MÁSTER EN INGENIERÍA INDUSTRIAL

TRABAJO FIN DE MÁSTER

TECHNO-ECONOMIC ASSESSMENT OF WATER ELECTROLYSIS TECHNOLOGIES FOR THE PRODUCTION OF GREEN HYDROGEN

Autor: Álvaro Esteban Otero

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Madrid

Mayo de 2023

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Fdo.: Álvaro Esteban Otero Fecha: 12/ 05/ 2023

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EL DIRECTOR DEL PROYECTO

Fdo.: Elke Schropp Fecha: 12/ 05/ 2023

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ANÁLISIS TECNO-ECONÓMICO DE TECNOLOGÍAS DE ELECTRÓLISIS DE AGUA PARA LA PRODUCCIÓN DE HIDRÓGENO VERDE

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Entidad colaboradora: Technische Universität München.

RESUMEN DEL PROYECTO

1. Introducción

Esta tesis se centra en el estudio de las tecnologías de electrólisis del agua para la producción de hidrógeno verde. Impulsados por el hecho de que el aumento de las emisiones tiene un impacto negativo en el medio ambiente, gobiernos de todo el mundo se han comprometido a reducir la emisión de contaminantes para controlar el cambio climático [United Nations 2015a]. Entre estos contaminantes destaca el CO_2 como principal gas de efecto invernadero, debido a la profunda dependencia de la economía de los combustibles fósiles. Esta materia prima ha permitido a la sociedad alcanzar niveles de bienestar nunca vistos en la historia; sin embargo, su utilización, que implica la emisión de dióxido de carbono como subproducto, está afectando al medio ambiente al aumentar la temperatura.

Por ello, se ha vuelto primordial diseñar nuevas fuentes de energía más respetuosas con el medio ambiente para hacer frente al desafío climático. La generación de energía solar y eólica se presentan como las principales alternativas a las fuentes de energía tradicionales. Sin embargo, su introducción en la red eléctrica actual supone una amenaza para la estabilidad del sistema [Parra et al. 2019]. Debido a la falta de capacidades reales de almacenamiento de energía, la energía producida en la red debe ser siempre igual a la cantidad de energía que se está consumiendo. Por lo tanto, la intermitencia de los recursos naturales, como el viento y el sol, dificulta la flexibilidad del sistema para responder a fluctuaciones inesperadas tanto de la producción como del consumo. Aquí es donde entra en juego el hidrógeno como forma de almacenamiento de energía [Acar and Dincer 2019].

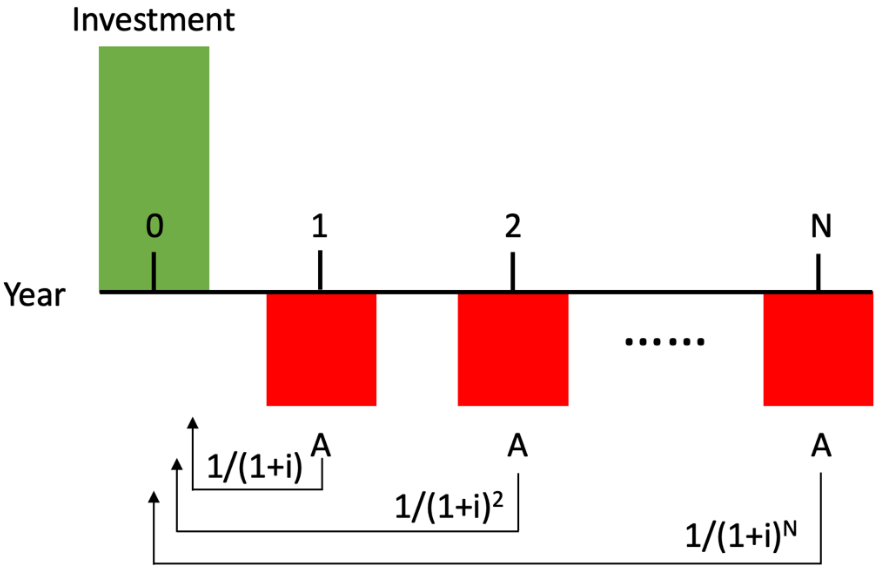
El hidrógeno es ya una materia prima muy extendida en la economía actual, ya que su importancia es capital en muchos procesos industriales [Rasul et al. 2022]. Hoy en día, el hidrógeno se utiliza en las refinerías para el hidrocraqueo. Además, también se emplea en la síntesis de productos químicos, como el amoníaco y el metanol, que tienen una gran relevancia para la sociedad [World Nuclear Association 2021]. Sin embargo, la mayor parte del hidrógeno que se utiliza hoy en día procede del procesamiento de combustibles fósiles [Gür 2021]. Por lo tanto, es necesario idear una nueva forma que sea eficiente y respetuosa con el medio ambiente para sustituir el hidrógeno no renovable actual y ampliar las aplicaciones potenciales de este producto de forma sostenible.

Esto puede lograrse realizando la electrólisis del agua, que la descompone en sus elementos fundamentales: oxígeno e hidrógeno [Ajanovic et al. 2022]. De esta forma, la energía eléctrica se almacena en los enlaces químicos de la molécula de hidrógeno, obteniéndose así un nuevo tipo de hidrógeno sostenible que se denomina hidrógeno verde. Este compuesto puede sustituir al hidrógeno existente y proporcionar a la industria una alternativa sostenible. Además, este tipo de hidrógeno es también la respuesta a los problemas de almacenamiento de energía que afectan a la red eléctrica [Falcone et al. 2021]. El hidrógeno verde obtenido puede procesarse mediante pilas de combustible para producir energía eléctrica.

Este estudio tiene un objetivo doble. En primer lugar, se lleva a cabo una profunda investigación técnica sobre el sector del hidrógeno y las tecnologías de electrólisis. A continuación, se diseña un estudio económico para evaluar la viabilidad económica de los principales tipos de electrólisis. Estas tecnologías son: la electrólisis alcalina (AWE), la electrólisis por membrana de intercambio de protones (PEMWE), la célula de electrólisis de óxido sólido (SOEC) y la electrólisis por membrana de intercambio de aniones (AEMWE). Los resultados de este estudio son relevantes para legisladores e inversores que pretenden dedicar fondos al desarrollo de nuevas plantas de electrólisis para la producción de hidrógeno verde.

2. Metodología

La metodología de la evaluación económica se basa en el cálculo de tres indicadores económicos para el proyecto [Bejan et al. 1996]: el coste nivelado del hidrógeno (LCOH), el valor actual neto (NPV) y la tasa interna de rentabilidad (IRR). Estos parámetros se calculan para las cuatro tecnologías en tres escenarios de funcionamiento diferentes: la planta de electrólisis se alimenta únicamente de energía eólica; la planta se alimenta únicamente de energía solar; y la planta está conectada a la red. También cabe mencionar que se supone que la región de instalación de la planta se encuentra en Alemania. El cálculo de estos indicadores económicos se basa en el descuento de los flujos de caja futuros generados por la central, como se muestra en la siguiente figura:



El LCOH se define como el coste del hidrógeno producido que tiene en cuenta los costes operativos, así como la inversión necesaria con la tasa adicional requerida por los inversores. La ecuación que da como resultado el LCOH es la siguiente

$$LCOH = CAPEX + OPEX = \frac{Investment * f_a}{H_2\ Production} + \frac{C_{x,0} * f_{\Sigma,x} * f_a}{H_2\ Production}$$

Por otro lado, el valor actual neto se define como la diferencia entre los flujos de caja futuros descontados y la inversión necesaria. Estos flujos de caja futuros dependen de los costes incurridos en la producción de hidrógeno y de los ingresos generados por su venta. La ecuación que da como resultado el NPV es la siguiente:

$$NPV = \frac{Income_N - Cost_N}{f_a} = (Price_N - LCOH) * \frac{Production}{f_a}$$

En cuanto a la IRR, se define como el tipo de interés que hace que el NPV sea igual a cero. Es decir, la rentabilidad máxima que pueden pedir los inversores dadas las condiciones en las que se desarrolla el proyecto. Si la IRR resulta cero, significa que el proyecto no generará beneficios bajo ninguna condición de financiación. La IRR se obtiene resolviendo la siguiente ecuación

$$P_0 * Production * f_\Sigma - Costs_0 * f_\Sigma = Investment$$

Estos tres indicadores se calculan tanto para el estado actual de la tecnología como para el estado estimado de la tecnología para 2030. Además, se analiza la estructura de costes de las cuatro técnicas para determinar cuáles son los principales factores que contribuyen al coste de la tecnología. Esto se completa con un análisis de sensibilidad que investiga el impacto potencial de la variación de cualquiera de estos factores en el coste final. Además, el análisis de las estimaciones para el estado de la tecnología en 2030 se amplía con la introducción de simulaciones Monte Carlo, que arrojan luz sobre la variabilidad potencial del rendimiento esperado de cada una de las técnicas.

En definitiva, este estudio pretende ofrecer un análisis exhaustivo del rendimiento económico y su variabilidad potencial de una tecnología aún en desarrollo como la electrólisis del agua para la producción de hidrógeno.

3. Resultados

En primer lugar, se aplicó la metodología al estado actual de la tecnología. En la tabla siguiente se presentan los resultados de los tres parámetros económicos evaluados:

		Power Scenario		
Indicator	**Technology**	**Wind**	**PV**	**Grid**
LCOH (€/kg)	AWE	4,35	6,87	3,29
	PEMWE	5,51	8,93	3,45
	SOEC	11,70	13,66	10,85
	AEMWE	79,93	81,60	74,98
NPV (million €)	AWE	10,693	0,930	6,549
	PEMWE	6,201	-6,997	5,938
	SOEC	-17,720	-25,293	-22,679
	AEMWE	-281,561	-288,004	-270,678
IRR (%)	AWE	21,57	6,04	24,93
	PEMWE	12,14	0,6	21,65
	SOEC	-0,57	-3,49	-3,49
	AEMWE	-16,24	-18,46	-18,88

En este primer caso, los resultados dividen las tecnologías en dos grupos. Por un lado, AWE y PEMWE se revelan como tecnologías que ya podrían ser rentables como alternativas de producción de hidrógeno a gran escala. Por otro, SOEC y AEMWE no tienen aún el nivel de madurez necesario para ser económicamente viables.

		LCOH (€/kg); Variation (%)			
	Variation	**AWE**	**PEMWE**	**SOEC**	**AEMWE**
Utilization factor	+15%	4,17;(-4,1%)	4,97;(-9,8%)	13,99;(+19,6%)	78,12;(-2,3%)
	-15%	4,72;(+8,5%)	5,79;(+5,1%)	13,34;(+14,1%)	82,38;(+3,1%)
Capital cost of the stack	+15%	4,62;(+6,2%)	5,96;(+8,2%)	12,87;(+10%)	91,28;(+14,2%)
	-15%	4,07;(-6,4%)	5,06;(-8,2%)	10,44;(-10,8%)	68,59;(-14,2%)
Energy consumption	+15%	4,65;(+6,9%)	5,81;(+5,4%)	11,89;(+1,6%)	80,27;(+0,4%)
	-15%	4,06;(-6,7%)	5,22;(-5,3%)	11,42;(-2,4%)	79,60;(-0,4%)
Price of energy	+15%	4,65;(+6,9%)	5,81;(+5,4%)	11,89;(+1,6%)	80,27;(+0,4%)
	-15%	4,06;(-6,7%)	5,22;(-5,3%)	11,42;(-2,4%)	79,60;(-0,4%)
OPEX	+15%	4,46;(+2,5%)	5,64;(+2,36%)	11,77;(+0,6%)	80,08;(+0,2%)
	-15%	4,24;(-2,5%)	5,38;(-2,36%)	11,54;(-1,4%)	79,78;(-0,2%)

El análisis de la estructura de costes y el análisis de sensibilidad arrojan luz sobre el factor que más contribuye al coste de la tecnología. Se observa que, para las tecnologías no rentables, el factor que determina el coste es la inversión de capital en la pila. En cambio, para PEMWE y AWE el consumo de energía tiene un peso equivalente al coste de capital sobre el precio final de la tecnología.

Pasando al análisis del estado esperado de la tecnología para 2030, a continuación, se presenta el LCOH obtenido con estos valores futuros:

		Power Scenario		
Indicator	**Technology**	**Wind**	**PV**	**Grid**
LCOH (€/kg)	AWE	4,27 (-1,8%)	6,77 (-1,5%)	2,89 (-12,1%)
	PEMWE	5,08 (-7,8%)	8,33 (-6,7%)	3,13 (-9,3%)
	SOEC	5,26 (-55,1%)	7,08 (-48,2%)	3,39 (-68,8%)
	AEMWE	6,98 (-91,3%)	8,78 (-89,2%)	5,98 (-92,1%)

Como muestra la tabla anterior, las tecnologías que previsiblemente reducirán más sus costes son SOEC y AEMWE. Al beneficiarse de las economías de escala y mejorar el rendimiento de la tecnología, estas dos alternativas podrían ser ya competitivas con las otras dos a finales de esta década. Sin embargo, el riesgo asociado a cada una de estas técnicas no es el mismo, como se muestra en las siguientes figuras obtenidas mediante Simulaciones Monte Carlo:

Las simulaciones de Monte Carlo introducidas a continuación muestran cómo la variabilidad del coste futuro de AEMWE es mayor que la asociada a las otras tres. Esto es un indicador de que 2030 podría ser demasiado pronto para desplegar una planta de producción de hidrógeno a gran escala apoyada en un dispositivo AEMWE. Sin embargo, la reducción de costes conseguida es muy prometedora para una tecnología que aspira a desempeñar un papel importante en el futuro del sector energético.

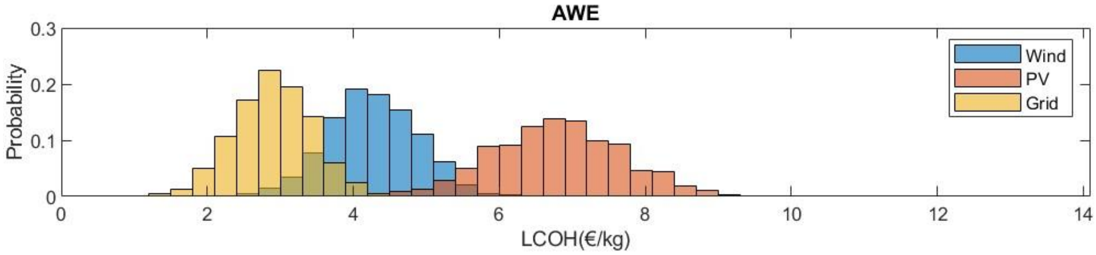


Figure 1. Results of MC simulations for AWE

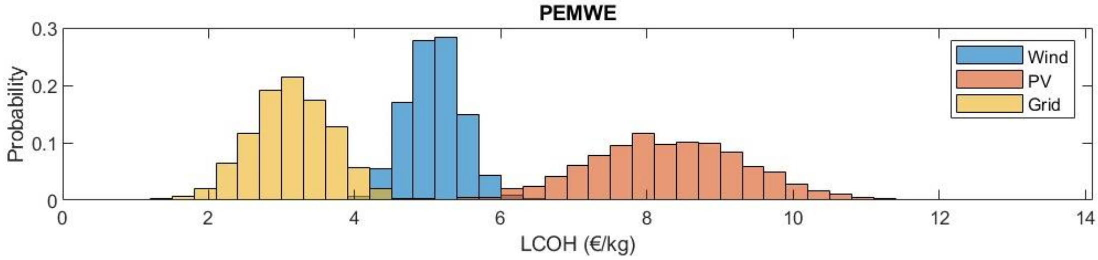


Figure 2. Results of MC simulations for PEMWE

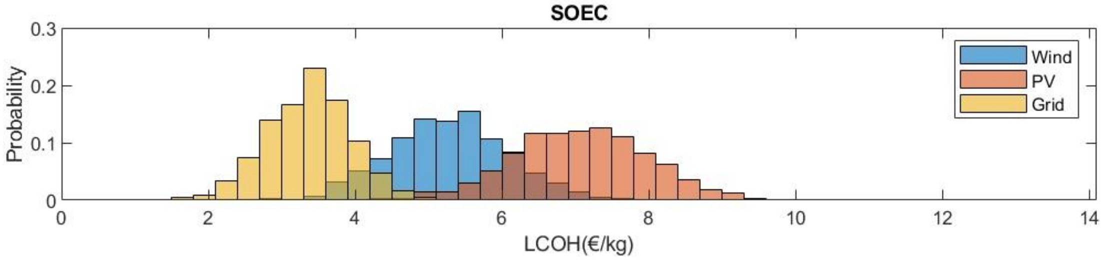


Figure 3. Results of MC simulations for SOEC

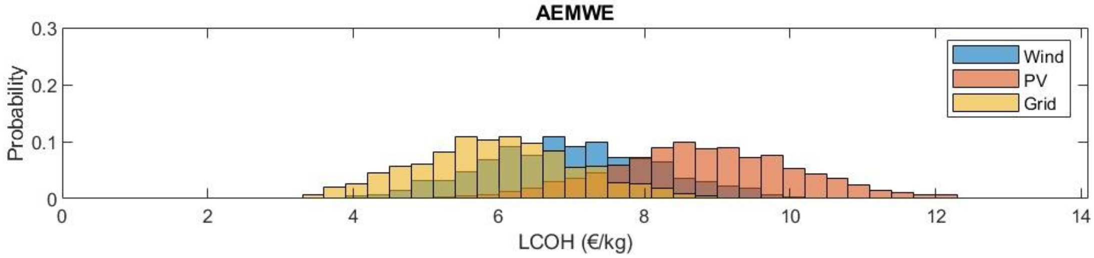


Figure 4. Results of MC simulations for AEMWE

4. Conclusiones

Los resultados obtenidos en este estudio permiten extraer las siguientes conclusiones. En primer lugar, el estado actual de la tecnología sugiere que sólo AWE y PEMWE podrían ser rentables ahora mismo para la construcción de una planta de producción de hidrógeno a gran escala. Sin embargo, para 2030 SOEC y AEMWE podrían alcanzar a las otras dos alternativas en términos de coste.

