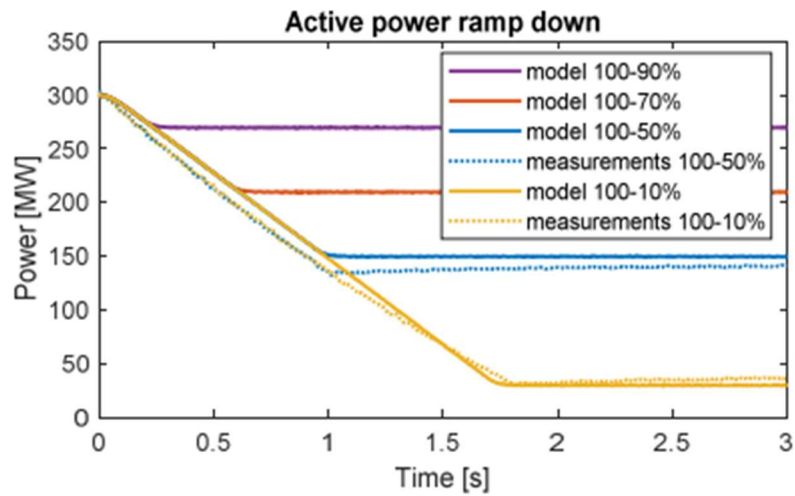
Figure 26 - Comparison between the simplified, scaled-up electrolyser model and the

field measurements (ramp down)

The test set up will be a sum of ramp inputs (simulating the continuous evolution of electrical power transmitted by a solar panel) connected to a derivative. The derivative is then connected to a filter, which will only pass through the ramps that do not surpass the limit (4MW/s for the Alkaline and 10MW/s for the PEM). Then it is connected to an integrator for the signal to go back to its original form.
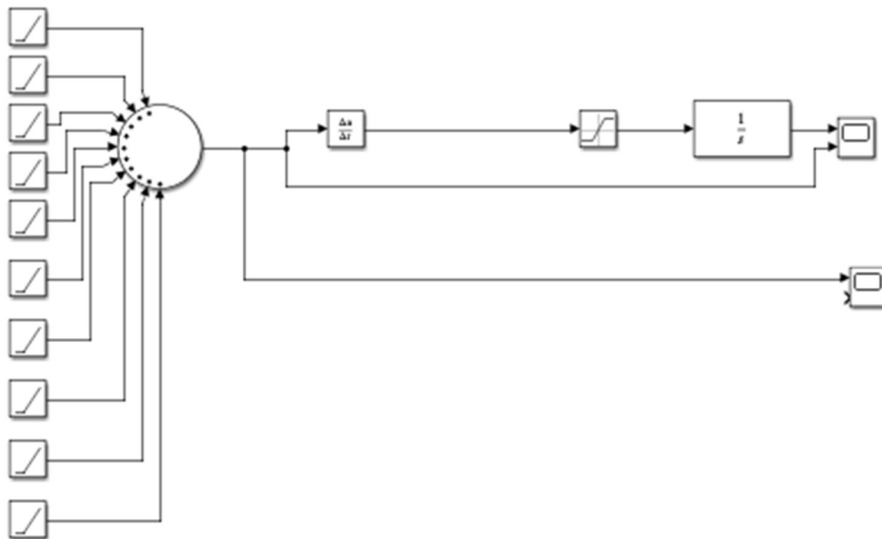

Figure 26.a – Set up of the intermittent power supply test

TEST 6 RESULTS

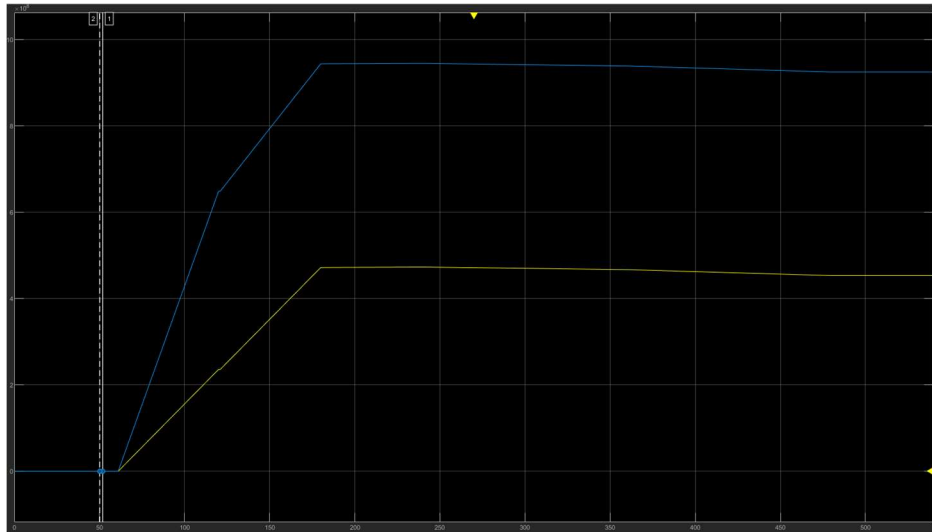Results from test 6 can be summarised with the following figure.

Figure X - Filtered input signal due to high-speed input power increase (Alkaline)

The blue curve is the input power, directly coming from the solar panel. The yellow curve is the power that was actually used by the electrolyser. We can see how the yellow curves cannot keep up with the blue curve since they have a slope bigger than 4 MW/s.

TEST 7 RESULTS

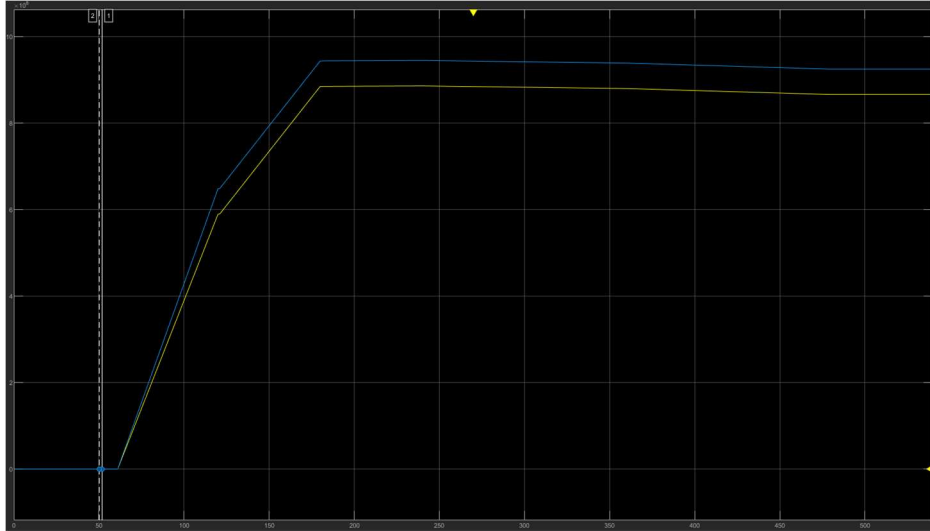Results from test 7 can be summarised with the two following figure.

Figure 26.b – Filtered input signal due to high-speed input power increase (PEM)

The blue curve once again is the input power, directly coming from the solar panel. The yellow curve is the power that was actually used by the electrolyser. We can see how the yellow curves cannot keep up with the blue curve since they have a slope bigger than 10 MW/s.

CONCLUSIONS

By comparing figures 26.a and 26.b we can see that the consumed input power is much larger for the PEM than for the Alkaline given a same power profile. The PEM can keep up with increasing power speeds that the Alkaline cannot. This result coincides with the theoretical findings claiming that PEM (due to its higher current density) responds better to intermittent power supplies.

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4. Economic assessment

A comprehensive economic analysis of the investment, operation and maintenance costs associated with the four prominent hydrogen electrolysers will be performed in this chapter. We want to evaluate the economic viability of each technology for their large-scale implementation, which is why we will consider electrolysers with a capacity of the order of the megaWatt, as it was done in the last chapter. Also note that the access to certain prices for certain technologies is restricted due to commercial purposes. Consequently, we will need to make good approximations to get accurate results.

4.1. Definition of the economic parameters

Let us first define the economic parameters that will be used in this section. The LCH (Levelized Cost of Hydrogen) shows the cost per kg of hydrogen production as it can be seen in equation 4.1.1:

$$LCH = \frac{\sum_{y=1}^{N} \frac{CapEx_y + E_y}{(1+d)^y}}{\sum_{y=1}^{N} \frac{m_{h,y}}{(1+d)^y}} \text{ (Equation 4.1.1)}$$

The NPV (Net Present Value) is a commonly used parameter to evaluate financial investments, since it gives the projected value of an investment over time. That is, it takes into account the discount factor d, which quantifies how much present money is valued compared to future money.

$$NPV = \sum_{y=0}^{N} \frac{Cash_{in} - Cash_{out}}{(1+d)^y} \text{ (Equation 4.1.2)}$$

The IRR (Internal Rate of Return) is another commonly used parameter, and it is defined as the discount factor yielding a net present value equal to 0 (that is, making the investment worthwhile).

$$0 = \sum_{y=0}^{N} \frac{Cas_{in} - Cash_{out}}{(1+IRR)^y} \text{ (Equation 4.1.3)}$$

The variables are defined in the figure below:

Variable	Description (Unit)
LCOH	Levelized Cost (EUR/kg Hydrogen)
y	Year index
N	Electrolyzer lifetime (year)
$CapEx_y$	Capital expenses in year y (EUR)
$OpEx_y$	Operational expenses in year y (EUR)
E_y	Electricity cost in year y (EUR/kWh)
$m_{h,y}$	Produced hydrogen in year y (kg/year)
d	Discount factor (%)
NPV	Net present value (EUR)
$Cash_{in}$	Cash inflow (EUR)
$Cash_{out}$	Cash outflow (EUR)
IRR	Internal rate of return (%)

Figure 27 - Definition of the variables of the economic parameters

4.2.   Economic analysis of the Alkaline electrolyser

The cost analysis will be performed on a 6 MW capacity Alkaline Water Electrolysis plant scaled up from a 3.5 MW capacity pressure electrolysis as it is described in the paper Kuckshinrichs, W., Ketelaer, T., & Koj, J. C. (2017), Economic Analysis of Improved Alkaline Water Electrolysis.

The goal of this scaling is to obtain results that are applicable to industrial plants. The following analysis will be centered in a German Alkaline Electrolysis site (the most cost optimal one) but will also be compared to other countries.

COST BREAKDOWN & SCALING UP

The following costs are gathered from Bertuccioli et al., 2014. We may consider two different cost breakdowns, one for the system and the other for the

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stack. The elements of the system can be splitted into different categories: stack, balance of plant, gas conditioning and power electronics. As it can be seen in the pie chart below, the main costs of the plant originate from the stack which takes half of the overall cost. The second most expensive element is the balance of the plant, which refers to all the supporting components and auxiliary systems a power plant needs to deliver energy. The rest is equally covered by power electronics and gas conditioning, which refers to the compressors and purifiers that prepare the hydrogen for commercialization.

We will now do the breakdown of the stack itself. The Cathode and the Anode make up for half of the stack cost. This is due to their high rate of degradation due to their key role in electrolysis. Both the Cathode and Anode need to be replaced frequently. Structural rings also make up a relevant percentage of the stack cost while other components such as the membrane, the pre-electrode, PTFE sealing etc. are less significant individually.
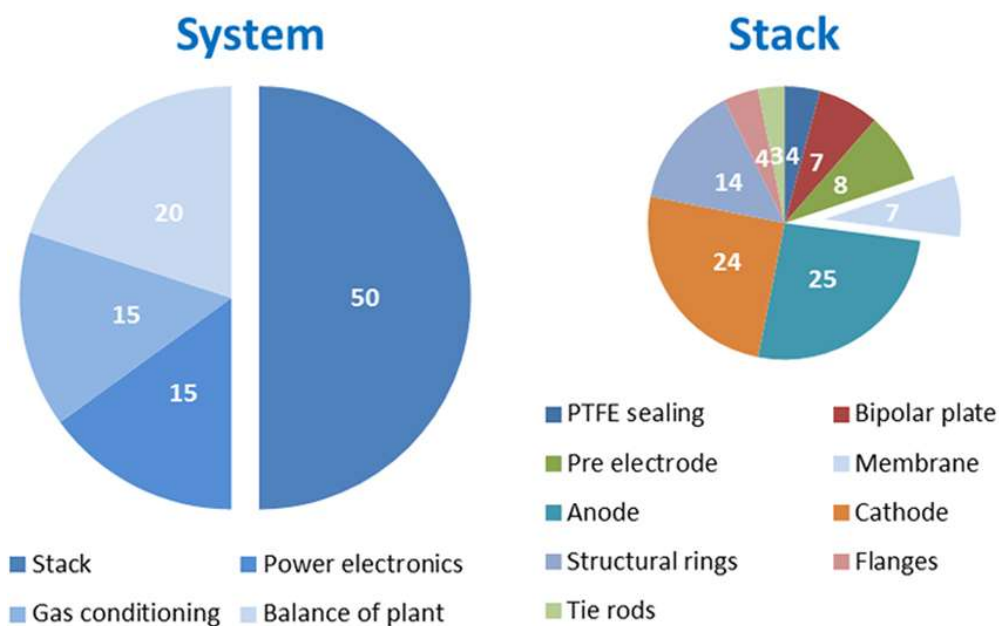

Figure 28 - Cost breakdown of the Alkaline Water Electrolysis Stack

Then, to scale up the investments corresponding to the costs mentioned above, equation 5.2.1 has been used, using a scaling exponent α equal to 0.85 which corresponds to the Alkaline technology (high level of maturity).

$$I_x = I_{base} \cdot \left(\frac{Cap_x}{Cap_{base}}\right)^{\alpha} \text{ (Equation 4.2.1)}$$

It was found that the direct depreciable capital cost (physical components cost) for the 6 MW plant was 6.1 million Euros. This investment corresponds to the overall cost described in Figure X, which is the cost of the system. To the 6.1 million Euros, 1.2 million Euros should be added to cover for the indirect depreciable capital cost, which includes site preparation, upfront permissions and engineering design.