Como se ha visto en la sección teórica de este estudio, AWE y PEMWE son tecnologías más maduras, lo que se traduce en menores costes de capital. Sin embargo, presentan inconvenientes críticos que dificultan su potencial para reducir aún más sus costes. En el caso de AWE, no es ideal para operar en condiciones de cambio rápido, que son las que se experimentan en la explotación de energías renovables. En el caso de la PEMWE, se basa en metales nobles para sus electrodos, lo que tiene un impacto significativo en el coste global de la tecnología.

Por otro lado, SOEC y AEMWE son tecnologías que aún se encuentran en fases iniciales de desarrollo, lo que se traduce en mayores costes de fabricación debido al bajo nivel de producción. Además, todavía tienen que hacer frente a altas tasas de degradación, lo que implica un elevado ratio de sustitución en comparación con las otras dos. Sin embargo, no necesitan metales nobles y las predicciones sobre su rendimiento los sitúan a la cabeza del mercado del hidrógeno en la próxima década.

En definitiva, este estudio demuestra la viabilidad del hidrógeno verde como alternativa al hidrógeno no renovable actual. La combinación de las distintas tecnologías alimentadas por recursos energéticos complementarios dará lugar a un sector del hidrógeno muy competitivo en costes.

5. Referencias

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TECHNO-ECONOMIC ANALYSIS OF WATER ELECTROLYSIS TECHNOLOGIES FOR THE PRODUCTION OF GREEN HYDROGEN

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Collaborating organization: Technische Universität München.

PROJECT SUMMARY

1. Introduction

This thesis focuses on the study of water electrolysis technologies for the production of green hydrogen. Driven by the fact that increasing emissions have a negative impact on the environment, governments from all around the globe have pledged to reduce the emission of pollutants in order to control climate change[United Nations 2015a]. Amongst these pollutants CO_2 stands out as the main greenhouse gas, due to deep dependence of the economy on fossil fuels. This raw material has enabled society to reach levels of welfare never seen before in history; however, its utilization, which implies the emission of carbon dioxide as by-product, is harnessing the environment by increasing temperature.

Thus, it has become paramount to design new and environmentally friendlier sources of energy to face the climate challenge. Solar and wind power generation present themselves as the main alternatives to traditional energy sources. Nevertheless, its introduction in the current power grid poses a threat to the stability of the system [Parra et al. 2019]. Due to the lack of real energy storage capabilities, the energy produced in the grid must always be equal to the amount of energy that is being consumed. Therefore, the intermittency of natural resources, such as wind and sun, hinders the flexibility of the system to respond to unexpected fluctuations of both production and consumption. This is where hydrogen comes in as a way of energy storage [Acar and Dincer 2019].

Hydrogen is already a well extended commodity in the current economy since its importance is paramount in many industrial processes [Rasul et al. 2022]. Today, hydrogen is used in refineries for hydrocracking. Moreover, it is also employed in the

synthesis of chemical products, such as ammonia and methanol, which have a significant relevance to society [World Nuclear Association 2021]. However, most of the hydrogen that is being used today comes from the processing of fossil fuels [Gür 2021]. Therefore, it is necessary to devise a new way that is both efficient and environmentally friendly so as to replace the current non-renewable hydrogen and to expand the potential applications of this commodity in a sustainable way.

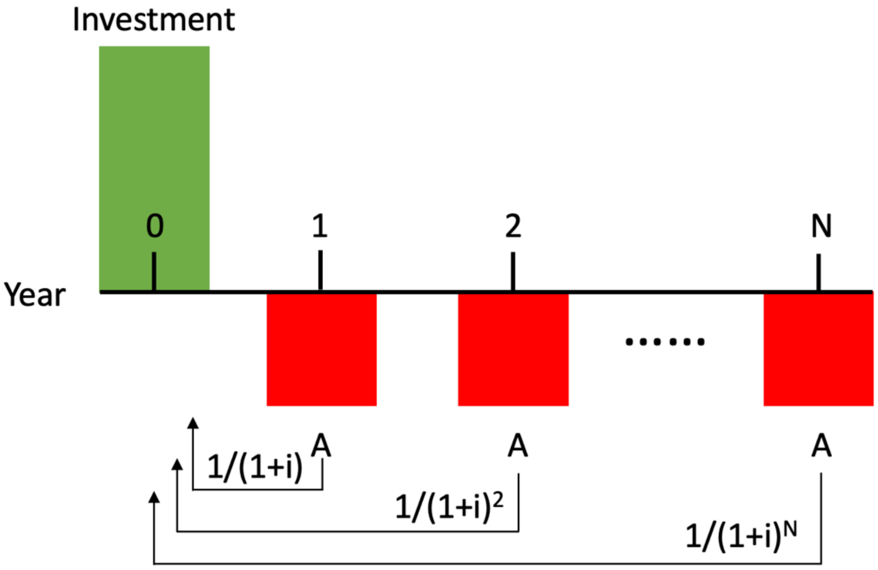
This can be achieved by performing electrolysis on water, which decomposes it into its fundamental elements: oxygen and hydrogen [Ajanovic et al. 2022]. This way, the electrical energy is stored in the chemical bonds of the hydrogen molecule, thus, obtaining a new type of sustainable hydrogen which is addressed as green hydrogen. This compound can replace the existing hydrogen and provide the industry with a sustainable alternative. Moreover, this type of hydrogen is also the answer to the energy storing problems that affect the electrical grid [Falcone et al. 2021]. The obtained green hydrogen can then be processed by means of fuel cells to produce electrical energy.

The objective of this study is twofold. First, deep technical research on the hydrogen sector and the electrolysis technologies is carried out. Then, an economic assessment is design to evaluate the economic feasibility of the main electrolysis types. These technologies are: alkaline water electrolysis (AWE), proton exchange membrane water electrolysis (PEMWE), solid oxide electrolysis cell (SOEC) and anion exchange membrane water electrolysis (AEMWE). The results of this study are relevant to policy makers and investors that aim to direct funds to the development of new electrolysis plants to produce green hydrogen.

2. Methodology

The methodology of the economic assessment is underpinned by the calculation of three economic indicators for the project [Bejan et al. 1996]: the levelized cost of hydrogen, the net present value, and the internal rate of return. These parameters are calculated for the four technologies under three different operating scenarios: the electrolysis plant is power solely by wind energy; the plant is powered solely by solar energy; and the plant is connected to the grid. It is also worth mentioning that the installation region of the plant is assumed to be in Germany.

The calculation of the economic indicators is based on the discounting of the future cashflows generated by the plant as shown in the following figure:



The LCOH is defined as the cost of the produced hydrogen that considers the operational costs as well as the required investment with the additional rate required by the investors. The equation that yields the LCOH is the following:

$$LCOH = CAPEX + OPEX = \frac{Investment * f_a}{H_2\ Production} + \frac{C_{x,0} * f_{\Sigma,x} * f_a}{H_2\ Production}$$

On the other hand, the net present value is defined as the difference between the discounted future cashflows and the required investment. These future cashflows depend on the costs incurred in the production of hydrogen and the income generated by its selling. The equation that yields the NPV is the following:

$$NPV = \frac{Income_N - Cost_N}{f_a} = (Price_N - LCOH) * \frac{Production}{f_a}$$

With regards to the IRR, it is defined as the interest rate that makes the NPV equal to zero. This is, the maximum profitability that can be asked by the investors given the conditions under which the project is develop. If the IRR results in zero, this means the project will not generate profits under any financing conditions. IRR is obtained by solving the following equation:

$$P_0 * Production * f_\Sigma - Costs_0 * f_\Sigma = Investment$$

These three indicators are calculated for both the current state of the technology and the estimated state of the technology by 2030. Moreover, the cost structure of the four techniques is analyzed to determine which are the main contributing factors to the cost of the technology. This is completed by a sensitivity analysis that investigates the potential impact of the variation of any of these factors in the final cost. Furthermore, the analysis of estimations for the 2030 state of the technology is broadened by the introduction of Monte Carlo simulations, which shed light on the potential variability of the expected performance of each of the techniques.

All in all, this study aims to provide a full comprehensive analysis of the economic performance and its potential variability of a still developing technology like water electrolysis for the production of hydrogen.

3. Results

First, the methodology was applied to the current state of the technology. The results for the three assessed economic parameters are presented in the following table:

		Power Scenario		
Indicator	**Technology**	**Wind**	**PV**	**Grid**
LCOH (€/kg)	AWE	4,35	6,87	3,29
	PEMWE	5,51	8,93	3,45
	SOEC	11,70	13,66	10,85
	AEMWE	79,93	81,60	74,98
NPV (million €)	AWE	10,693	0,930	6,549
	PEMWE	6,201	-6,997	5,938
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	PEMWE	12,14	0,6	21,65
	SOEC	-0,57	-3,49	-3,49
	AEMWE	-16,24	-18,46	-18,88

For this first case, the results divide the technologies into two groups. First, AWE and PEMWE reveal themselves to be technologies that could already be profitable as large-scale hydrogen production alternatives. On the other, SOEC and AEMWE do not still have the maturity level required to be economically feasible.

		LCOH (€/kg); Variation (%)			
	Variation	**AWE**	**PEMWE**	**SOEC**	**AEMWE**
Utilization factor	+15%	4,17;(-4,1%)	4,97;(-9,8%)	13,99;(+19,6%)	78,12;(-2,3%)
	-15%	4,72;(+8,5%)	5,79;(+5,1%)	13,34;(+14,1%)	82,38;(+3,1%)
Capital cost of the stack	+15%	4,62;(+6,2%)	5,96;(+8,2%)	12,87;(+10%)	91,28;(+14,2%)
	-15%	4,07;(-6,4%)	5,06;(-8,2%)	10,44;(-10,8%)	68,59;(-14,2%)
Energy consumption	+15%	4,65;(+6,9%)	5,81;(+5,4%)	11,89;(+1,6%)	80,27;(+0,4%)
	-15%	4,06;(-6,7%)	5,22;(-5,3%)	11,42;(-2,4%)	79,60;(-0,4%)
Price of energy	+15%	4,65;(+6,9%)	5,81;(+5,4%)	11,89;(+1,6%)	80,27;(+0,4%)
	-15%	4,06;(-6,7%)	5,22;(-5,3%)	11,42;(-2,4%)	79,60;(-0,4%)
OPEX	+15%	4,46;(+2,5%)	5,64;(+2,36%)	11,77;(+0,6%)	80,08;(+0,2%)
	-15%	4,24;(-2,5%)	5,38;(-2,36%)	11,54;(-1,4%)	79,78;(-0,2%)

The analysis of the cost structure and the sensitivity analysis shed light on the factor that contribute the most to the cost of the technology. It can be observed that for the non-profitable technologies, the factor that determines the cost is the capital investment on the stack. On the other hand, for PEMWE and AWE the energy consumption has an equivalent weight compared to the capital cost on the final price of the technology.

Moving on to the analysis of the expected state of the technology by 2030, the LCOH obtained with these future values is presented below:

		Power Scenario		
Indicator	**Technology**	**Wind**	**PV**	**Grid**
LCOH (€/kg)	AWE	4,27 (-1,8%)	6,77 (-1,5%)	2,89 (-12,1%)
	PEMWE	5,08 (-7,8%)	8,33 (-6,7%)	3,13 (-9,3%)
	SOEC	5,26 (-55,1%)	7,08 (-48,2%)	3,39 (-68,8%)
	AEMWE	6,98 (-91,3%)	8,78 (-89,2%)	5,98 (-92,1%)

As shown in the above presented table, the technologies that are expected to reduce their costs the most are SOEC and AEMWE. By benefiting from economies of scale and by improving the performance of the technology, these two alternatives could already be competitive with the other two by the end of this decade. However, the risk associated with each of these techniques is not same as shown in the following figures obtained by means of Monte Carlo Simulations:

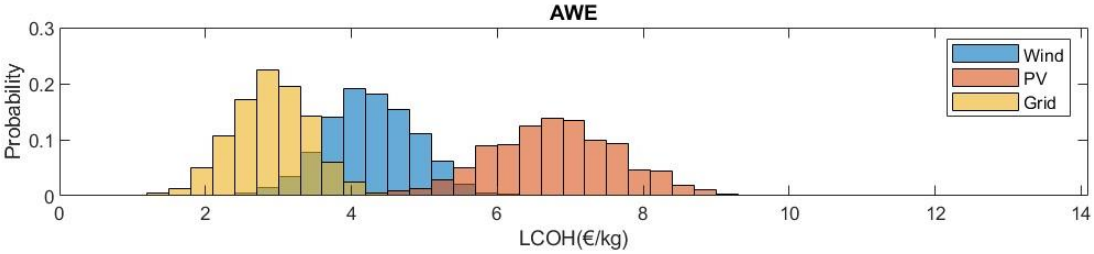

Figure 5. Results of MC simulations for AWE

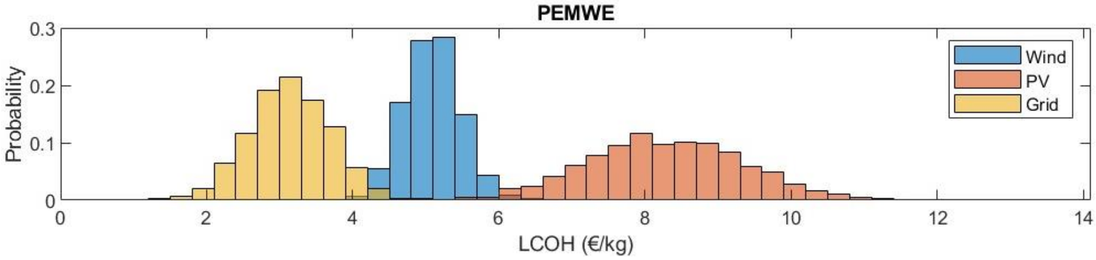

Figure 6. Results of MC simulations for PEMWE

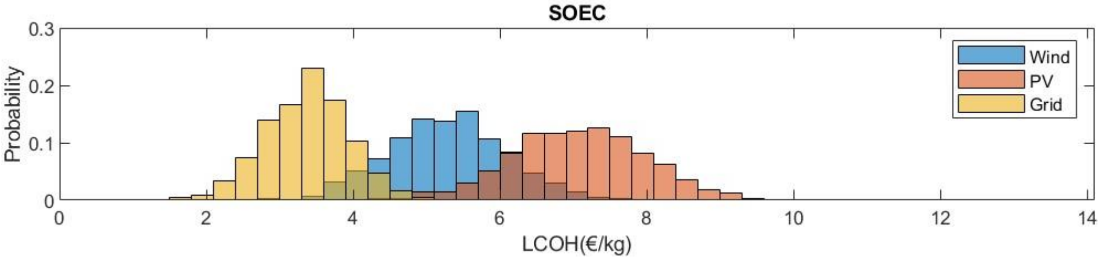

Figure 7. Results of MC simulations for SOEC

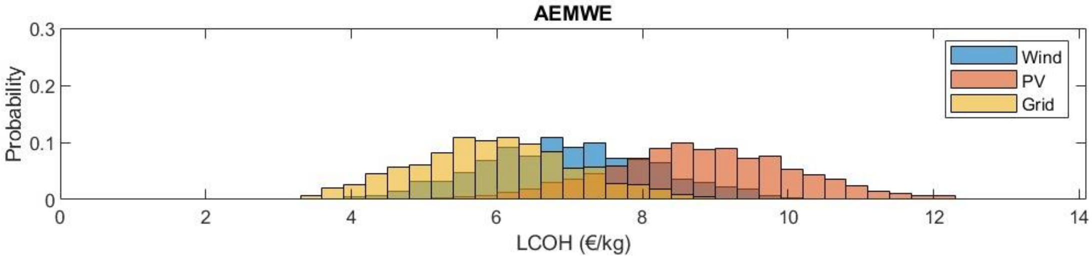

Figure 8. Results of MC simulations for AEMWE

Monte Carlo simulations show how the variability of the future cost of AEMWE is higher than that associated with the other three. This is an indicator that 2030 might be too soon to deploy a large-scale hydrogen production plant supported by a AEMWE device. However, the achieved cost reduction is very promising for a technology that aims to play a significant role in the future of the energy sector.