The latter results as well as the fix and variable operation and management expenses can be seen in Table X below. Note that the Euros from the study are 2015 Euros and therefore a 19.98% cumulative price increase has been considered with respect to the values found in the Economic Analysis from the paper Kuckshinrichs, W., Ketelaer, T., & Koj, J. C. (2017).

Expense name	Expense value	Unit
Investment - Direct depreciable cost	6.1 million	€
Investment - Stack replacement	3.05 million	€
Investment - Plant decommissioning	0.366 million	€
Investment - Indirect depreciable capital cost	1.2 million	€
Fix O&M - Material	0.153 million	€
Fix O&M - Labor	0.153 million	€
Variable O&M - Deionized water	0.012	€/kg
Variable O&M - KOH	3.012	€/kg
Variable O&M - Steam	0.012	€/kg

Expense name	Expense value	Unit
Variable O&M - Nitrogen	0.334	€/kg

Table 17 - Scaled up expenses of an Alkaline Water Electrolysis System (6 MW)

From the above table, adding all the Investment expenses we obtain a CAPEX requirement of 10.716 mllion Euros. OPEX requirements will vary, in function of hydrogen production.

Cash Flows

Expenses were evaluated in this section only considering the cash outflows, except for tax redemption. Therefore, positive values represent losses and negative values represent income in the figure below.
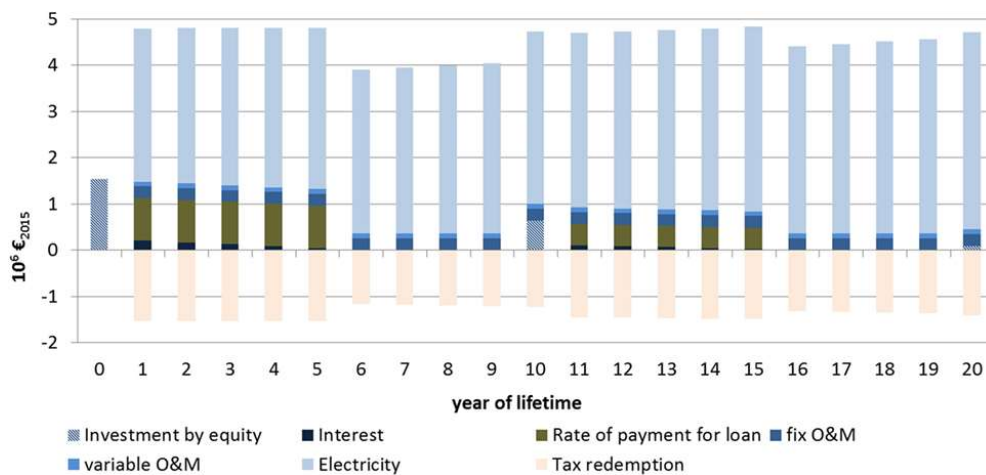

Figure 29 - Current value cash flow (expenses) of the alkaline water electrolysis site

We observe that expenses fluctuate between values of 4 and 5 million Euros. The figure also shows how significant electricity prices are in the expenses of an electrolyser: they account for three quarters or more of the annual expenses. We can also determine how this plant has been financed: two major initial investments by equity (one in year zero and the other in year ten) together with a loan made

possible the purchase of such a plant. Both the interest and the rate of payment for the loan is decreasing through time. The fix and variable O&M (which do not include electricity costs) are relatively low with respect to the rest of expenses. Moreover tax deductibility should not be overlooked, as it reduces the expenses approximately in one quarter.

Levelized Cost of Hydrogen

The levelized cost of hydrogen is an important parameter for the analysis because it gives a value for the cost of hydrogen in €/kg taking into account present and future costs with a discount factor. For instance, if the direct depreciable cost of the investment takes place in the future instead of in period the levelized cost will decrease ("present money is worth more than future money").
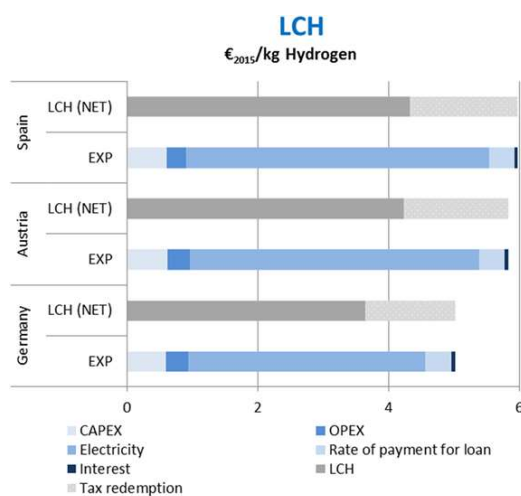

Figure 30 - Levelized Cost of the Hydrogen from alkaline water electrolysis sites of three countries

The figure above presents the LCH of the same facility but located in three different countries. Germany is the most attractive country because of electricity expenditures, which are significantly lower than in Spain or Austria. The rest of expenses are equal between countries. Tax redemption plays an important role in all

three countries since it can pay for all the expenses aside from electricity. Converting to 2023 euros, this leads to Germany having an LCH of 4.37 €/kg.

Net Present Value

The net present value of the site in three different countries is presented below, together with the expenditures. Notice that the NPVs presented are all negative, and this is because cash inflows (apart from tax redemption) are not yet considered as it was the case in the Cash Flows part.
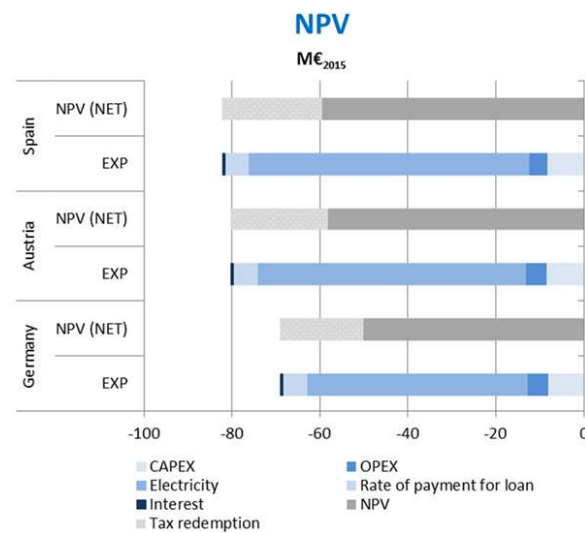

Figure 31 - Net Present Value of the same alkaline water electrolysis site in three countries

Forcefully, since the same expenses have been evaluated in the NPV and the LCH, the ranking of most attractive countries will be the same as in the previous part, with Germany having the less negative NPV. In 2023 euros, this NPV should be of -8.04 Million Euros.

Profitability

One last yet important information is that the only site that is profitable in the 20 year period evaluation, assuming that prices for Hydrogen are constant and high,

is the German one. This can be seen in the diagram below as the German line is the only one constantly below the line of 5 €/kg.
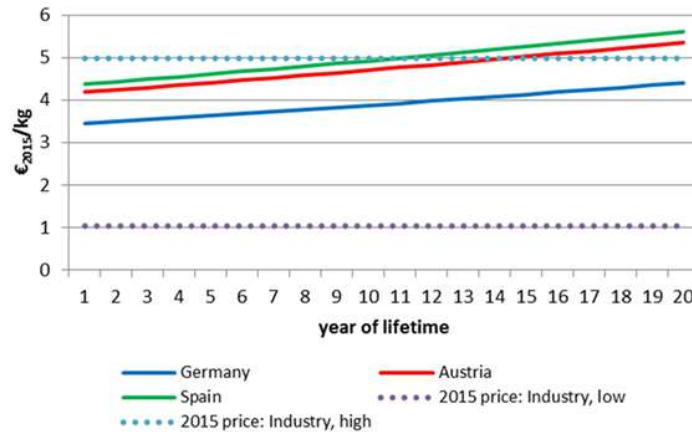

Figure 32 - Net Present Value of the same alkaline water electrolysis site in three
        countries

4.3.   Economic analysis of the PEM electrolyser

The cost analysis of the PEM electrolyser will include four different scenarios so as to find out the conditions for optimal production making use of this technology. Unlike what was done in the last section, this time we will also take into account the revenues from hydrogen production for the LCH, NPV and IRR. For simplification, the only operational expense that will be considered is electricity, calculated using 0.06 EUR/kWh which is the lower price limit for industrial electricity in Germany. This assumption is reasonable, as we have seen in the last section that electricity makes up for the vast majority of operational expenses.

BASE SCENARIO

This scenario will compare the three main economic parameters that were defined at the beginning of this chapter for PEM setups of 2, 5, 10 and 20 MW.

Different life times were also considered since not all cells have the same life time and accidents can happen thus reducing the lifespan of the setup.
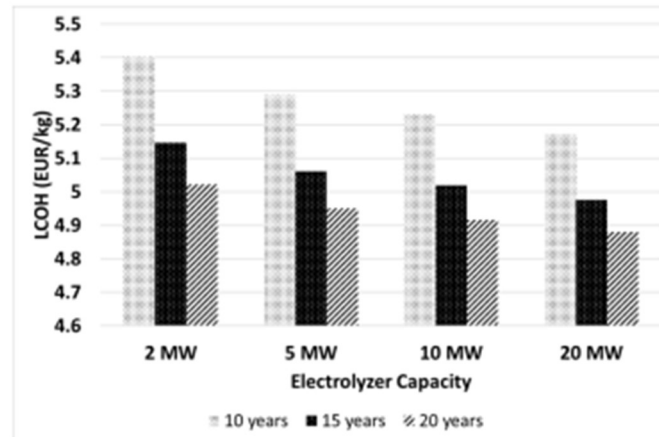

Figure 33 - LCH of electrolysers with respect to capacity and lifetime

In the figure above we see how, for any capacity, the LCH decreases with time (which is logical, since the more time passes the more we accumulate Cash Inflows). Moreover this decrease is not linear: for any of the capacities, the cost reduction from lifetimes 10 to 15 years are larger than from 15 to 20 years. This should highlight the importance of maintenance: it plays a key role in profitability.
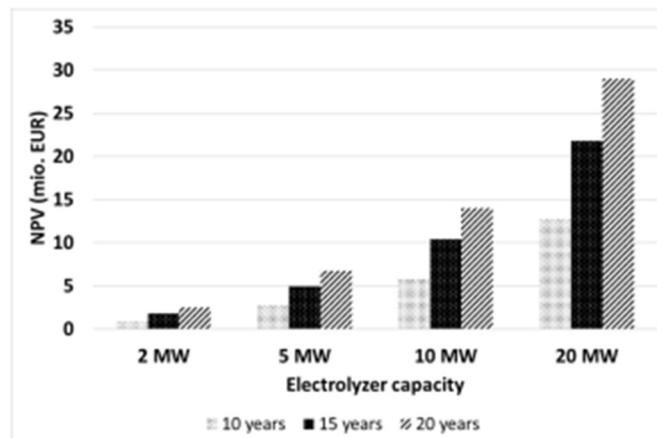
Figure 34 - NPV of electrolysers with respect to capacity and lifetime

The NPVs presented above vary largely in function of their capacity. They also vary in function of lifetime but this variation becomes more visible the bigger the capacity of the electrolyser. This can be explained once again by the fact that the more time passes the more we accumulate Cash Inflows, and such cash inflows are larger for electrolysers with larger capacities since they can produce more. In this way, we can see how hydrogen is a very scalable product: NPVs are at a bit less than 2.5 Millions of Euros for 2MW electrolysers and rise up to 8 times their value for 20 MW electrolysers.
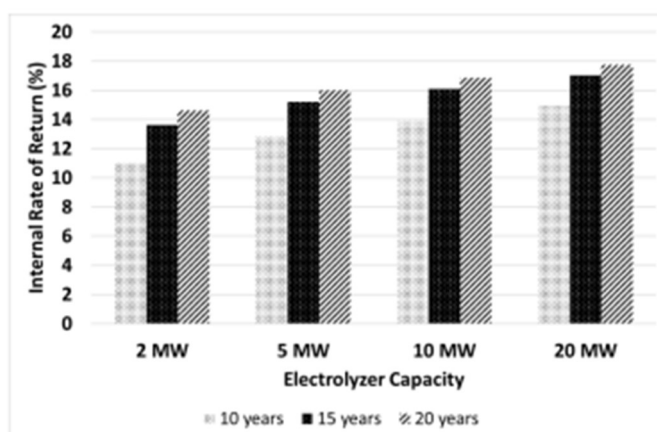

Figure 35 - IRR of electrolysers with respect to capacity and lifetime

Concerning IRRs, they are less variable than the NPV and the LCH. We see that IRR values vary between 11 and 18% approximately. These values can be interpreted as how much the investor has to value present money so as to obtain a profitable investment through time. For instance, for an investor to invest in a 10 MW PEM electrolyser, her discount rate should be of 14% at most. Equity firms consider that reasonable business valuations have 12 to 20 % discount rate, which means that the values obtained would attract investors.