4. Conclusions

The results obtained in this study allow for the drawing of the following conclusions. First, the current state of the technology suggests that only AWE and PEMWE could right now be profitable for the construction of a large-scale hydrogen production plant. However, by 2030 SOEC and AEMWE might catch up with the other two alternatives in terms of cost.

As seen in the theoretical section of this study, AWE and PEMWE are more mature technologies, which translates into lower capital costs. However, they present critical drawbacks that hinder their potential to further reduce their costs. In the case of AWE, it is not ideal to operate under fast-changing conditions, which are the ones experienced under renewable energy operation. In the case of PEMWE relies on noble group metals for its electrodes, which has a significant impact on the overall cost of the technology.

On the other hand, SOEC and AEMWE are technologies that are still under initial stages of development, which translates into higher manufacturing costs due to low level of production. Moreover, they still struggle with high degradation rates, which imply a high substituting ratio compared to the other two. However, they do not need of noble group metals and the predictions on their performance place them in the position of leading the hydrogen market in the next decade.

All in all, this study shows the viability of green hydrogen as an alternative to the current non-renewable hydrogen. The combination of the different technologies powered by complementary power resources will yield a very cost competitive hydrogen sector.

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Abbreviations

η. *Overpotential*
α_a. *Anode charge transfer coefficient*
α_c. *Cathode charge transfer coefficient*
°C. *Degree Celsius*
ΔG_H. *Free Gibbs energy*
µm. *micrometer*
A. *Ampere*
AEMWE. *Anion exchange membrane water electrolysis*
atm. *Atmospheric pressure*
AWE. *Alkaline water electrolysis*
BOP. *Balance of plant*
CAPEX. *Capital expenditures*
CCUS. *Carbon capture use and storage*
C_E. *Cost of energy*
CH_4. *Methane*
C_L. *Cost of labour*
Co. *Cobalt*
CO_2. *Carbon dioxide*
CO_2eq. *Carbon dioxide equivalent*
C_W. *Cost of water*
DC. *Direct Costs*
F. *Faraday constant*
f_a. *Distribution factor*
g. *gram*
GDC. *Gadolinia-doped ceria*
H. *Atomic hydrogen*
H_2. *Molecular hydrogen*
H_2O. *Water*
HER. *Hydrogen evolution reaction*
i. *Interest rate*

IC. *Indirect costs*

IEM. *Ion exchange membrane*

IRR. *Internal rate of return*

J. *Joule*

j_0. *Intrinsic exchange current density*

K. *Kelvin*

kg. *Kilogram*

KOH. *Potassium hydroxide*

kW. *Kilowatt*

kWhAC. *Kilowatt hour in alternate current*

LCA. *Life cycle assessment*

LCOH. *Levelized cost of hydrogen*

LSC. *Lanthanum-strontium-cobaltite*

LSCF. *Lanthanum strontium ferrite cobaltite*

LSM. *Lanthanum strontium manganite*

m. *meter*

MEA. *Membrane electrode assembly*

MJ. *Megajoule*

Mo. *Molybdenum*

Mt. *Megaton*

N. *Nitrogen*

NaOH. *Sodium hydroxide*

Ni. *Nickel*

N_L. *Number of operators*

NO_X. *Nitrogen oxide*

NPV. *Net present value*

OER. *Oxygen evolution reaction*

OFC. *Offsite costs*

OH. *Hydroxide*

ONC. *Onsite costs*

OPEX. *Operational expenditures*

p. *Pressure*

PCET. *Proton coupled electron transfer*
PEMWE. *Proton exchange membrane water electrolysis*
PGM. *Platinum group metals*
Pt. *Platinum*
PTL. *Porous transport layer*
Q_r. *Reaction quotient*
R. *Gas universal constant*
R&D. *Research and Development*
RFNBO. *Renewable fuels of non-biological origin*
Ru. *Ruthenium*
r_x. *Nominal rate*
S. *Sulfur*
SDG. *Sustainable development goal*
SOEC. *Solid oxide electrolysis cell*
SOFC. *Solid oxide fuel cell*
T. *Temperature*
Ti. *Titanium*
TW. *Terawatt*
V. *Volts*
WACC. *Weighted average cost of capital*
Y_2O_3. *Yttria*
YSZ. *Yttrium stabilized zirconia*
ZrO_2. *Zirconia*

1. Introduction

The topic of this master’s thesis is the production of green hydrogen by means of water electrolysis. This first chapter of the study aims to provide an overview of the research that serves as a starting point for the thesis. Therefore, Chapter 1 of this master thesis is divided into three parts: motivation, objectives, and structure. The motivation provides the rationale for the study, highlighting the urgency to reduce greenhouse gas emissions and the potential of hydrogen to contribute to sustainable development. The objectives outline the technical and economic goals of the study, including the technical research on electrolysis technologies and the economic analysis of the four main types of electrolysis. Finally, the structure provides an overview of how the study is organized, highlighting the key chapters and sections. The structure of the introduction section ensures a clear understanding of the purpose, scope, and organization of the master thesis.

1.1.Motivation

The motivation of this study is driven by the urgent need to reduce greenhouse gas emissions and mitigate the impacts of climate change. Governments worldwide have made ambitious pledges to reduce their emissions to net-zero by 2050 or earlier, as part of the Paris Agreement. The transportation and industrial sectors are significant contributors to global emissions, and decarbonizing these sectors is crucial to achieving the Paris Agreement goals [United Nations 2015a].

Hydrogen, particularly green hydrogen produced by electrolysis powered by renewable energy, has emerged as a promising solution for decarbonizing the transportation and industrial sectors. Hydrogen can be used as a fuel for vehicles, power generation, and industrial processes, replacing fossil fuels and reducing emissions. The United Nations has also recognized the potential of hydrogen to contribute to sustainable development, as outlined in the Sustainable Development Goals (SDGs).

The production and use of green hydrogen align with several SDGs, including SDG 7 (Affordable and Clean Energy), SDG 9 (Industry, Innovation, and Infrastructure), and SDG 13 (Climate Action) [United Nations 2015b]. Green hydrogen can provide affordable and clean energy to remote areas and support the development of sustainable infrastructure. Hydrogen can also support the transition to a circular economy by enabling the use of renewable energy to produce green hydrogen, which can be stored and transported to areas with high energy demand.

However, a major challenge in the widespread adoption of renewable energy is the intermittency of these resources. Solar and wind power are highly dependent on weather conditions and are not always available when needed. This intermittency can result in imbalances in the electricity grid and challenges in meeting energy demand during peak periods. Hydrogen can help solve this issue by storing energy during times of excess supply and releasing it when demand exceeds supply [Parra et al. 2019]. Hydrogen storage can provide a flexible solution for balancing the electricity grid, reducing the need for fossil fuel-based backup generation, and supporting the integration of renewable energy into the grid.

In conclusion, this study is motivated by the urgent need to reduce greenhouse gas emissions and mitigate the impacts of climate change. The production and use of green hydrogen can contribute to achieving the Paris Agreement goals and the Sustainable Development Goals. Hydrogen offers a flexible solution for storing and releasing renewable energy, addressing the intermittency issue associated with these resources. The findings of this study will be useful for policymakers, industry stakeholders, and investors who are interested in the potential of hydrogen to contribute to sustainable development and decarbonization of the transportation and industrial sectors.

1.2. Objectives

The primary objectives of this study are to conduct a technical research on the electrolysis technology and to perform an economic analysis of the four main types of electrolysis methods. The technical research involves an investigation into the underlying principles of electrolysis and the different types of electrolysis technologies that are available. It also involves an analysis of the operating parameters that affect the performance of the electrolysis systems, such as current density, temperature, and pressure. The technical research explores the challenges associated with the different types of electrolysis technologies, such as electrode degradation and gas crossover. The research identifies the technical barriers that need to be overcome to increase the efficiency and reliability of electrolysis systems.

The economic analysis of this study evaluates the capital and operating costs of each technology, including the costs of the electrolysis stack, and balance of plant equipment. It estimates the levelized cost of hydrogen for each technology and the net present value of the project. It identifies the main drivers of cost reduction for each technology, such as economies of scale, technological improvements, and renewable energy cost reductions.

In conclusion, this thesis has two primary objectives: to conduct technical research on electrolysis technologies and to perform an economic analysis of the four main types of electrolysis technologies. The technical research provides a deeper understanding of the underlying principles and technical challenges of electrolysis technology, while the economic analysis provides insights into the cost performance of the technology and its variability depending on the assessed scenario.

1.3.Thesis Structure

This thesis is divided into five main chapters. The present Chapter 1 introduces the background and motivation of the study. This chapter also serves as an introduction to the importance of hydrogen as an energy carrier and its potential to contribute to the transition towards a more sustainable energy system.

Chapter 2 focuses on the economic impact of hydrogen as a commodity in today’s society. First, a classification of the different types of hydrogen depending on their production technique is described. Then, hydrogen main current applications are presented to provide evidence of the present impact of this compound in the industrial sector. Last, the concept of hydrogen economy is introduced, which serves as basepoint to discuss the potential applications of hydrogen in the future and how these could reshape the economic paradigm.

Moving on to Chapter 3, it reviews the literature on electrolysis technologies for the production of green hydrogen. First, the chapter discusses the fundamentals of the electrochemical decomposition of water. Then, various types of electrolysis technologies are introduced, together with their advantages and disadvantages, and their potential for commercialization. The chapter also reviews the current status of the technology in terms of cost and efficiency.

Chapter 4 is dedicated to the economic analysis of the assessed electrolysis technologies. The chapter describes first the model employed for the economic valuation of the techniques. The elements involved in the analysis are the input variables and the economic indicators estimated for each of the technologies. Second, the results provided by the model are analyzed by means of a comparison of these economic indicators. These are analyzed under different scenarios and operating conditions to further broaden the dimension of the analysis. Thus, this section provides insight on the factors contributing to the cost and efficiency of the technology and that affect its commercial viability.

Last, Chapter 6 concludes the study by summarizing the main findings and providing recommendations for future research. The chapter also discusses the implications of this research for policymakers, industry stakeholders, and investors.

In summary, this thesis aims to provide a comprehensive analysis of electrolysis technologies for the production of green hydrogen. The study evaluates the commercial viability of the technology and identify the key parameters that affect the cost and efficiency of the technology. Thus, the study aims to contribute to the efforts directed to the development and rollout of a sustainable energy system.

2. Hydrogen Economy

Hydrogen is an important commodity in today's economy, and it is predicted to increase its importance in the following decades. The need for developing new forms of energy is driving a growing research interest in this technology among the scientific community [Yue et al. 2021]. The idea of storing electrical energy as chemical energy by means of renewable sources has inspired many who believe hydrogen could play a main role in the path towards sustainability. However, it is important to fully understand the principles behind this technology in order to navigate the transition from the current polluting hydrogen sector to the projected sustainable energy vector. By comprehending today's paradigm, light could be shed on the development and integration of this technology in the energy mix.

Therefore, this chapter is dedicated first to analyze the current state of the hydrogen sector, its relevance in today's economy and the potential it has to become a key driver in the future. Then, Chapter 3 focuses on discussing the technology on which the transition towards a sustainable hydrogen production is based: water electrolysis. Working principles, employed materials, areas of improvement and current performances are studied for four different electrolysis techniques, accomplishing a solid theoretical basis that underpins the later economic assessment.

2.1. Types of Hydrogen

Hydrogen is a well extended commodity in the industrial sector. Similar to many other areas of the economic activity, its production configuration is being reassessed with the objective of finding fully sustainable ways of obtaining the desired product. In the case of hydrogen this transformation process of its production paradigm is represented by the transition from grey hydrogen, going through blue hydrogen, towards green hydrogen [Ajanovic et al. 2022]. This section is dedicated to developing a complete understanding of the different types of hydrogen, comparing its production fundamentals, and picturing the potential transition from a CO_2-emitting synthesis to a sustainable hydrogen production.

The most extended type of hydrogen nowadays is grey hydrogen [Gür 2021]. This method consists of obtaining hydrogen using fossil fuels as raw material. Through steam reforming of natural gas or coal gasification, hydrogen is produced emitting CO_2 as by-product. Both techniques are very well established in today´s industry showing very solid ranges of efficiency (60-85%) and being the most cost-competitive method to produce hydrogen [Ajanovic et al. 2022]. Nevertheless, its high carbon intensity turns them into unviable processes in the long term, attending to the sustainable objectives set by policy makers and governments all around the globe. These will hinder the performance of grey hydrogen in terms of costs and improve the competitiveness of alternative, more environmentally sustainable methods.

A step forward from grey hydrogen towards sustainability is represented by blue hydrogen. This type of hydrogen is the result of a mild variation in the production process of grey hydrogen. Carbon capture use and storage (CCUS) units are put in place in order to balance the CO_2 emitted during the steam methane reforming. However, many are skeptical about the true benefits obtained by this enhancement of the process. The installation of CCUS units increases the total cost of the plant and reduces the efficiency up to 5-14% [Gür 2021]. Moreover, potential methane leaks also pose a substantial threat to the environmental improvements provided by the carbon capture units. Methane is a strong greenhouse-gas, and its use has dramatically increased during the last decades. Thus, many studies have been developed in order to determine the potential harm its leaks could inflict on the environmental performance of the energy system. Furthermore, there is not yet a clear production chain that gives CO_2 true importance as a potential usable commodity, making captured CO_2 a burden with no useful application. Underground carbon storage systems are put in place to accumulate the useless CO_2, further increasing the capital cost of the plant, and hindering the overall benefits of the technology. This is the reason why many see blue hydrogen as a transition method, not as a sustainable alternative, to shift from grey hydrogen to truly sustainable ways of production [Carlson 2020].

The ultimate sustainable method for hydrogen production is green hydrogen. However, other alternatives are being developed in order to serve as a transition to such a complex technology. Among these alternatives lies pink hydrogen, which uses nuclear energy to perform water electrolysis and produce hydrogen [Dawood et al. 2020]. This might not be a suitable alternative for many western countries, except for France, who have decided to forsake nuclear. Nevertheless, it can be a viable method for other countries like China and Russia, which could substitute their current coal-based production system with a nuclear based system, significantly reducing their CO_2 emissions.

Turquoise hydrogen is a new technique based in methane pyrolysis, which generates carbon as by-product but in a solid phase [Ajanovic et al. 2022]. Thus, the CO_2 is not emitted to the atmosphere, but rather formed into filamentous carbon or carbon nanotubes which present great value for many industrial sectors and can be further fed into other production processes. However, this process has not yet been commercialized and is still in on-going research phases.

Another interesting method that is being developed is aqua hydrogen. This new technique was invented by the University of Calgary and tested in collaboration with Proton Technologies in Canada [Yu et al. 2021a]. They use as base for the production depleted oil sands and oil fields, emitting no CO_2 through the process. This process consists of injecting oxygen to the underground oil reservoirs, where oxidation takes place at a temperature of 350°C. Oil and water split generating carbon oxides and hydrogen. These oxides are kept underground while the obtained hydrogen is pumped back up to the surface. This technique is midway between green and blue hydrogen, since it uses fossil fuels as raw material but still no CO_2 is emitted to the atmosphere. Moreover, advocates of this technology argue this technique could be cost-competitive compared to grey hydrogen [Yu et al. 2021a]. This cost effectiveness is driven by the fact that the oil used would be otherwise useless for its normal industrial extraction. Nevertheless, there are still concerns to be resolved in relation to the actual environmental performance of this method. The authors recognize that an LCA is needed in order to determine the potential harms of this technique, namely the effects of increasing underground temperatures in nearby ecosystems and the potential CO_2 leakages from the ground. They also mention difficulties regarding the scalation of production and public resistance against this technology, which might favor green hydrogen [Yu et al. 2021a].

The aforementioned types of hydrogen constitute intermediate steps in the path towards the ultimate goal of this sector: the development of green hydrogen. Green hydrogen is a fully sustainable way of producing hydrogen since no hydrocarbons participate in the process. It consists of performing electrolysis on water, using renewable energy sources as the driver of this chemical process, such as solar and wind energy [Ajanovic et al. 2022]. By applying an electrical current on water, the oxygen and hydrogen atoms that build up the water molecules are separated, thus, obtaining highly pure hydrogen, and only producing oxygen as by-product. This is a great advantage compared to other techniques of hydrogen production that require further steps in order to separate hydrogen from other compounds involved in the process. This method of producing hydrogen is also cherished by the scientific community because it can help solve the main challenge the energy system has in its pursuit of sustainability: large scale energy storage [Falcone et al. 2021].

The current electrical grid has no real capacity for storing energy since the size of batteries is simply not big enough. Therefore, the system is forced to constantly match the produced and consumed power. This is where the intermittency of renewable sources, such as solar and wind, becomes an issue. Its availability cannot be controlled, and it can happen that the resources are available when there is no use for them, thus hindering their potential for enhancing the environmental performance. Hydrogen gives the system an alternative to store this unwanted and untimely excess of renewable energy: this electrical energy is transformed into chemical energy stored in the hydrogen bonds. These are the reasons why green hydrogen is for many such a promising solution for the current energy mix [Acar and Dincer 2019]. Within the water electrolysis technique there are many variations that differ from each other mainly in components and materials; these are thoroughly analyzed in the chapter specifically dedicated to water electrolysis.

Beyond water-electrolysis-obtained hydrogen, there are other types of hydrogen that can be included in the green category. This is the case of for example hydrogen obtained via biogas steam reforming. Through a similar process of that of grey and blue hydrogen, this technique varies in the employed raw material. The fact that it uses biogas instead of fossil fuels as base for the process transforms this method into a carbon neutral technology [Ajanovic et al. 2022]. However, the energy content of biogas relative to its mass is low, and the overall efficiency of the system is not as high. Moreover, this type of hydrogen lacks the main advantage offered by electrolysis-produced hydrogen, namely its ability to store electrical energy. Another technique for obtaining hydrogen in a carbon neutral way is photohydrogen. This method uses bacteria or algae that, by means of natural or artificial light, split water into hydrogen and oxygen [Dawood et al. 2020]. However, it lies currently in the very first stages of development and at a very small scale.

New different ways of producing hydrogen keep appearing. Several studies propose various classification systems and try to keep up with the new developments. In this study, the assessed types of hydrogen are gathered in the following Figure 9:

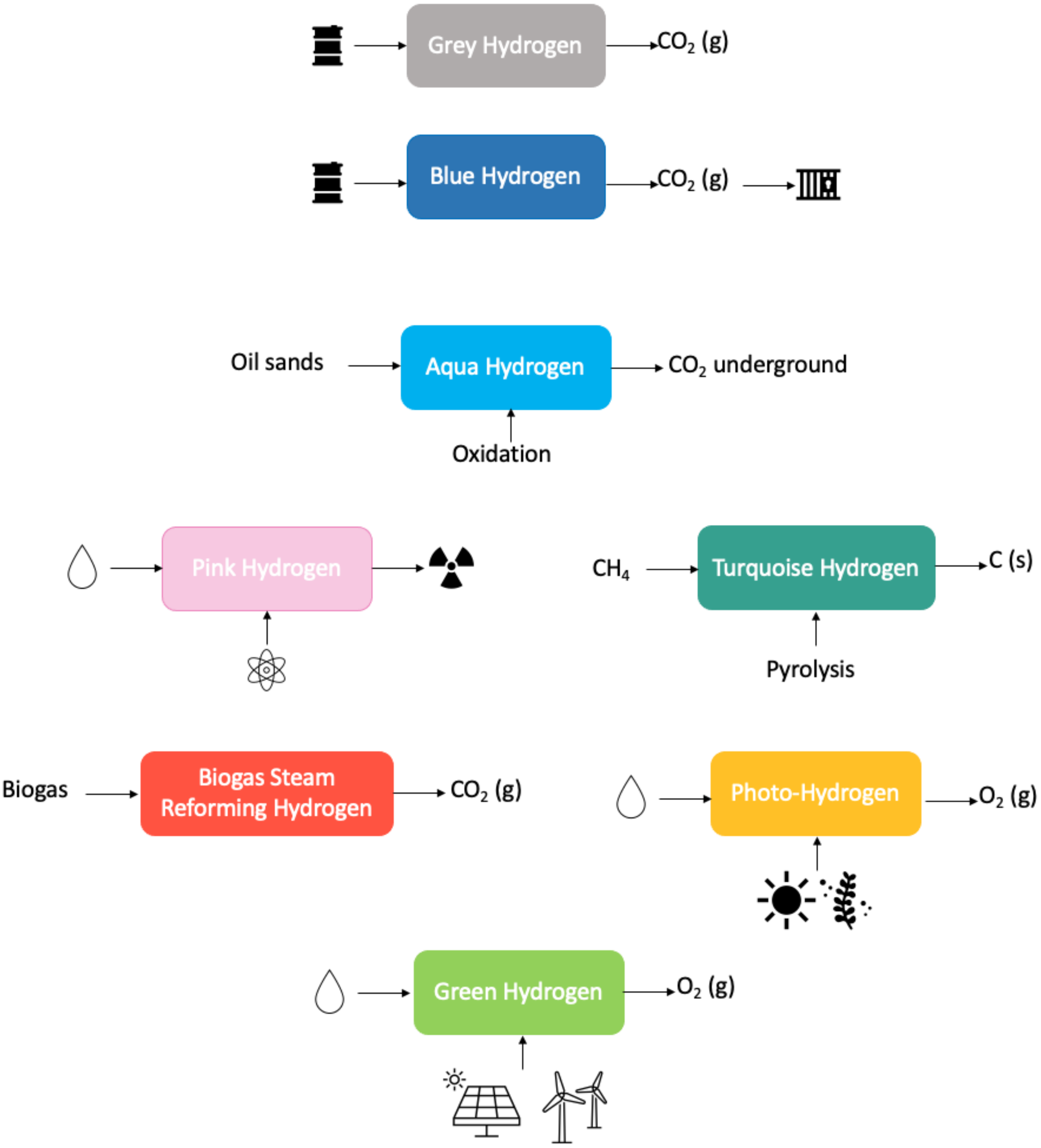

Figure 9. Color-based classification of hydrogen production techniques

2.2.Importance in Current Economy and Main Applications

Hydrogen is a well-established raw material in the current economy. Due to its characteristics, it has become a very valuable commodity for many different industrial processes. In figures, the total world production of pure hydrogen was 85 Mt in 2020 as seen in Figure 10, adding to this number an extra 45 Mt mixed with other gases in the form of syngas [Rasul et al. 2022]. Prospects predict a substantial increase in hydrogen production in the following decades, mainly achieved through new and more sustainable methods. By 2050, the annual worldwide production of hydrogen is expected to reach 530 Mt, roughly five times more of today's current output [World Nuclear Association 2021]. Nearly 70% of today's hydrogen is employed in three main industrial activities: hydro processing in refineries, ammonia synthesis and methanol synthesis [World Nuclear Association 2021].

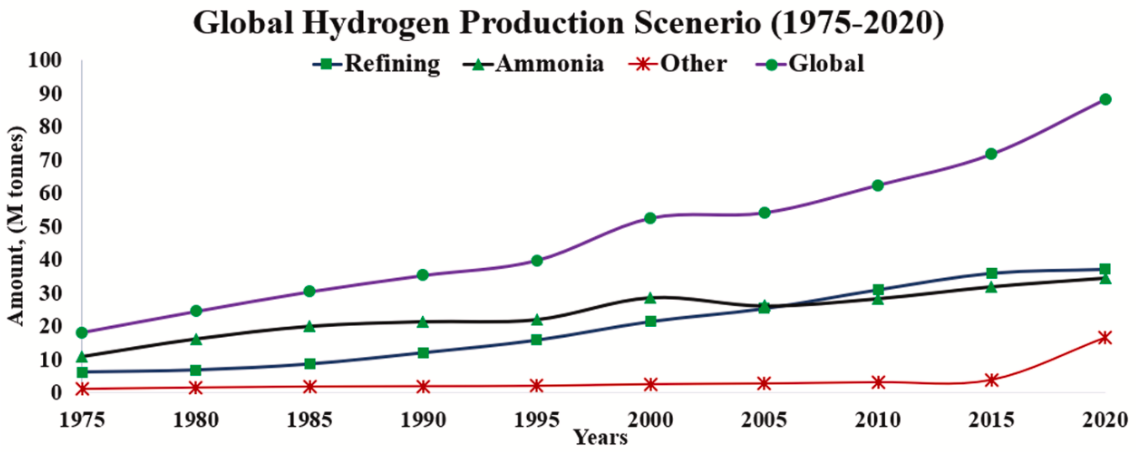

Figure 10. Hydrogen production development 1975-2020 [Rasul et al. 2022]

There exist two main processes in which hydrogen is used in refineries: hydrocracking and hydrofining [Abe et al. 2019]. The first of them, hydrocracking, is a process by which heavy hydrocarbons are converted into lighter compounds that present a higher hydrogen-to-carbon ratio. This is achieved through catalytic hydrogenation, which consist of a sequence of cracking and hydrogenation of hydrocarbons to break its carbon bonds [Abe et al. 2019]. These new lighter products are more valuable since they have fewer impurities. Moreover, the post-processing steps are reduced significantly, which implies a simultaneous cost reduction. Furthermore, hydrocracking plays also a role in the obtention of benzene, toluene and xylene, using by-products of oil refining as raw material [Saab et al. 2020]. Although hydrocracking has been applied mainly to petroleum, new techniques are being developed in order to apply this method to other types of feedstocks in order to produce biofuels. These new feedstocks range from non-edible vegetable oils to municipal waste and biomass, thus providing a sustainable pathway for the production of such fuel. Regarding the second process, hydrofining, is the method used in refineries with the objective of eliminating impurities in fuels. These impurities appear in the form of sulfur and sulfur dioxide [Acar and Dincer 2019], which are commonly related with acid rain. Therefore, hydrofining is a necessary step in the synthesis of gasoline and diesel, which need to comply with the limitations imposed by institutions to the sulfur content in fuels. Recently, the Fischer-Tropsch process has gained momentum for the development of cleaner fuels by using syngas to produce complex hydrocarbons without the characteristic sulfur impurities present in traditional fuels [Dodaro 2015].

The other main sector in which hydrogen is widely demanded is ammonia production. Ammonia is the leading inorganic chemical produced in the industrial sector due to its various applications [Zhang et al. 2020]. The main relevance of this compound, which is formed by nitrogen and hydrogen in a one to three molar fraction via the Haber-Bosch process, lies in the agricultural sector, where the ammonia-based fertilizers have become essential in the past century [Chai et al. 2021]. Moreover, it is employed for refrigeration of building and industrial processes, and for the fabrication of different materials, fibers and plastics. In the future, in addition to all these applications, ammonia is expected to play a role in the energy sector as a potential energy carrier. Its higher energy density, its cheaper costs and its more stable and matured production chain, place ammonia in a competitive position against pure hydrogen for the role of the future energy vector [Chai et al. 2021]. Nevertheless, there are other drawbacks related to ammonia, such as low burning velocity and high NO_X emissions, which hinder the position of this compound as a fully sustainable energy carrier [Chai et al. 2021].

The third most important application for hydrogen is methanol synthesis [World Nuclear Association 2021]. In this case, hydrogen is not employed as pure feedstock, instead it is included in the process as part of syngas. Synthetic gas is a mixture of hydrogen, carbon dioxide and carbon monoxide, which mainly comes from the reforming of natural gas. After the conversion of syngas to methanol, the effluent that comes from the reactor must be distilled in order to obtain the desired product [Bozzano and Manenti 2016]. Similar to ammonia, methanol is used for the synthesis of a wide variety of industrial products, such as formaldehyde and methyl-tert-butyl ether [Bozzano and Manenti 2016]. Moreover, it is employed for the synthesis of plastics, paints, resins, silicones, etc. Also, methanol is used in the fuel sector since its mixture with gasoline provides an enhancement of the octane number of the compound. Methanol can also be utilized as a sole fuel for internal combustion engines; nevertheless, issues like corrosion of materials are a challenge yet to be overcome [Rasul et al. 2022]. In the future, however, it is expected that methanol plays an even more important role in the energy and transport sector as a hydrogen carrier. Instead of acting alone as a fuel, methanol could be employed for fuel cell vehicles, thus providing an additional alternative to hydrogen and ammonia and further enhancing the flexibility of the transport sector [Rasul et al. 2022].

Beyond these three main applications, hydrogen has also relevance in other industrial sectors. This is the case of the electronics industry, where hydrogenation is employed in a reduction process in order to obtain silicon. Furthermore, hydrogen is used in the metallurgical sector as a reducing agent when the employability of carbon is not a suitable option [World Nuclear Association 2021]. Another possible use for hydrogen is to utilize it as an alternative fuel, for both electric power generation and household heat generation, although in those areas it is not widely extended. The spacecraft industry uses liquid hydrogen, not only as a fuel, but also as the power source for the shuttle electronics and to produce water for the ship’s crew [Rasul et al. 2022].

In recent years, with the appearance of modern fuel cells, hydrogen importance for the energy and transport sector has been redefined. This new technology transforms the chemical energy stored in the hydrogen bonds to electricity, which can be then converted into mechanical energy. Thus, the development of hydrogen technologies can be rethought as a whole in the current economy, acquiring a new and more important role at all levels of production and consumption. In combination with renewable energy sources, the production of hydrogen as a clean energy vector can be decisive for the future sustainability of society's consumption patterns, giving to this commodity a key role in many economic and industrial applications. By postulating hydrogen as the most promising alternative to fossil fuels, many have elaborated predictions on how that potential economic system would look like and the opportunities that might arise from this new paradigm. This novel concept for the economy of the future has been named hydrogen economy.

2.3.Hydrogen Economy in the Future

Hydrogen is a compound that has been known in the scientific community for the past two centuries. Since its first specific aimed synthetization in 1761 by Robert Boyle, the history of hydrogen has gone through several important milestones. It was in 1800 when water electrolysis was first used to produce hydrogen. A few years later, in 1839 Sir William Robert Grove managed to develop the first functioning fuel cell powered by hydrogen [Dawood et al. 2020]. In the 20th century several applications were reserved for the utilization of this commodity, such as aerospace applications. By 1960's NASA was the world's main user of liquid hydrogen, which they employed to produce water for the space shuttles as discussed in the previous chapter [Rasul et al. 2022]. However, accidents like the Hindenburg disaster in 1937, in which 35 people were killed due to the ignition of an airship, raised the concerns regarding the operational hazardousness posed by hydrogen [Dawood et al. 2020]. These safety issues related to the high inflammability of hydrogen, united with the convenience and rapid spread of fossil fuels displaced hydrogen from any potential main role in the energy sector.

Thus, the 20th century became the oil century by reaching an efficiency along the whole value chain that found no other competitors. Fossil fuels became then the basis that underpinned the greatest phase of economic growth in the history of humanity. Nevertheless, many remained skeptical and insisted in the necessity of continuing with the search of alternatives for long term sustainability given the potential harms that oil could pose to the environment. In 1970's, the hydrogen economy concept was introduced at the General Motors Technical Centre and since then it has become one of the main research topics in the scientific community [Abe et al. 2019]. It is presented normally as a complementary strategy towards reaching a fully sustainable economy, but not as the only answer to this challenge. For example, hydrogen could be very useful for sectors where electrification is especially difficult, such as the maritime transport sector [Atilhan et al. 2021]. These research efforts are trying to shed some light onto the future structure and sectors of the so-called hydrogen economy. Bottom-up, these sectors are potential uses, storage and production.

As seen in Chapter 2.3, hydrogen is already a well-extended commodity that is widely used in the industrial sector. However, the mass production predicted by the idea of a hydrogen economy opens up an ocean of possibilities for this material and allows for a reconsideration of its use in sectors where it was before unfeasible to employ such an expensive compound. This is the case of the power sector which, as discussed in the previous chapter, could really benefit from cheap hydrogen. The main problem with the current electrical grid is its lack of flexibility caused by the inability to store significant amounts of energy at an affordable price [Parra et al. 2019]. This makes the operation of such system really challenging, since generation and consumption must be equal at all times. This is where hydrogen could play a main role in the future economy, by harnessing the excess renewable energy in order to produce green hydrogen via water electrolysis.