DEPENDENCY ON COSTS AND PRODUCT PRICE VARIATION

After viewing how the lifetime of a technology and the capacity affect the principal economic parameters, it can be interesting to evaluate the technologies given a decrease in all expenses and then a decrease in all expenses and the cost of hydrogen.

In the first scenario we only consider a 10% decrease in each expense type. The consequences can be appreciated in the following column diagram.
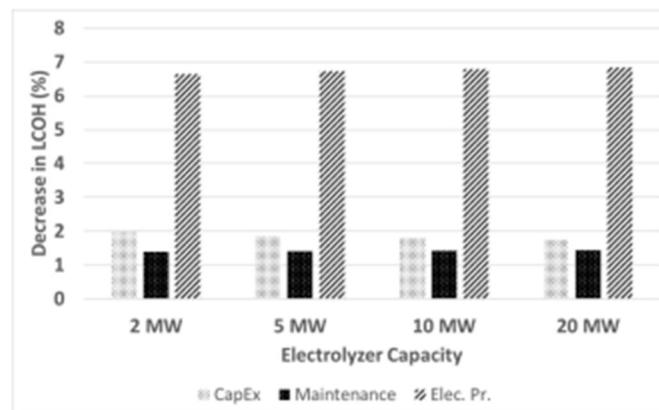
MW electrolysers.

Figure 36 - Decrease in LCH with respect to 10% decrease in each expense type

We first notice that the most impacted expense is electricity price. Decreasing electricity prices by 10% produces a decrease in LCH two times bigger than the one

achieved by decreasing both Maintenance and CAPEX costs by 10%. Therefore, companies will have to put effort in finding cheap electricity rather than cheap CAPEX or Maintenance. This has also been seen in the economic evaluation of the Alkaline electrolysis: the high Spanish electricity prices are the main reason why the investment was viable in Germany and not in Spain.

Now let us observe how NPV reacts to a 10% decrease in each of the expenses combined with a 10% increase in the Hydrogen selling price. Note that this change is likely to become true in the medium run due to the PEM being a hot research topic and an increasingly common energy source.
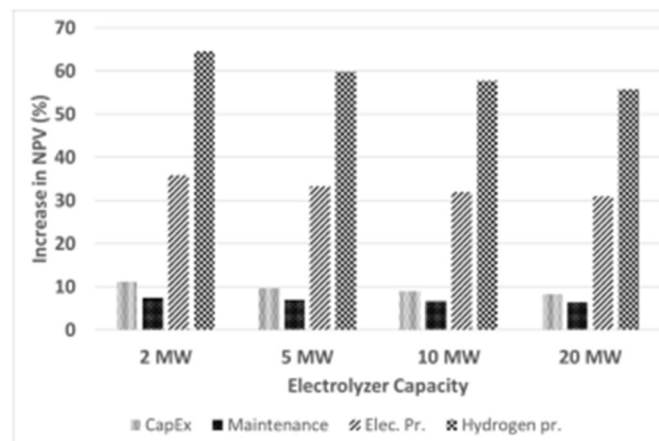
MW electrolysers.

Figure 37 - Increase in NPV with respect to 10% increase in hydrogen selling price and 10% decrease in each expense type

Here it is observed that what makes the NPV increase the most is the 10% increase in Hydrogen selling price, even more than decreasing by 10% the three main expenses, no matter the capacity. We can also notice how the lower the capacity, the higher the 10% increase in price impacts the NPV. The 10% increase in hydrogen selling price can eventually come after an increase in the demand of hydrogen (since it is needed to reach market equilibrium).

ELECTRICITY PRICE

As we have seen earlier, electricity prices play a key role in the profitability of PEM electrolysis. Expensive electricity scenarios have been evaluated in the figure below in order to expect worst case LCH values. With an 86.37% increase in electricity prices from the base case scenario of a 15-year life time, 2 MW capacity electrolyser, we found a value of LCH being equal to 9.5 EUR/kg (a 4.35 EUR/kg increase).

10 years	LCOH (EUR/kg)	% increase
2 MW	9.8	82.28
5 MW	9.7	84.05
10 MW	9.6	84.97
20 MW	9.6	85.91
15 years	LCOH (EUR/kg)	% increase
2 MW	9.5	86.37
5 MW	9.5	87.82
10 MW	9.4	88.56
20 MW	9.4	89.32
20 years	LCOH (EUR/kg)	% increase
2 MW	9.4	88.5
5 MW	9.3	89.77
10 MW	9.3	90.41
20 MW	9.3	91.07

Figure 38 - LCH for the high electricity price and percent increase from the base
scenario

4.4. Economic analysis of the SOEC and the AEM electrolyser

The difficulty to find relevant costs for the SOEC and AEM electrolysers is higher than PEM and Alkaline technologies due to their low readiness level. Indeed, the SOEC is considered to be in a Demonstration stage while the AEM is still in a Large Prototype stage.

Concerning the SOEC technology, Bui et al. show the breakdown of the LCH for three different types of four different types of SOEC: low-temperature recirculation blower (LP-LTBL), High-power high-temperature recirculation blower (HP-HTBL), High-power high-temperature recirculation blower (HP-HTBL) and a HP-EJT (High-power ejector).
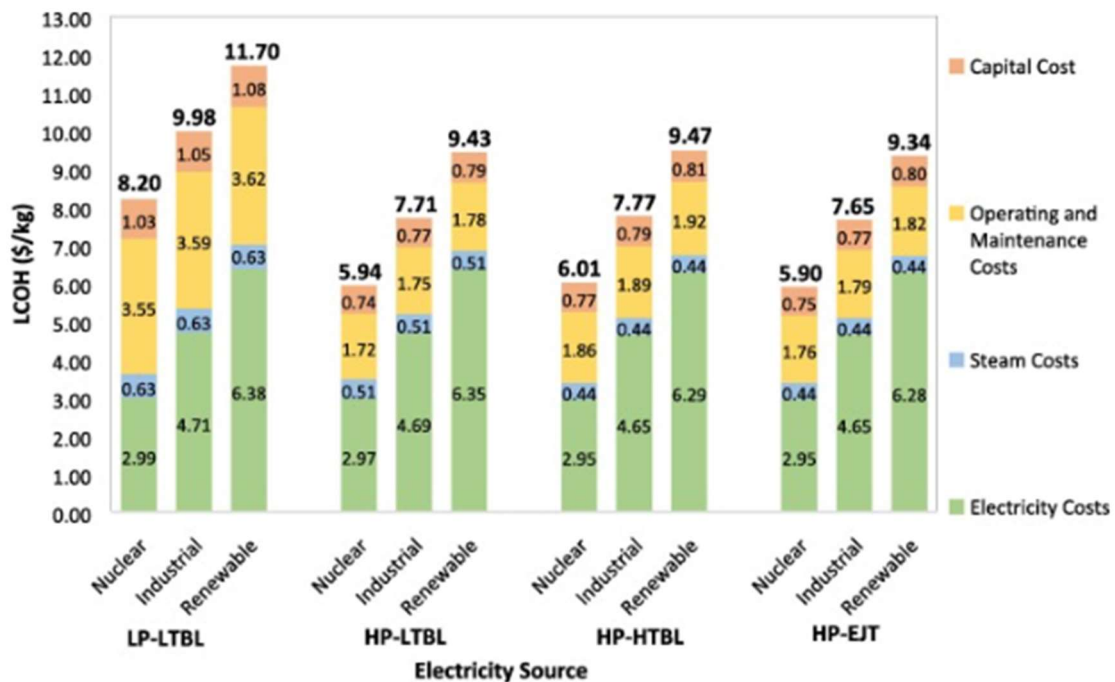
increase).