Thus, the production of hydrogen will become a goal itself since it will provide storing service to the power grid. Once the hydrogen has been produced there will be several pathways, in the future hydrogen economy, to employ this material efficiently. As mentioned before, hydrogen will remain a reliable raw material for many well-established industrial processes that will see how their environmental performance improves with the new greener product. Moreover, hydrogen could be employed directly in the electrical grid, not only as a storing mechanism, but also provide ancillary services like voltage and frequency regulation and helping reduce negative prices occurrences [Yue et al. 2021]. The later have become frequent during the last years in Germany, where an overestimated installation of wind capacity has been leading the German electric market to relapse many times these negative prices [Amelang and Appunn 2018]. For such purposes, it is also key to develop cost competitive fuel cells, that allow for an efficient conversion of hydrogen into electricity.

The aforementioned fuel cells will also be fundamental in the efficiency improvement of co- and trigeneration. Cogeneration is the simultaneous generation of heat and power. On the one hand, the system produces electricity in order to meet the electric power demand; on the other, thermal units are put in place for the production of heat destined to certain thermal loads. Trigeneration is an extended version of cogeneration in which not only heat is produced, but also cold. By combining heat and power generation, the overall efficiency of the system improves significantly [Ferrucci et al. 2018]. Such systems are already operational in large scale thermal plants, where the excess heat of the electrical generator is employed for thermal purposes. In the future hydrogen economy, the addition and integration of hydrogen fuel cells in such systems could enhance their environmental performance and also their cost competitiveness. Moreover, micro versions of this technology could be developed for households and, in combination with PV-cells, provide consumers with actual green energy independence [Yue et al. 2021]. In fact, some projects are already in development in that sense. Figure 11 shows a schematic of the configuration of a trigeneration system:

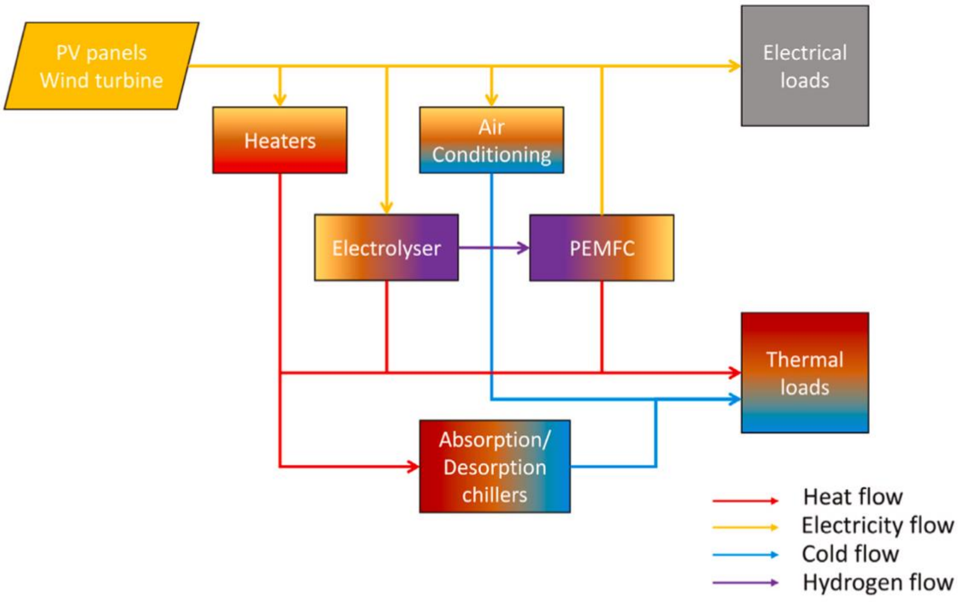

Figure 11. Trigeneration schematic [Yue et al. 2021]

Moreover, power-to-gas is an application that could also be paramount in the future hydrogen economy [Gahleitner 2013]. It makes a reference to the path of production of methane, in which electricity is turned into hydrogen and then, by adding CO_2, it is transformed into CH_4. This could provide an additional environmental advantage since this carbon dioxide could be originated by its capture in high carbon intensive processes. From then on, this methane could be injected in the natural gas grid and easily distributed, achieving a competitive cost efficiency [Gondal 2019]. This application has also been referred to as e-fuels and has been proposed as way of harnessing internal combustion engines in an environmentally friendly manner. This way, such a mature technology can remain useful during the transition to a fully sustainable economy by employing fuels that are carbon neutral. For instance, such an e-fuel is being used for the flight route between Madrid and Bilbao [Aiestaran 2021], providing a sustainable alternative to the airplane sector which is extremely difficult to electrify.

Another key aspect for the development of the so-called hydrogen economy is the storage of such commodity. For most applications, hydrogen will not be consumed immediately after its production and in the same location where it was first generated; on the contrary, a flexible and affordable storage and transportation system will be required in order to allow for a fully functional deployment of this technology. For such purposes, there exist three different storage possibilities depending on the state of the hydrogen: gaseous, liquid and solid [Ren et al. 2017]. Currently, the most extended method involves the storing of hydrogen in gaseous state. This method is also convenient for transportation of hydrogen in very large quantities, since it can be injected into the already existing natural gas grid, which translates into significant savings in capital expenditures. However, when it comes to the static storage of gaseous hydrogen, several issues arise regarding the low density of this compound: massive, pressurized vessels are required [Hirscher 2009]. Beyond the space such installations occupy, the pressurization process takes up too much energy, harnessing the overall efficiency of the system. Moreover, this kind of pressurized systems normally come with leakages which, in this case, pose a serious safety hazard due to the high inflammability of hydrogen.

Liquid hydrogen storage presents similar problems to those of gaseous hydrogen. In addition to them, liquefaction of hydrogen introduces extra costs to the process that really harness the cost competitiveness of this method [Niaz et al. 2015]. Moreover, this cooling process is very energy intensive and reduces the efficiency and the possibilities of a widespread roll out of this technology. However, in terms of volume requirement, this technique employs more compact vessels, since the density of liquid hydrogen is roughly twice that of gaseous hydrogen. Therefore, liquid state hydrogen storage is reserved for very specific small-scale applications where cost requirements are not as paramount, such as the space industry [Rasul et al. 2022].

The less developed, but still the most promising alternative to solve this challenge is the solid-state storage systems. These systems are safer, more compact and lighter than those based on gaseous or liquid state hydrogen [Zhang et al. 2015]. Moreover, they have the potential of becoming more economical than the other two alternatives. The storage of hydrogen in these systems occurs through two different processes: physisorption and chemisorption. On the one hand, physisorption consists of the adsorption of hydrogen molecules in the surface of the material. Afterwards, the stored hydrogen can be released again by the application of a thermal stimulus. This method offers a very good efficiency; however, its capacity is low at ambient conditions [Abe et al. 2019]. On the other hand, chemisorption consists of chemical reactions occurring between the material of the storing device and hydrogen, which is stored in atomic form building compounds with the storing material. Such storing device can be formed of different materials, but the most promising are metals [Zhang and Wu 2017]. The resulting metal hydrides are considered to be the best alternative for the future hydrogen economy, since various research have begun to show its potential to provide high density and safe storage capabilities.

The other sector that will concentrate most of the efforts in the future hydrogen economy is hydrogen production. As discussed in Chapter 2.1, there are many different types of hydrogen depending on their production path, which are classified employing a color ranking. However, most of the predictions point to the fact that, in order to have a fully sustainable hydrogen sector in the long term, green hydrogen is the answer to most of the challenges society will face in the deployment of the so-called hydrogen economy. That is the focus of this study, to thoroughly analyze the alternatives available for the best and most efficient production of green hydrogen. In the following chapter a full study is provided on the different variations of the technique employed to produce this sustainable form of hydrogen: water electrolysis.

2.4.New European Regulation on Renewable Hydrogen

The hydrogen sector is currently undergoing a process of deep transformation, in which regulations are being develop in order to clarify the path towards decarbonization of the technology. As a matter of fact, simultaneously to the elaboration of this research the European Commission made public two new Delegated Acts included in the Renewable Energy Directive. The objective of these two pieces of legislation is to define both rules and targets for the hydrogen sector in an attempt to clarify what the requirements are to classify hydrogen as green and to elaborate a comprehensive regulatory framework to provide investors with security. The production targets set by the Commission are ambitious, aiming at achieving by 2030 10 million tons of green hydrogen imports and 10 million tons of domestic production, which represents 14% of the European energy consumption [European Commission 2023].

The first Act aims to define the conditions under which hydrogen-based fuels and other compounds can be considered as renewable fuels of non-biological origin (RFNBO). This is achieved by the introduction of the concept of “additionality”, which varies depending on whether the plant is connected to the grid [European Commission 2023]:

- For renewable energy plants dedicated solely to the production of hydrogen independent of the main grid, this concept translates only into the requirement of new plant utilization. This means the plant employed to power the electrolyser must not have been in operation for longer than three years, in an attempt to incentivize the construction of new plants while not detracting resources from the main electrical grid.

- For plants that are connected to the grid, the concept of additionality is expanded with two premises: temporal and geographical correlation. The first refers to the fact that the produced hydrogen must be equivalent to the renewable energy produced by the grid to be considered green. This requirement must be fulfilled in a monthly basis. On the other hand, the geographical correlation limits the available energy for production to the energy produced in the location where the hydrogen plant is based.

The second Act defines the methodology to be employed in the calculation of the lifecycle emissions of the produced hydrogen. This method includes upstream emissions, emissions related to the processing of the compound and its transportation to consumption points. The key aspect to be discussed about this second piece of regulation is the established emission threshold to differentiate green hydrogen from non-renewable hydrogen. This value was set to 18 g CO_2eq/MJ which allows for the inclusion of hydrogen produced with nuclear energy as green hydrogen [European Commission 2023]. This was decided after long deliberations in which France was the main representative of pink hydrogen, given the country’s strong dependence on this source of energy.

With these two Delegated Acts Europe moves forward in its attempt to develop a hydrogen economy. This legal framework provides investors with the necessary security to act and start deploying new resources for the execution of green hydrogen related projects. Also, it places Europe in the forefront of regions trying to attract investments intended for renewable energy projects. For the purpose of this research, this new legislation is included in the economic section as a limitation of the production capacity in the case where the electrolysis is carried out by means of the electricity provided by the main electrical grid. Given its importance for the determination of economic value of energy related projects, this new legislation is key in order to analyze projects deployed within the European Union.

3. Water Electrolysis

The intention of this chapter is to gather the most relevant research to date in relation to water electrolysis. This electrochemical process, known by the scientific community for many years, has gained attention during the last decade due to its potential to become the key feature in the development of a sustainable hydrogen economy. Within water electrolysis there exist different variations to the configurations through which such process can be performed. However, before analyzing the various types of electrolysis techniques, it is paramount to first provide a thorough assessment of the theoretical concepts and principles that underpin such technology.

3.1. General Principles of Water Electrolysis

Water electrolysis refers to the process by which the water molecule is chemically decomposed by the application of an electrical current. Such process is carried out in an electrolyser which can consist of various cells. This cell's structure is depicted in the following Figure 12:

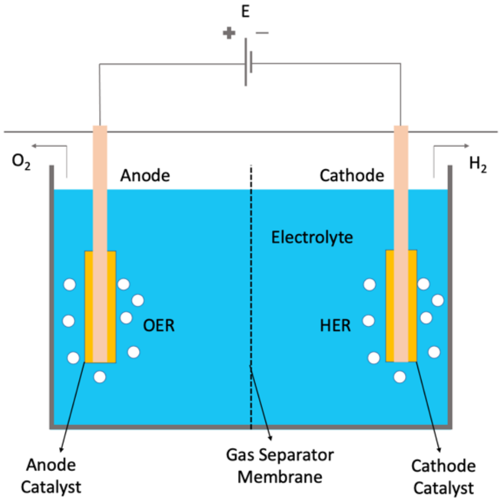

Figure 12. Cell schematic

As presented above, the electrolyser cell consists primarily of two electrodes, the anode and cathode, which are positively and negatively charged, respectively [Lei Zhang et al. 2020]. The tips of these electrodes are covered on specific catalysts that allow the chemical dissociation of water. In-between there is an electrolyte, which allows for the constant flow of current. The system is supplied with electrical energy by an external power source which, for the purpose of this study, is a renewable source. After the dissociation of the water molecule has occurred, oxygen and hydrogen gases appear, and it is paramount to maintain them separated so that they can be later processed. For such purpose, a gas separator membrane is installed in the middle.

This is the structure of a single electrolyser cell; however, in practice several of these cells are installed in series and in parallel in order to increase the voltage and the current density the overall system can sustain. In [Yue et al. 2021] a schematic is provided for a complete electrolyser system. As seen below, a separator system, accompanied by a purification system, is required for each of the gases stream in order to get rid of any excess water. Such excess is then recovered and reinjected in the water stream that goes in the electrolyser. Before entering the electrolyzing unit, the pressure and temperature conditions must be set. These parameters depend on the specific technology being used to carry out the process. Specifics related to this matter are discussed in following chapters.

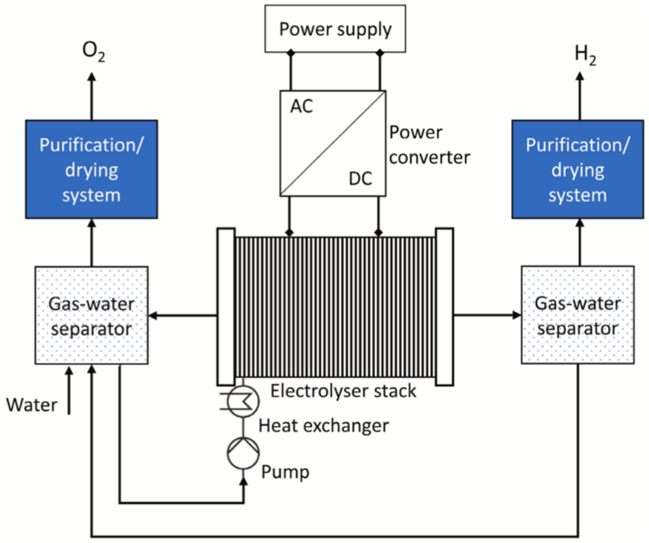

Figure 13. Schematic of a full electrolyser system [Yue et al. 2021]

From a general perspective, the process of water electrolysis can be summarized by equation 1. This is the so-called full cell reaction, which consists of the dissociation of the water molecule into molecular hydrogen and oxygen by the application of an electrical current. However, this process is two-folded, and it can be divided into two half-cell reactions: the oxygen evolution reaction (OER) and the hydrogen evolution reaction

(HER) [Lei Zhang et al. 2020]. OER occurs on the anode, the positive electrode, while HER takes place on the cathode, the negative electrode. Specifics to both evolution reactions are discussed in the following chapters.

$$2H_2O + Energy \rightarrow O_2 + H_2 \tag{1}$$

For the reaction to happen, a certain amount of voltage must be applied in order to initialize the decomposition of water. This threshold is called the equilibrium voltage. Under standard conditions (T = 298 K, p = 1 atm, pH 0), the standard equilibrium voltage can be derived from the following Gibbs free energy equation [Wikipedia 2023], resulting in a value of U_0 = 1,229V

$$\Delta G_0 = -z * F * U_0 \tag{2}$$

where z=2 is the number of electrons converted per H_2 molecule; and F=96485 $Cmol^{-1}$ is the Faraday Constant. Gibbs free energy is a term used in thermodynamics that refers to the maximum amount of work a closed system can provide under constant temperature and pressure. The equation includes the variation of the Gibbs free energy, which corresponds to the maximum amount of non-expansion work that can be performed by a closed system in a fully reversible process, in this case the electrolyser. If practical application conditions do not correspond to the standard, thus a factor must be added to the previous standard baseline. This factor is dependent on concentrations, partial pressures, temperature and activities, and is derived from the Nernst Equations. Therefore, the variation of Gibbs free energy is related to the standard free energy through the following equation [Wikipedia 2023]

$$\Delta G = \Delta G_0 + R * T * \ln Q_r \tag{3}$$

where R=8,314 $JK^{-1}mol^{-1}$ is the gas universal constant; T is temperature in K; and Q_r is the reaction quotient, which is equal to the ratio of the chemical activities of the reductant and the oxidant. By substituting (2) in (3), the Nernst equation can be expressed in terms of equilibrium voltages as follows.

$$U_{eq}^{cell} = U_0 - \frac{R * T}{z * F} * \ln Q_r \tag{4}$$

This equation yields the theoretical voltage value at which decomposition of water begins for certain conditions. However, in practice there are other inefficiencies that increase the voltage requirement. This additional effort is called overpotential, and it is primarily caused by the flow of electrical current.