Figure 39 - LCH with different electricity sources

Since only green hydrogen is in the scope of this study, we will only focus on the renewable energy LCHs. LCH values for green hydrogen oscillate between of 10.73 EUR/kg and 8.56 EUR/kg. We will note that once again electricity costs are responsible for most of the cost. CAPEX costs approximately double or even triple OPEX costs, but the sum of them is still inferior to electricity costs in all cases. So far, electricity costs are a major issue for the three most up-to-date technologies.

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From [40] we can also gather the LCH breakdown together with expected decreases in the long run.
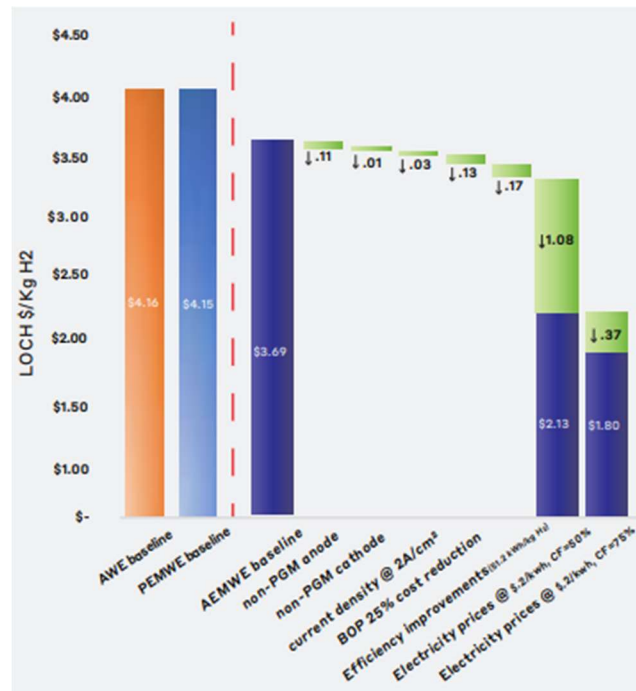
increase).

Figure 40 - Cost breakdown and expected adjustments in the long run of a 5 MW AEM electrolyser

We are only concerned about the right part of the column diagram. Converting dollars into euros, we obtained an LCH for the AEM (5 MW capacity plant) of 3.38 EUR/kg H. Note that the cost of electricity in this analysis is remarkable lower than for the previous technologies because it is electricity that come from the power lines, which are exceptionally low in the US. Thus, the value obtained should only be looked as an indicative one.

4.5. Key takeaways and cost comparison

The below table aims to summarize our findings by comparing costs and commenting on them.

	Alkaline	PEM	SOEC	AEM
CAPEX level	Moderate	High	Very high	High
Comments on CAPEX	Primary cost drivers are stack, power supply and balance-of-plant components.	Proton Exchange Membranes are made of a particularly expensive material and require a complex design. Hydrogen purification, system integration and power electronics are also a big part of the Capital Expenditures.	Top-notch materials and high temperature operation justify the very high CAPEX.	Similar to PEM electrolysis due to the cost of anion exchange membranes and catalysts.
OPEX level	Moderate	High	Moderate - High	Moderate - High
Comments on OPEX	Primary cost drivers are electricity consumption, water usage, and routine maintenance. Periodic replacement of electrodes and membranes is necessary.	The main reason why operational expenditures are higher than the Alkaline is because of the higher electricity consumption, together with the membrane replacement and electrode cleaning costs.	Lower electricity consumption due to high-temperature operation. Occasional cell replacement and control system upkeep are necessary.	Lower electricity consumption than PEM electrolysis but higher maintenance costs due to frequent membrane replacement and cleaning.

Table 18 - Cost comparison table of the four state-of-the-art electrolyser technologies

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The economic analysis reveals that the most cost-optimal alternative in terms of CAPEX and OPEX is the Alkaline technology. Nonetheless, other alternatives such as the PEM or the AEM can be even more attractive due to their higher efficiency levels, which are translated into more cash income to compensate CAPEX and OPEX expenses. The SOEC, although being a promising solution, has not the maturity yet to combine technical efficiency with profitability. Thorough research in material science should be able to replace the costly specialized materials by a cheaper material having similar properties.

Thus, large industrial corporations willing to produce hydrogen are advised to purchase a PEM electrolyser plant (and once in a commercially available stage, an AEM electrolyser plant) since they can cover a high CAPEX and OPEX. In exchange, they will benefit from a more efficient production. Smaller corporations, with less purchasing power, are advised to purchase an Alkaline electrolyser plant due to their lower initial investment and maintenance costs.

5. Project timeline and cost

The timeline of this project can be checked in the Gantt Chart that is in the Annex (Annex 8). From there, we can estimate that this project would eventually have, if it would have been a professional project instead of an educational one. Since this project is theoretical, the estimation can be done by only considering manpower costs, that is, all information has been gathered in a cost-zero manner. Considering myself as the only worker (and all external help as the help of work colleagues, which implies a cost of 0 EUR) a recently graduated student in Industrial Technologies would typically earn 13,82 €/h according to talent.com . Taking into account that the dedication of this project has been of approximately three hours per day, five days a week, during twenty-five weeks, the cost for such project would result in 5 182.5 EUR.

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6. Conclusions

The four state-of-the-art hydrogen electrolyser technologies have been evaluated through this study.

Alkaline electrolysis is the most mature, reliable technology of the four. Other remarkable advantages of the technology are its high durability and gas purity. It is easy to implement, and until today it is the most affordable option in terms of levelized cost of hydrogen (4.37 EUR/kg), capital expenditures (450-1300 EUR/kWe) and operational expenditures.

PEM electrolysis can be considered as the upgrade of Alkaline electrolysis. It operates in a similar way to the latter, but has the advantage of reaching higher current densities, thus leading to higher electrical efficiencies. It also has a highly pure and compressed output. The high current density is the most remarkable advantage since it is responsible for the excellent dynamics making it a perfect candidate for green hydrogen as we have seen in the simulation section. Nevertheless, these advantages come to a certain cost: the levelized cost of hydrogen, capital expenditures and operational expenditures will be more expensive. Indeed, the levelized cost of hydrogen will be 5.2 EUR/kg, capital expenditures 1000-1650 EUR/kWe and operational expenditures will be higher due to faster membrane degradation.

SOEC electrolysis is one of the next promises. Its electrical efficiency is even higher than for the PEM, and it also allows significant heat integration unlike other technologies. Nonetheless, it is still at a demonstration stage and has important concerns beginning with its difficulty to manage intermittent power supplies and the large amounts of heat needed. Currently, the levelized cost of hydrogen for this technology is at 9.65 EUR/kg, its capital expenditures 2550-5000 EUR/kWe and operational expenditures can be lower or similar to the one of the PEM.

AEM electrolysis is the other next promise. Although still at a small prototype stage, this technology is expected to become even cheaper than the PEM electrolysis while reaching similar levels of efficiency. Its main advantage is the fact that it uses a non-noble metal catalyst, which makes it cheaper than the SOEC alternative. Other advantages are its compact format, high purity and pressure output as well as its relatively easy scalability.

This study also allowed us to notice a major bottleneck affecting the feasibility of all technologies: electricity prices. High electricity prices are the main cause for the elevated levelized costs of hydrogen, no matter how they were generated.

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Annexes

Annex 1. Matlab code for the Alkaline Electrolysis Cell

```
function [Efficiency,Prod_H2,Vstack,Current_density_cm2,P_consumed,V,Vrev] =
fcn(Current,Temperature,Pressure,Concentration,Gibbs_coefficient,Area,N)

%Input data

T = Temperature; %[ºC]
P = Pressure; %[Bar]
C = Concentration; %[%]

Current_density_cm2=Current/Area; %[A/cm^2]
Current_density = Current_density_cm2*10000; %[A/m^2]

%Model constants (found with non linear regression)

s = 0.338242335018428; %[V]
r1 = 4.45153181441e-5; %[Ohm*m^2]
r2 = 6.88873922e-9; %[Ohm*m^2/ºC]
t1 = -1.53933355588e-2; %[m^2/A]
t2 = 2.00180112171; %[ºC*m^2/A]
t3 = 15.2417849654; %[(ºC^2)*(m^2)/A]
j1 = 4.16338920245e-5; %[Ohm*m^2]
j2 = -1.08260057566e-5; %[Ohm*m^2/M]
j3 = 7.00873474477e-7; %[Ohm*m^2/M^2]
d1 = -3.12995926063e-6; %[Ohm*m^2]
d2 = 4.47137037234e-7; %[Ohm*m^2/bar]

%Faraday's constant in Coulombs/mol

F=96485; %[C/mol]

%Reversible voltage

Vrev = -Gibbs_coefficient/(F*2); %[V]

%Equations of the model (found experimentally)

r = r1+r2*T; %[Ohm*m^2]
t = t1+t2/T+t3/(T^2); %[m^2/A]
d = d1+d2*P; %[Ohm*m^2]
```

```matlab
j = j1+j2*C+j3*C^2; %[Ohm*m^2]

% Total voltage needed for the electrolysis to occur
V = Vrev + (r+j+d)*Current_density+s*log10(t*Current_density+1); %[V]

% Power consumed by the electrolyser
P_consumed = N*V*Current; %[W]

% Production of H2
Prod_H2 = N*(Current/(2*F)); %[A/(C/mol)]=[mol/s]

% Efficiency
Efficiency = 286000/(2*F*V); %[]

% Vstack
Vstack = V*N; %[V]
```

Annex 2. Matlab code for the PEM Electrolysis Cell

```matlab
function [Eficiencia,Produccion_H2,Vstack,Densidad_i,Potencia_Electrica, Uocv,
nact, nohm] = fcn(Corriente,Temperatura,Presion,Coeficiente_Gibbs,Area,N)

%Parámetros de entrada

T = Temperatura+273.15  %Temperatura en K

P = Presión

%Datos electrolizador

Densidad_i=Corriente/Area; %A

%Constante Faraday

F=96485

%constante de gases

R = 8.3145

%voltaje reversible

Vrev = -Coeficiente_Gibbs/(F*2)

%PRESIONES

PH2O = 6.1078e-03*exp(17.2694*((T-273.15)/(T-34.85)))  %atm

PH2 = P-PH2O

PO2 = P-PH2O

%PARAMETROS DEL VOLTAJE DE LA CELDA

ALFAan = 0.7353

ioan = 1.1*10^-7

Espesor_membrana = 0.0178

Conductividad_mebrana = 0.1604

Rmenb = Espesor_membrana/Conductividad_mebrana
```

Uocv = Vrev + (R*T/(2*F))*(log(PH2*PO2^0.5/PH2O)) %para una celda

nact = (R*T/(2*ALFAan*F))* sinh (Densidad_i/2* ioan)

nohm = Rmenb * Densidad_i

V = Uocv + nact + nohm

Potencia_Electrica = N*V*Corriente

Produccion_H2 = N*Corriente/(2*F)

Eficiencia = 286000/(2*F*V)