Cell current density has an impact on electrode voltage for four reasons. First, the flow of electrical current through the electronic conductors causes potential losses proportional to the resistance of these as predicted by Ohm’s Law [Lei Zhang et al. 2020]. Moreover, significant values of current density produce the appearance of bubbles on both the catalysts’ surface, which hinders the activity, and in the electrolyte, which further increase the ohmic losses in transport. Also, the kinetics at electrochemical interfaces are problematic, specially at the anode since the OER consists of several steps that hinder the speed of the process and require an overvoltage to overcome it. And last, ions must be transported through the electrolyte, which requires as well an overpotential to beat any limitations or resistances.

The relationship between density current and electrode voltage is paramount in the operation of electrochemical cells. Most of these cells are current controlled, and therefore rely on this relationship to function at the desired rate. This response function is called polarization curve, and it is the main characteristic function of a cell. The Butler-Volmer equation, through which this relationship between current density and voltage (or overvoltage) is obtained, states the current density in a simple and single-molecule redox reaction depends on the voltage difference between the electrode and the electrolyte. This equation divides the current density into two components, one anodic and another cathodic, simplified as follows [Chatenet et al. 2022]

$$j = j_a + j_c \tag{5}$$

$$j = j_0 * \left\{ exp\left[\frac{\alpha_a * z * F * \eta}{R * T}\right] - exp\left[-\frac{\alpha_c * z * F * \eta}{R * T}\right] \right\} \tag{6}$$

where α_a and α_c the anode and cathode charge transfer coefficient, respectively; η the over potential; j_0 the intrinsic exchange current density, which corresponds to the current at zero overpotential and the absence of electrolysis. The following Figure 14 shows an example of the polarization curve of a cell.

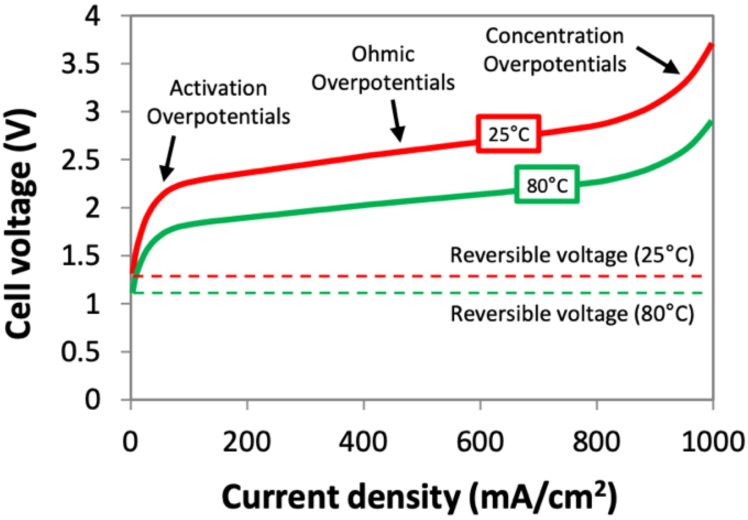

Figure 14. Polarization curve depending on the temperature [Amores et al. 2017]

From equation (7) it is relevant to note the importance of both the transfer coefficient and the intrinsic exchange current, which are material dependent. Therefore, they are the two key parameters that define the adequacy of the potential electrocatalyst's properties [Amores et al. 2017]. However, its values are deeply dependent on the overpotential, meaning that for different ranges of overpotential the sensitivity of the measurements varies. Moreover, from equation (7) the Tafel equation can be derived, which expresses the logarithmic relation between the overpotential and the current density. This equation introduces the concept as well of Tafel slope

$$\eta = A + \frac{R * T}{\alpha * F} * \log_{10} j = A + b * \log_{10} j \tag{7}$$

where b is the Tafel slope and A is an offset term related to the standard exchange current. Since the Tafel slope depends on the value of the transfer coefficient, it value is also subject to the same variations. These fluctuations of the measurements are due to the multi-step character of the electrochemical reactions that are taking place [Chatenet et al. 2022]. Such complexity is not considered in the simplified Butler-Volmer equation, which is important to keep in mind for the later technical analysis.

3.2.Half-Cell Reactions: HER and OER

As already stated in the previous section, the overall water decomposition in an electrochemical cell can be divided into two half-cell reaction: the hydrogen evolution reaction and the oxygen evolution reaction. Each one of these processes has different characteristics in terms of compounds involved in the reaction, velocity and steps required, and adequate materials for each of the electrodes. The objective of this section is to provide a thorough understanding of each of the half-cell reactions, which rounds up the theoretical concepts presented in the previous chapter.

3.2.1. Hydrogen Evolution Reaction (HER)

The Hydrogen Evolution Reaction (HER) takes place on the cathode of the cell. HER has more simple, faster kinetics compared to the oxygen evolution reaction (OER) since it consists merely of a two-step electron transfer [Lei Zhang et al. 2020]. This process unfolds following different pathways depending on various factors, such as pH, which is the potential of hydrogen [Conway and Salomon 1964]. This term is used to characterize the acidity or basicity of a given solution measuring the presence of free H^+ ions: in acidic medium, the concentration of free protons is higher compared to that of OH^- ions, which is defined with lower pH values; in alkaline medium, pH values are higher since the concentration of OH^- is greater than that of H^+. When these concentrations are equal, pH is assessed with a value of 7. In acidic conditions, the two-step HER begins with the adsorption of hydrogen by the cathode [Lei Zhang et al. 2020]. This step is called the Volmer reaction, and is defined as follows

$$M + H_3O^+ + e^- \rightarrow M - H_{ads} + H_2O \tag{8}$$

where M refers to the catalyst material, and M-H_{ads} is the adsorbed hydrogen atom. From (8) two different steps can lead to the desorption of hydrogen. On the one hand, the hydrogen molecule can be formed through an electrochemical desorption, which is also called the Heyrovsky reaction. In this step, an adsorbed hydrogen joins with a hydronium ion to produce the desired hydrogen molecule as follows

$$M - H_{ads} + H_3O^+ + e^- \rightarrow M + H_2 + H_2O \tag{9}$$

On the other hand, two adsorbed hydrogen atoms can directly join on the surface of the cathode, which is known as chemical desorption. This step is also called the Tafel reaction, and is defined as follows

$$M - H_{ads} + M - H_{ads} \rightarrow 2M + H_2 \tag{10}$$

In acid medium, the HER is the preferred half-cell reaction. Since it takes place in the negative electrode, the reaction is favored by the presence of extra H^+ in the solution in the form of hydrated protons, or hydronium ions [Chatenet et al. 2022]. On the other, in alkaline or neutral medium, the presence of protons is negligible compared to water, thus, the reactant that is reduced is the water molecule itself. Therefore, the overall process is similar to that of acidic medium but substituting the hydronium ions with water molecules, beginning with the following Volmer reaction.

$$M + H_2O + e^- \rightarrow M - H_{ads} + OH^- \qquad (11)$$

Similar to acidic medium, in alkaline medium the desorption can also follow two different paths. First, the electrochemical desorption or Heyrovsky reaction shown in (12)

$$M - H_{ads} + H_2O + e^- \rightarrow M + H_2 + OH^- \qquad (12)$$

or the chemical desorption, also called the Tafel reaction, which is the same as equation (10). These equations show the important role that the catalytic material plays in the HER. It is paramount that the materials, of which the cathode is made, have outstanding adsorption and desorption capabilities. This means that a certain material can have great hydrogen adsorption qualities; however, it is not ideal to work as catalyzer since its bonds with hydrogen are too difficult to break [Pomerantseva et al. 2017]. Therefore, the free energy of Gibbs (ΔG_H) ideal value is 0, where neither the adsorption nor the desorption forces trump each other to allow for good catalytic characteristics. This is what is called the Sabatier Principle of catalyzers and can be graphically represented through a Volcano diagram as shown in Figure 15:

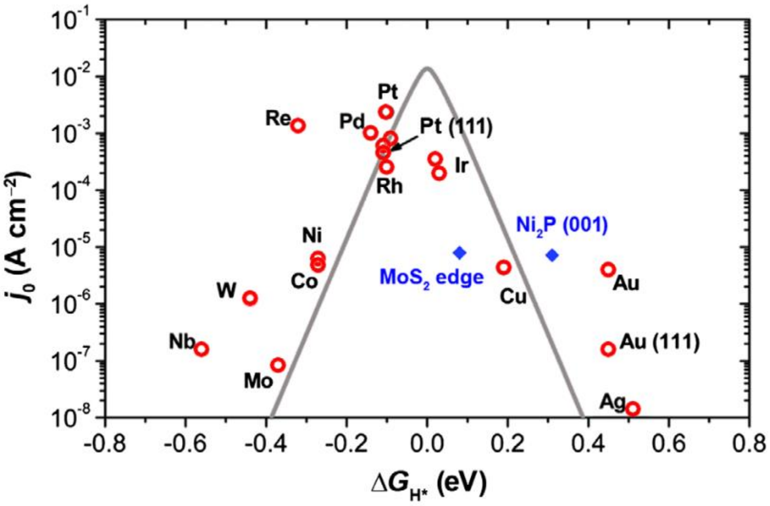

Figure 15. Volcano plot including several catalyzers [Pomerantseva et al. 2017]

This Volcano plot represents the exchange current density versus the free Gibbs energy. As it can be observed, there exists a Sabatier optimum near $\Delta G_H=0$ where the current density is maximized. This region corresponds to the platinum group metals (PGM) which are the most efficient to carry out the HER. However, the scarcity of such materials and their high price is driving new promising research regarding non-PGM catalyzers which can further decrease the overall cost of the technology. Later on, a chapter is dedicated to discussing the developments in such field of study.

3.2.2. Oxygen Evolution Reaction (OER)

The Oxygen Evolution Reaction (OER) takes place on the anode of the cell. In contrast to HER, the OER kinetics are much slower since it consists of a four-step electron transfer, thus, determining the overall efficiency of the electrolysis [Lei Zhang et al. 2020]. Moreover, three different reaction intermediates appear along the cycle. This process, known as proton-coupled electron transfer (PCET) [Chatenet et al. 2022], involves the transfer of protons and electrons between different atoms, which begin and end at different atomic orbitals. Unlike HER, OER is favored in alkaline and neutral conditions. When pH is higher, the concentration of OH^- is higher than the concentration of H^+, thus, being the anode the positive electrode, attractive interactions with those anions are the preferred reaction. In acid medium, the OER develops following two possible pathways [Lei Zhang et al. 2020]:

$$M + H_2O \rightarrow M - OH_{ads} + H_2 + OH^- \tag{13}$$

$$M - OH_{ads} \rightarrow M - O_{ads} + H^+ + e^- \tag{14}$$

$$M - OH_{ads} + M - OH_{ads} \rightarrow M - O_{ads} + M + H_2O \tag{15}$$

$$M - O_{ads} + M - O_{ads} \rightarrow 2M + O_2 \tag{16}$$

The first pathway is dictated by the equations (13)→(14)→(16); the second follows the order (13)→(15)→(16). It can be observed that under acidic conditions, the interactions happen within the electrode, where the adsorbed elements couple with each other in order oxidize. This is explained by the fact that, under these conditions, the majority of the ions present in the solution are positive, thus, attracted to the opposite electrode where the HER is taking place. On the other hand, under alkaline conditions, the kinetics of OER are favored through the presence of hydroxide anions. The chemical balances of the steps of the reaction are described as follows:

$$M + OH^- \rightarrow M - OH_{ads} + e^- \tag{17}$$

$$M - OH_{ads} + OH^- \rightarrow M - O_{ads} + H_2O + e^- \tag{18}$$

$$M - O_{ads} + M - O_{ads} \rightarrow 2M + O_2 \tag{19}$$

$$M - OH_{ads} + 2OH^- \rightarrow M - OOH_{ads} + H_2O + e^- \tag{20}$$

$$M - OOH_{ads} + OH^- \rightarrow M + O_2 + H_2O + e^- \tag{21}$$

The first pathway is the so-called Eley-Rideal (ER-type) mechanism, described by the order (17)→(20)→(21) [Lei Zhang et al. 2020]. For this type of OER it is required the formation of the intermediate peroxide OOH, which leads to the desorption of the oxygen molecule by its combination with a hydroxide anion. On the other hand, the path described by (17)→(18)→(19) directly adsorbs oxygen anions on the surface of the anode, which later combined result in the desorption of oxygen molecules. This mechanism is called Langmuir-Hinshelwood (LH-type).

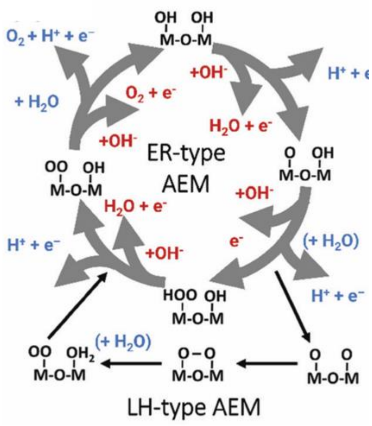

Figure 16. OER Pathways [Chatenet et al. 2022]

Whether the ER-type or the LH-type is the dominant process in the OER of an electrolyser depends on the material of the anode. ER-type is related to Ru- and Ir-based catalyzers, while LH-type is characteristic for Co-based catalysts [Chatenet et al. 2022]. More aspects regarding the materials of the electrons are discussed later on.

3.3.Electrolysis Types

Electrolysis is an electrochemical process that has been known by the scientific community for over two centuries. During this period, different ways of carrying it out have been developed, each with several advantages and drawbacks compared to the others. Specially during the last two decades, with the development of renewable energy, electrolysis technologies have gained momentum in the race towards a sustainable future. The idea of converting that electrical energy into chemical energy stored in the hydrogen molecule is a very promising solution to solve the storing hindrances the energy supply system is facing. The various electrolysis solutions differ from one another in their configuration, their working electrolyte, the separator membrane and the operating conditions, i.e., temperature and pressure. In this section, an analysis on the four main electrolysis techniques is provided, which serves as the theoretical basis for the later techno-economic analysis. These technologies are: alkaline water electrolysis, proton exchange membrane water electrolysis, solid oxide electrolysis cell and anion exchange membrane water electrolysis.

3.3.1. Alkaline Water Electrolysis (AWE)

AWE is the most mature electrolysis technique [Yu et al. 2021b]. It follows the same cell schematic presented in Figure 12, with alkaline conditions. For commercial purposes, several electrolysis cells can be configured both in parallel and in series, thus, providing enhanced voltage, current and power capabilities. These configurations are named monopolar and bipolar, respectively. Monopolar systems are those in which the positive electrodes of all the cells are connected to each other; same for the negative electrodes, which provides the system with a greater current density limit while maintaining low the voltage requirement. The whole parallel connected system is then introduced in a single electrolyte tank. The lower voltage condition provides higher safety standards; however, higher current densities lead to higher ohmic losses. Also, the ancillary electronic equipment needs to be adapted to the more demanding current requirements, which leads to an increase in cost of materials [Santos et al. 2013].

On the other hand, the bipolar assembly provides higher voltage at lower current densities. In this case, the cathode and anode of neighboring cells are connected, and the current is collected using endplates. Lower current density means lower ohmic losses, which translates into better overall energy efficiency [Santos et al. 2013]. However, the bipolar arrangement is more complex than the monopolar, which in terms of manufacturing is significantly simpler, thus, reducing potential leakages of both electrolyte and gas. Moreover, in the bipolar arrangement cathodes and anodes are very close, which might lead to potential shortcuts in case of failures. Both configurations can be enhanced by combining these strategies, i.e., various monopolar systems can be connected in series and several bipolar systems can be coupled in parallel. In Figure 17 is presented the scheme of both configurations:

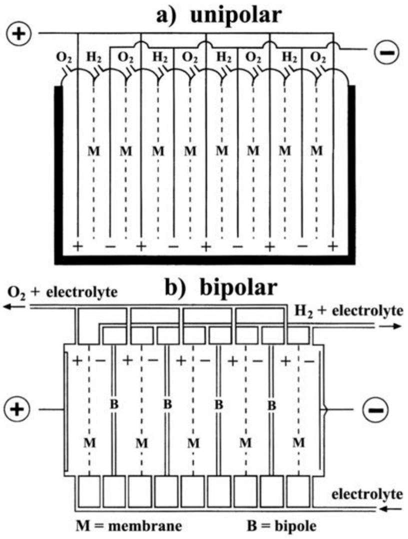

Figure 17. Uni- and bipolar configuration of cell stacks [Santos et al. 2013]

The electrolysis process takes place on the region where the electrolyte and the electrodes meet [Amores et al. 2017]. This area of contact, where the liquid phase interacts with the solid phase, has certain characteristics that are worth discussing. Around the electrode's surface a boundary layer is established, which is called the electrical double layer. Each of the electrodes, depending on the sign of their charge, attract the solvated ions of their opposite charge. On a molecular level, a first layer of ions is established on the surface of the catalyst, followed by another layer of opposite charged ions. This electrical configuration yields an electrical field divided into two regions: the compact layer, which is the region of space occupied by the two electrical layers, where the electrical voltage decreases linearly; and the diffusive layer, beyond the two-fold layer and where the voltage decreases exponentially until it stabilizes at a certain value in the electrolyte. The difference between this stabilized value and the potential at the electrode is called Galvani voltage [Zhang and Zhao 2009], which refers to the difference in voltage between two different phases and is paramount for the determination of the current density.

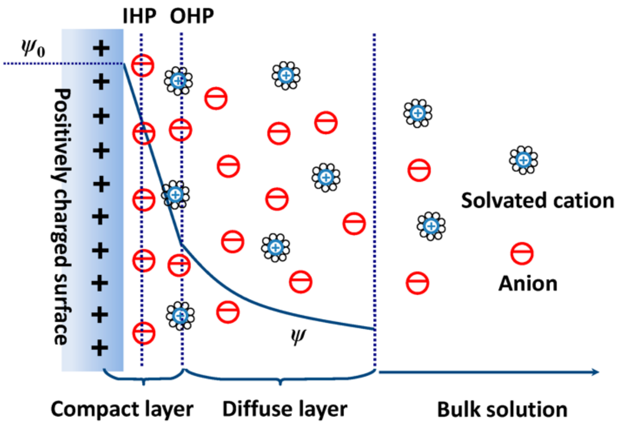

Figure 18. Surface behavior of the electrolyte around the catalyst [Zhang and Zhao 2009]

Electrically, that double layer behaves as two capacitances, which require for a charging current to assemble. This translates into poor transient behavior and harness the efficiency of the system in reaching steady state conditions. This impediment is the greatest when trying to integrate AWE into the electric power grid, since the dynamics of intermittent renewable resources, such as wind and solar power, require for fast response ancillary systems [Chatenet et al. 2022]. In commercial electrolyser, the longitude of the electrodes can lead to fluctuations of this characteristic along the surface. This phenomenon can cause non-desired forces which may harness the performance of the overall system. This is a key factor to be considered when manufacturing and operating these devices.

Moreover, the performance of the electrode-electrolyte interface can also be hindered by certain substances depositing on the surface of the catalyst. The adsorption of such species leads to so-called deactivation of the catalyst since the effective active surface has shrunk [Zhang and Zhao 2009]. Therefore, the design of proper electrodes and the election of their materials has become paramount in the pursuit of higher efficiencies. These materials must, first, present very good conductivity, which mean that under current, the voltage drop along the conductor is minimal. Moreover, they must have outstanding stability and corrosion properties to allow for an optimal performance during the longest period of time possible.

In AWE the typically preferred material for the electrodes is the Ni-based [Yu et al. 2021b]: for the anode, Ni oxides are the most common alternative; for the cathode, Ni and iron alloys are amongst the best options. Introducing iron as a companion of Ni reduces the deactivation caused by the formation Ni hydroxide due to the higher concentration of H_2 near the cathode.

The electrolyte is another key aspect to consider in the design of an AWE system. Typically, a potassium hydroxide (KOH) solution (25-30wt.%) [Lei Zhang et al. 2020] is employed for this purpose. Another alternative is sodium hydroxide (NaOH); however, the efficiency of the former is higher. The ions of the electrolyte are responsible for carrying most of the current across the cell, from one electrode to the other [Gandia et al. 2013]. The major drawback generated by the circulating current through the electrolyte is the formation of bubbles. These bubbles cause severe ohmic drops, which harness the efficiency of the cell. This hindrance can be assessed from both the electrode point of view and the electrolyte point of view [Chatenet et al. 2022]. On the one hand, several perforation techniques have been proposed for the electrodes which reduce the potential formation of bubbles at their surface. On the other, the addition of surfactants to the aqueous solution also reduces the bubble formation phenomenon, which is paramount for the optimization of the system [Chatenet et al. 2022].

Submerged in the aqueous solution, a separator is installed in between the anode and the cathode. This separator consists of a porous membrane whose objective is to ensure that the hydrogen gas and the oxygen gas do not mix upon formation. The mixing of these two gases is problematic from two points of view: first, it poses a safety threat due to the high inflammability of hydrogen; second, it requires for a later energy consuming purification step to separate both gases [Gandia et al. 2013]. However, the presence of this membrane causes ohmic losses due to the resistance introduced in the system.

There are three types of separators: first, porous spacers, which their main function is to avoid contact of cathode and anode; second, diaphragms, with much smaller porous that function as convection and diffusion barriers; and third, ion exchange membranes (IEM), which allow for a selective migration of anions and cations. IEMs are very thin polymer sheets built of a combination of fluoro- and hydrocarbons, which allow passage for either positive or negative ions [Chatenet et al. 2022]. These membranes are the basis for new electrolysis technologies that are discussed in the following chapters.

The aforementioned elements of an alkaline electrolysis cell lead to mechanical and electrical obstacles interfering with the electrical current. These obstacles translate into voltage drops, also called ohmic losses. Based on Joule’s law, these losses are emitted in the form of heat and harness the performance of the system. Therefore, during the design phase, all the elements involved in the configuration must be considered from the point of view of reducing both mechanical and electrical losses, which can be achieved through electrochemical engineering and the use of high conductivity materials, respectively.

All in all, the commercialized AWE systems operate in a temperature range of 80-90°C, pressures of around 35 bar and are able to provide a current density of 1000-3000 Am^{-2} [Chatenet et al. 2022]. An overall efficiency of 50% is considered acceptable for this technology.

3.3.2. Proton Exchange Membrane Water Electrolysis (PEMWE)

PEMWE is a technology that was invented in the 1950s by General Electric and was initially employed in specific sectors such as the aerospace sector [Chatenet et al. 2022]. However, the focus was placed in the generation of oxygen rather than the production of hydrogen. Throughout the last decades, PEMWE has evolved in order to be a competitive alternative to the traditional steam reforming hydrogen production. Nowadays, PEMWE has reached remarkable energy efficiency levels at high hydrogen production rate, become one of the main alternatives for the future hydrogen economy [Ayers 2019].

The structure of PEMWE cells presents fundamental differences with that of AWE systems. In this case, instead of an alkaline liquid electrolyte, a solid polymer electrolyte is used to transport the current from the cathode to the anode. Moreover, in PEMWE there is no net consumption of electrolyte and, with a constant and steady supply of water the concentration of the electrolyte remains constant throughout the whole process [Carmo et al. 2013]. This membrane is highly acidic and is usually made of perfluorinated sulphonic acid. The most commonly used material for such membranes is Nafion® [Chatenet et al. 2022]. Its general width varies around 150μm and shows better conductivity than alkali liquid electrolytes; however, due to the minimal value of the membrane's width, gases might leak from one side to the other, leading to the safety and purity issues already discussed for AWE [Gandia et al. 2013]. Nafion® is an ionomer that shows very good stability capabilities and which allow the passage of cations, i.e., allows for the protons to go from the anode to the cathode, while simultaneously denying passage to the electrons [Ayers 2019].

This selective conductivity is called charge-based exclusion. On each side of the membrane, the positive and negative electrodes are placed right on the surface, without any gap in between. This way, the catalysts are in direct contact with the membrane forming an assembly that is called membrane electrode assembly (MEA) [Bareiß et al. 2019]. This MEA is then placed between to porous transport layers (PTL), again following a no-gap criteria to minimize losses. The whole system is then placed in between two bipolar plates, whose purpose is to isolate the cell from other cells in case several of these are stacked together to fulfill certain requirements. These bipolar plates are designed including channel-like structure which, in practice, serve as pipes for gases and water. Water is fed to the anode, where the water molecule is breakdown into an oxygen molecule and two hydrogen ions [Bareiß et al. 2019]. These positively charged ions travel through the membrane until they reach the cathode, where the HER takes place and hydrogen is obtained. The electrons obtained in the previous OER find their electric path through the external circuit and power source, since the charged-based exclusion performed by the membrane prevents them from following the same path as the protons. A comprehensive scheme of the PEMWE cell is provided in the following Figure 19:

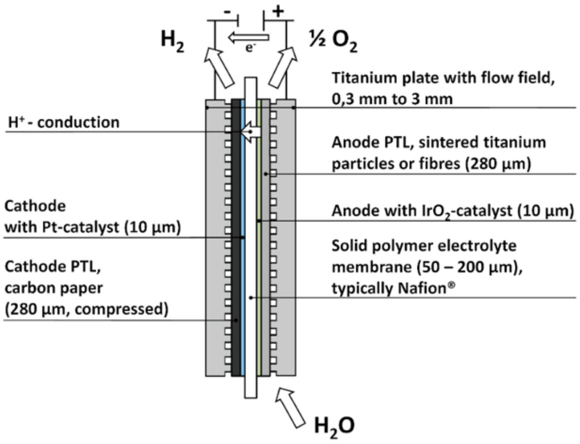

Figure 19. Configuration of a PEM electrolyser [Bareiß et al. 2019]

Regarding the adequate materials for each of the elements, perfluorinated sulphonic acid ionomer has already been discussed as the most widely used alternative for the fabrication of the solid electrolyte membrane [Lei Zhang et al. 2020]. On the one hand, the cathode catalyst is normally made of PGM, such as platinum and palladium. Regarding the cathode PTL, the conditions of HER allow for the use of non-noble metals such as carbon. Thus, the cathode transport layer is normally a carbon paper. On the other hand, for the anode catalyst, the best alternative is the Ir oxide. Ru-based catalyst also show very high catalytic activity for the OER; however, its stability is weak under acidic conditions [Lei Zhang et al. 2020].

Regarding the anode PTL, carbon cannot be employed as for the cathode PTL since it is not stable, therefore, the most common used layers are titanium based, which are more stable for the OER since it forms compact oxide layers [Ayers 2019]. Ti nanostructuring is more complex than that of carbon, which leads to heterogeneities along the catalyst-PTL connection [Gandia et al. 2013]. That added to the slower kinetics of OER contributes to the higher overpotential required for the anode activation, as shown in Figure 12. The thickness of both the anode and cathode PTLs are around 300µm, while the electrodes' width lies around the value of 10µm. With regard to the bipolar plates, these are Ti-based [Chatenet et al. 2022].

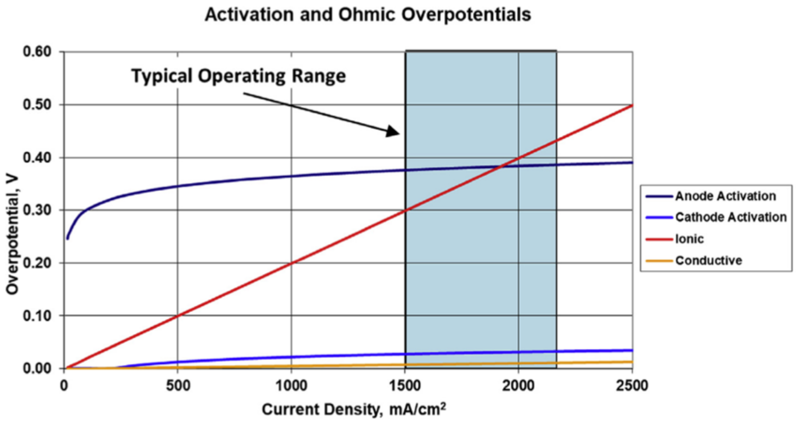

Figure 20. Breakdown of overpotentials in a PEM electrolyser [Ayers 2019]

Based on the previous paragraph, the main drawback of PEMWE compared to AWE can be deducted: the requirement of noble metals for several of the involved components translates into a higher capital cost. However, in terms of efficiency and energy performance PEMWE presents clear advantages compared to the alkaline technology [Ayers 2019]. First, it can operate at higher current densities and power requirements, which translates into a greater hydrogen throughput. This energy efficiency can reach values up to 70% and the current density up to 15000 Am^{-2} which is nearly ten times the current density provided by AWE [Chatenet et al. 2022]. Moreover, the kinetics and dynamics of the membrane-based system are much more agile, which turns it into a more suitable fit for its integration with fast changing energy sources, such as solar and wind power. In terms of operational temperature, the allowed is similar to that of AWE, ranging in 50-80°C. Also, in terms of pressure, PEMWE can be operational up until 70 bar, nevertheless, the most common is 35 bar similar to AWE [Chatenet et al. 2022]. Through new material configurations and material usage reduction the cost competitiveness is expected to improve in the following years. The reduction of catalyst loading for both anode and cathode is being thoroughly investigated so to provide the market with a competitive PEMWE [Ayers 2019].

3.3.3. Solid Oxide Electrolysis Cell (SOEC)

A solid oxide electrolysis cell (SOEC) is a solid oxide fuel cell (SOFC) functioning in inverse mode. This system is also regarded as high temperature electrolysis since the operational temperature is the main differentiating factor with the rest of electrolysis technologies. It is a better alternative to couple with a power plant which generates electricity or heat. Moreover, these cells can also be employed for the electrolysis of carbon dioxide or even simultaneous electrolysis of water and CO_2 [Hauch et al. 2020]. Thus, they are utilized for the production of syngas, hydrogen and oxygen, which find various applications. For instance, in the aerospace industry this kind of cells are being tested to generate oxygen on Mars surface alongside other efforts to make it habitable [Hecht et al. 2020].

The structure of SOEC adds a new variation to the two electrolysis concepts already explained. In this case, in contrast with PEMWE, the water is fed to the cathode, which is also referred to as the steam electrode; fuel electrode for SOFC. On the other hand, the anode is also referred to as air electrode. It is also important to note that the working fluid is in this case vapor, given the high temperatures at which the whole process occurs [Chatenet et al. 2022]. On the cathode’s surface the HER takes place and hydrogen gas is produced. In the same reaction oxygen anions (O^{2-}) are liberated and transported through the barrier separating both electrodes, as seen in Figure 21. Then, they reach the anode, where OER occurs, and oxygen molecules are emitted. Thus, the main structure of SOEC consists of three elements: the barrier, the cathode and the anode.

The barrier which contains the electrolyte is solid and is normally made of yttrium stabilized zirconia (YSZ) [Lei Zhang et al. 2020], which is coated with manganite. This ceramic is formed by oxides of the two aforementioned species namely zirconia (ZrO_2) and yttria (Y_2O_3) and its thickness ranges around 100 μm. The addition of yttria to pure zirconia generates oxygen vacancies on the anionic sublattice, i.e., the oxide part of the crystal structure. Thus, this ceramic has ionic conductivity properties, allowing for the electrical transport of oxide ions, specially at high temperatures. The higher the content of yttria, the better the conductivity of the obtained compound; however, for high temperatures an excessive content of the infiltrated oxide can become problematic: material decomposition begins and the content of yttria along the membrane becomes heterogenous, which leads to electrical degradation [Sohal et al. 2010]. Relative to this matter, new solutions are being proposed, such as co-doping the zirconia with scandium oxides.

Regarding the structural properties of both electrodes, it is worth mentioning they are both porous [Lei Zhang et al. 2020]. In addition to these three main elements of the cell, an extra layer is added to the system. This layer is made of gadolinia-doped ceria (GDC) whose function is to inhibit reactions between the air electrode materials, such as LSC, and the YSZ. GDC is another ceramic with higher ionic conductivity than YSZ. Also, it has lower reactivity to the electrode materials, thus, it is used as a separator element [Hauch et al. 2020]. Although GDC electrochemical properties might trump YSZ properties, the latter is still preferred as the main material for the SOEC since it provides higher mechanical strength. Moreover, at very high temperatures there is potential for the reduction of GDC when exposed to hydrogen [Hauch et al. 2020].