Vstack = V*N

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Annex 3. Matlab code for the 'Gibs_coefficient' block

```matlab
function Gibbs_coefficient = fcn(Temperature)

if Temperature <= 100
  Gibbs_coefficient = -
0.000181818181818182160*Temperature^2+0.182727*Temperature-
241.654545454546;
else
  Gibbs_coefficient = 4.46428571428546e-
06*Temperature^2+0.0484928571428575*Temperature-230.32;
end
```
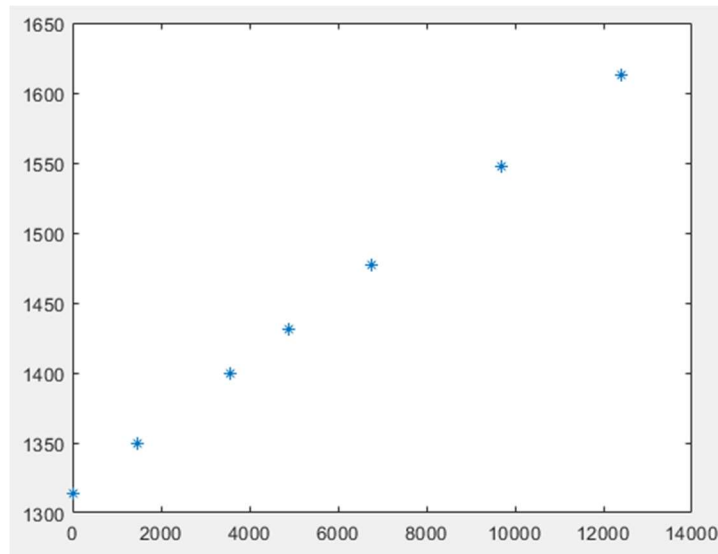
Annex 4. Polarization curve of the Alkaline electrolyser Simulink model (Current vs V$_{stack}$)
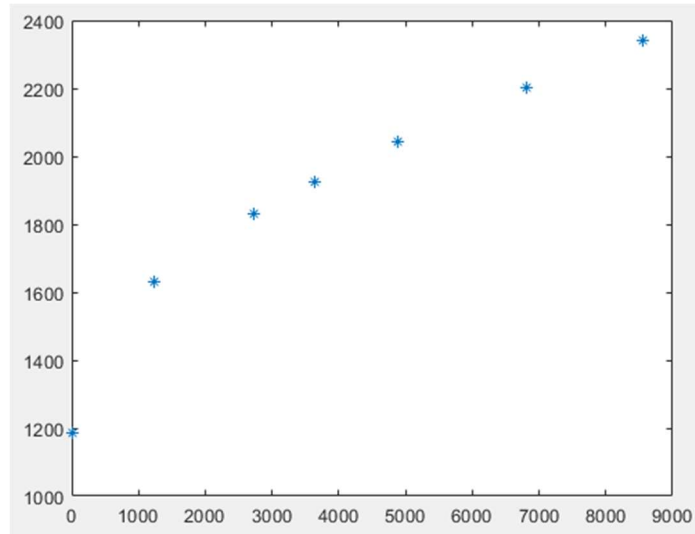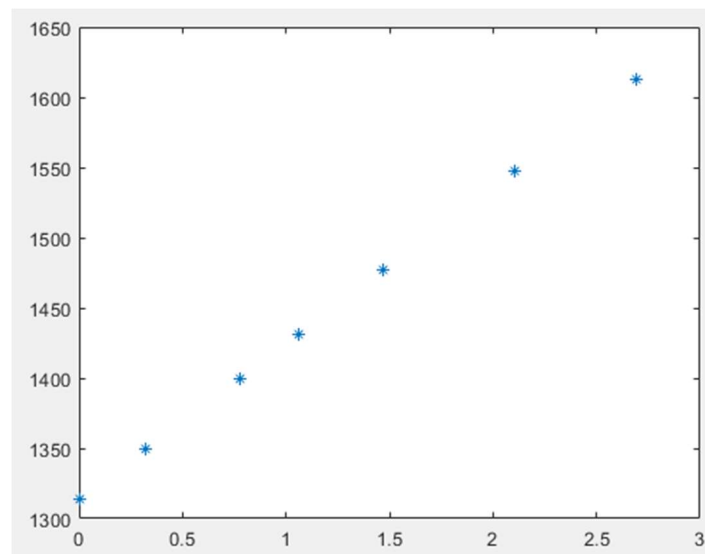

Annex 5. Polarization curve of the Alkaline electrolyser Simulink model (Current density vs V$_{stack}$)

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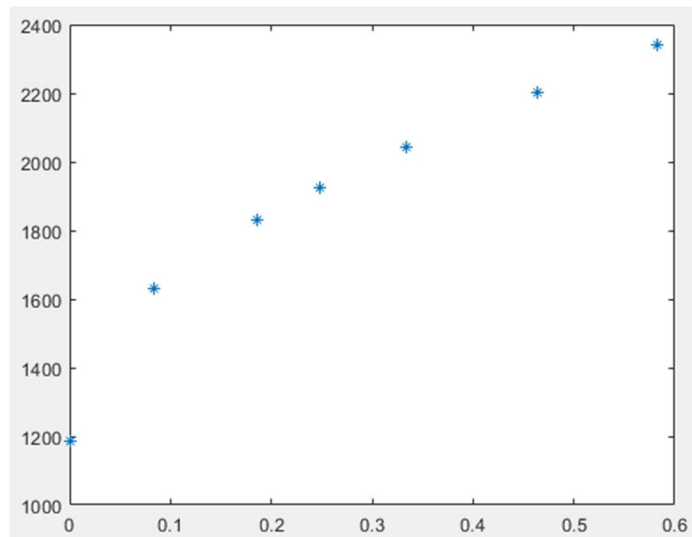
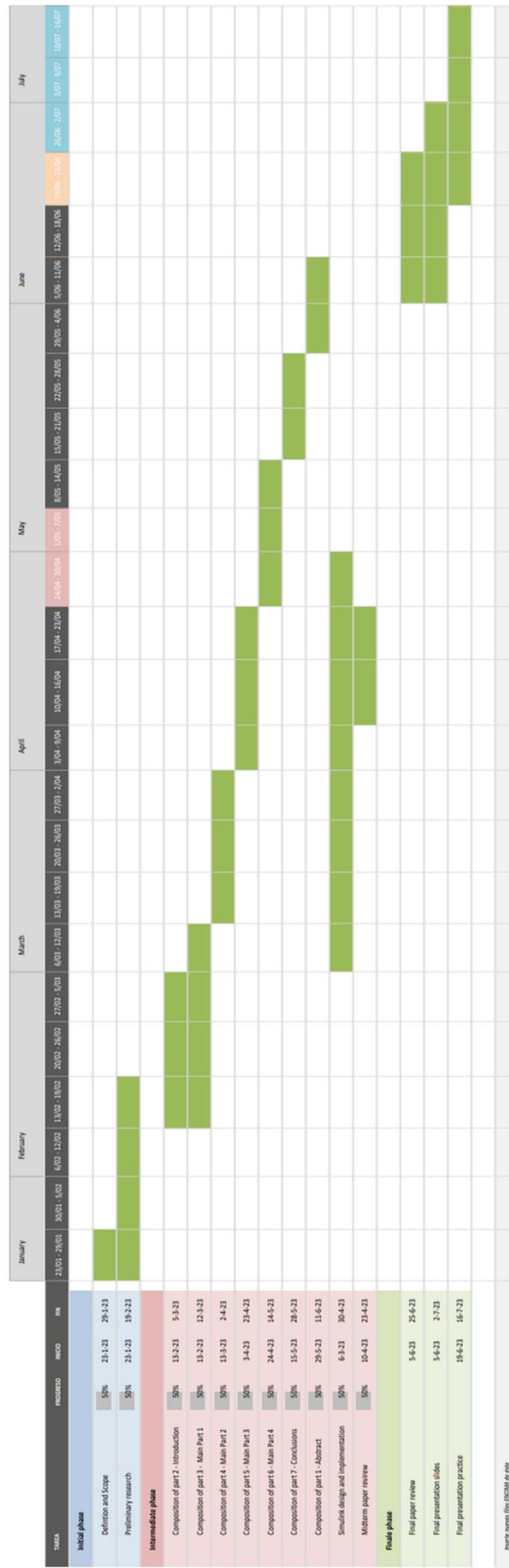**Annex 6.** Polarization curve of the PEM electrolyser Simulink model (Current vs V_{stack})

Annex 7. Polarization curve of the PEM electrolyser Simulink model (Current density vs V_{stack})

Annex 8. Gantt chart of the undergraduate thesis project