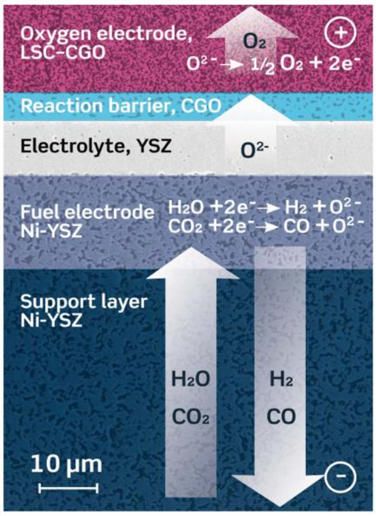

Figure 21. Schematic of a SOEC [Hauch et al. 2020]

Regarding the materials for the electrodes, it is worth mentioning that they are based on non-noble metal elements, as well as the membrane. For the fuel electrode, Ni is the main material employed, which is abundantly available [Lei Zhang et al. 2020]. On the other hand, the air electrode is normally composed of perovskite materials. Perovskite is originally a specific compound formed of calcium titanate; however, this denomination has been extended to other crystals with the same configuration. In the case of SOEC air electrode, the most common compound is lanthanum strontium manganite (LSM), with other higher performing materials under development such as lanthanum strontium ferrite cobaltite (LSCF) [Hauch et al. 2020]. Similar to the previous discussed electrolysis technologies, the LSM-electrolyte interface is one of the main rate limiting elements, given the slower OER kinetics [Lei Zhang et al. 2020].

The previous paragraph sums up one of the main advantages of SOEC compared to other electrolysis technologies like PEMWE: the components of the SOEC do not require noble metal-based materials. This is a great drawback PEMWE since it poses a great challenge to reduce the catalyst loading to reduce the overall cost of the system [Hauch et al. 2020]. As an example, if a 1 TW power plant were to be built using fuel cell technology and were it based on PEMWE, 53 months' worth of global platinum production would be needed. However, if it were to be SOEC based, the requirement of zirconia and yttria would be equivalent to 1 month and 21 months of their global annual production, respectively. Moreover, this comparison could be extended to include lithium-based batteries, which would require roughly 50 years' worth of this material production in 2021 [Hauch et al. 2020].

Furthermore, SOEC is not only more efficient in terms of materials' cost, but also in terms of electrical efficiency. Figure 22 shows the cell voltage relative to the current density in AWE, PEMWE and SOEC. This comparison shows that, for the same current density SOEC reports lower overpotential than the other two. This higher efficiency is especially driven by the specific temperature condition under which SOEC occurs, which provides this technology with several thermodynamic advantages [Chatenet et al. 2022].

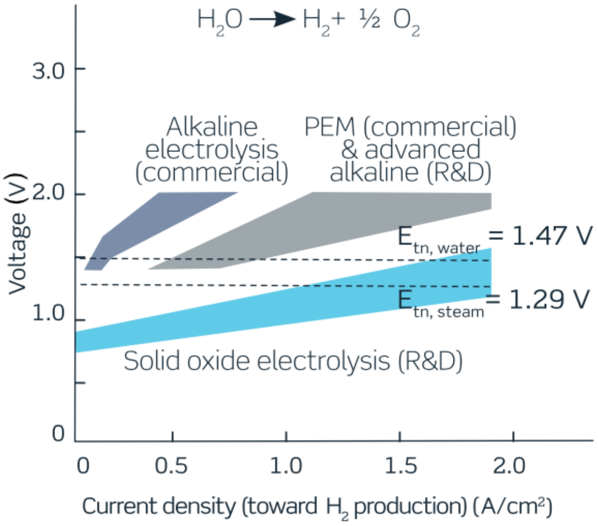

Figure 22. Comparison of performances between AWE, PEM and SOEC [Hauch et al. 2020]

However, this technology is also accompanied with certain drawbacks. SOEC occurs under especially harsh temperature conditions (over 700°C). This causes severe thermal stress to the material, both mechanically and chemically, which can lead to degradation [Sohal et al. 2010]. This degradation is specially aggravated during ramp-up and shut-down processes. Such degradation mechanisms occur specially on the steam electrode and leads to Ni migration. Moreover, the manufacturing impurities of the steam electrode are also a source of degradation, leading to the formation of crystals. These glass phases lead to the inhibition of active sites, which causes a depletion of the catalyst activity. In addition to that, cleaning of inlet gases has become paramount to reduce the potential degradation and the migration of nickel [Sohal et al. 2010]. Thus, a great deal of the research efforts in the field of SOEC are focused on discovering new configurations of materials that provide better stability capabilities and reduce degradation. Along with that, operating at lower temperatures could also be an alternative to improve the performance of this technology, which is a real candidate to provide with mass production of clean hydrogen.

3.3.4. Anion Exchange Membrane Water Electrolysis (AEMWE)

Anion exchange membrane water electrolysis (AEMWE) is the newest development in the field of water electrolysis for the production of hydrogen. This new technique combines aspects of the already existing AWE and PEMWE. Similar to AWE the process in AEMWE occurs in an alkaline medium; however, the configuration of the system mimics that of PEMWE with a membrane-electrodes assembly (MEA) [Hua et al. 2023]. Since this new technique aims to benefit from the advantages of both these technologies, it appears to be the most promising alternative for mass production of green hydrogen supported by intermittent renewable energy sources such as solar and wind energy. However, these are just projections that need to be confirmed by further research that addresses the two main challenges this development of this new technology poses: long-term stability of the materials and high current density operation [Blain 2022].

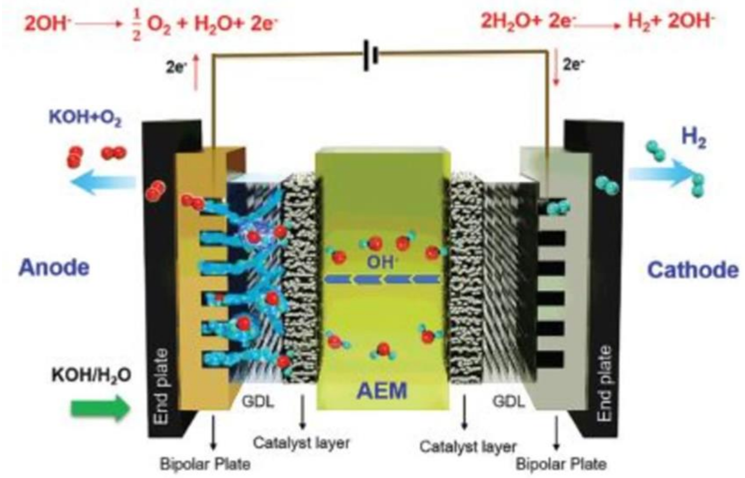

Figure 23. AEM electrolyser schematic [Blain 2022]

The structure of AEM electrolysers is similar to that of PEM electrolysers, in fact, the anion exchange-based devices can be configured by taking a proton exchange-based device and substituting its membrane with a hydroxide exchange membrane. In this case, the composition of water occurs at the cathode where, through the HER, hydrogen molecules are liberated [Lei Zhang et al. 2020]. As a result of this reaction, hydroxide anions are produced and transferred through the membrane to the anode, where the OER takes place. This whole process occurs in an alkali medium just as it develops in AWE [Henkensmeier et al. 2021]. It is worth noting that, given the high pH, i.e., the low presence of protons in the electrolyte, the kinetics of the HER are more sluggish than under acidic conditions, which leads to a higher overpotential corresponding to the activation energy of the reaction at the cathode.

Both electrodes are separated by an AEM which is composed of a polymer backbone together with anchored cationic groups, which provide with anion conductivity and selectivity. Among these backbones, several have already been studied: polysulphone type, polystyrene type, fluorinated type, polyethylene type… [Li and Baek 2021] Regarding the functional groups, these belong generally to nitrogen-based classes such as ammoniums and diammoniums. Moreover, other non-N-based groups have been studied, such as phosphonium and S-based groups, such as sulphonium [Chatenet et al. 2022]. These cationic groups can be integrated with the polymer backbone following different structures. For instance, they can be a part of the main chain, attached to it as a side chain or integrated by forming a hyper-branched polymer.

Compared to the PEM, these hydroxide exchange membranes present lower kinetics, which is associated to the higher molecular weight of the ions involved in the process. The transportation of these ions through the membrane can be explained through the vehicular and Grotthuss mechanisms [Miller et al. 2020]. These two principles refer to the transfer of proton defects through its diffusion along the polymer by the formation and division of covalent bonds with neighboring molecules. This conductivity of the material could be improved by increasing the concentration of functional groups in the polymer which leads to an enhancement of the ion exchange capacity.

Moreover, higher temperature and higher-pressure operation decrease the ohmic resistance of the membrane, as well as an increased hydration of the former. However, it is paramount to consider the relation between conductivity and water uptake. A high water uptake leads as well to higher mechanical stresses, which hinders the long-term stability and performance of the membrane [Mayerhöfer et al. 2022]. Therefore, new research is necessary to find new polymer configurations that are able to provide good ion exchange capacities while maintaining the water uptake as low as possible.

Moving on to the materials for the electrodes, in the case of the cathode these are selected with the main objective of accelerating the slower kinetics of HER in alkali medium. Currently, the best performing catalyst compounds are Pt-based groups, although recent advancements have been made regarding non-noble metal-based compounds. These new compounds are nickel-based, and research has shown promising results for NiMo-based alloys [López-Fernández et al. 2021]. The transition from noble to non-noble based catalyst would lead to a significant capital cost reduction of the AEMWE technology.

Concerning the OER catalyst, AEMWE shows the advantage as well, compared to the acidic conditions of PEMWE, of allowing non-noble based electrocatalysts [Lei Zhang et al. 2020]. Thus, similar to HER catalyst, Pt-based groups can be substituted by other non-noble metals, such as Ni and Co, and also compounds following perovskite’s structure. It is important to note that, during the OER, the adsorbed oxygen modifies the chemical structure of the surface by forming hydroxide structures, which further enhance the electrolysis performance [Hua et al. 2023]. However, this surface reconstruction phenomena can also be problematic for the long-term stability of the catalyst; therefore, it is paramount to further develop the knowledge on the relation between stability and activity of these materials.

Regarding other elements of the device, such as the PTLs and the bipolar plates, AEMWE has also an advantage compared to PEMWE devices since the titanium-based components required in the later can be substituted by steel-based components [Chatenet et al. 2022]. With regards to the electrolyte, if the feed consists of pure water, only the membrane provides anion conducting capacity. KOH solutions can also be added, which improves the conductivity of the system by providing alternative conducting paths [Lei Zhang et al. 2020]. However, this alkali solution is corrosive for the membrane, which can hinder its stability and long-term performance [Miller et al. 2020]. Therefore, the research efforts are focused on further developing systems in which the feed consists only of pure water.

AEMWE clearly shows potential to outperform other electrolysis technologies in terms of cost and performance. The fact that the whole device can be non-noble metal-based projects a future lower capital cost than for the rest of the technologies. However, anion exchange electrolysis is a recently developed technology; therefore, there is still many aspects to be researched to balance its development with the other techniques. For instance, there is still not enough information about long-term stability of the device, which is key to perform a meaningful comparison with the other methods. Moreover, the so-far made research regarding the relation between potential and current density have reached 3,5 Acm^{-2} for a voltage of 2 V, for an operation durability of only 50 hours, which is still far behind the other three technologies [Hua et al. 2023]. Other studies that have undertaken longer operation experiments yielded a 2,1 V voltage for a 1 Acm^{-2} current density for 12000 hours. This performance is still not competitive with other commercialized electrolysis devices; nevertheless, many agree that this technology can be the key for large-scale hydrogen production in the future.

4. Economic Assessment Model

The objective of this chapter is to perform a comprehensive economic analysis that provides a comparative cost overview of the four electrolysis technologies previously assessed in the technical section. For such purpose, the economic assessment is based in three parameters commonly used for the valuation of energy projects: the levelized cost of hydrogen (LCOH), the net present value of the investment (NPV) and the internal rate of return (IRR). These three economic parameters take in consideration the time value of money by the utilization of discount factors. Moreover, a sensitivity analysis, in combination with Monte Carlo simulations, is provided to enhance the insights offered by this study. With this addition light can be shed on the contribution of each of the factors driving the cost of the technology while also accounting for the potential variability of the assumptions and predictions of the selected parameters.

The model developed in this study is applied to all four electrolysis technologies. In order to do so, several modifications are introduced depending on the specific assessed technique. These are introduced and explained later on the analysis. Regarding the specifics of the model, its explanation is divided into four sections. First, the input variables are illustrated. These include the capital expenditures (CAPEX), the operational costs (OPEX), and the water and energy costs. With the aid of coherent assumptions and parameters, these input variables are processed in order to obtain the LCOH, NPV and IRR. Furthermore, the analysis is broadened with the inclusion of a sensitivity analysis that focuses on the impact of each of the contributing factors to the cost of the technology. It is also worth mentioning that the model is applied under several operating conditions. These operating scenarios are also explained later on the study. Figure 24 is a schematic of the structure of the analysis:

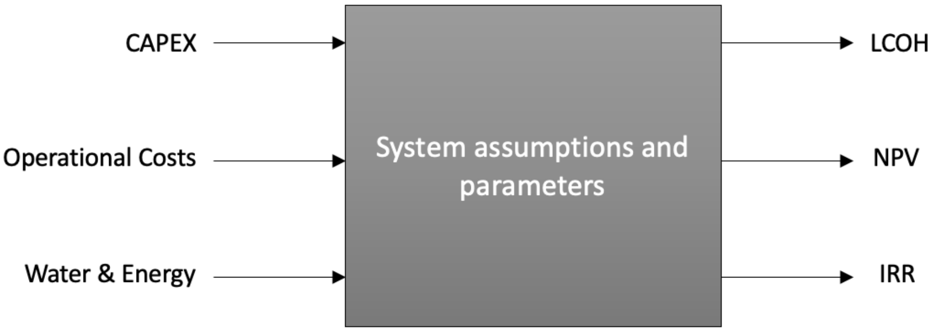

Figure 24. Model schematic

4.1.Input Variables

The input variables are the elements fed into the model, which are determined by the assessed technology and the conditions of the specific scenario under scrutiny. Before moving on to the explanation of each of the input variables it is necessary to first discuss several operating assumptions that are required to determine the size of the electrolysers.

For such purpose, the daily production of system is established to 1 ton of H_2 per day. Moreover, the amortization period of the plant is considered to be 20 years. Furthermore, a utilization factor is also introduced in order to reflect the availability of the energy source that varies depending on the assessed production scenario. These scenarios are: production of green hydrogen supported by a wind farm, production aided by PV generation and production driven by power obtained from the grid. The assigned parameters are selected assuming the construction of the plant in Germany [Destatis - Statistisches Bundesamt 2021].

Moreover, the electricity price also varies depending on the analyzed scenario. Regarding the factor assigned to the grid power scenario, it is worth mentioning that not all the hydrogen generated under this conditions can be considered as green as explained in Chapter 2.4, which discussed the new European regulation on renewable hydrogen. Furthermore, the new European regulation also establishes that for new electrolysis plants that operate independently of the grid, the power plant feeding the electrolyser must be of new construction. Therefore, the prices presented in Table 1 for both the wind and the

PV scenario refer to the levelized cost of the energy, thus, considering the construction of the plant in the analysis. On the other hand, the energy cost in the grid scenario represents an agreed price in the first year of operation, which has to be projected into the future as explained in the following chapters.

		Scenario		
		Wind power	PV power	Grid power
Utilization factor	%	20,9	10,5	80
Energy price	€/MWh	39,4	53	30

Table 1. Assessment scenarios data

4.1.1. Capital Expenditures (CAPEX)

CAPEX refers to the cost of building the plant. For the purpose of this research, this cost category is subdivided into two elements: the cost of the electrolyser and the balance of plant (BOP). The specifics of BOP are out of the scope this study; however, an estimation of its cost is provided in [Bejan et al. 1996].

First, the cost of the electrolyser is calculated by means of the estimation of the size of the plant and the capital cost estimation of the stack obtained in the literature. In addition to these parameters, the lifetime of the stack also plays a main role in the estimation of the capital expenses, since it determines the number of replacements required during the amortization of the project. Moreover, it is also required to provide with the specific energy and water consumption, which are used later on for the calculation of operational costs. All these parameters are obtained from [Taibi et al. 2020] except for the following: H_2 hourly production for AWE [Holst et al. 2021], PEMWE [Holst et al. 2021], AEMWE [Enapter 2023] and SOEC [Hauch et al. 2020]; and capital cost for AEMWE [Enapter 2023]. Table 2 reflects all these values. Regarding the power consumption, a bracket is provided in the literature; however, for the purpose of this research, the lower limit of the presented ranges is employed in the analysis.

Characteristics		***AWE***	***PEMWE***	***AEMWE***	***SOEC***
Stack unit size	[kW]	1000	1000	2,5	5
Power consumption	[kWhAC/kg]	50-78	50-83	57-69	40-50
Current density	[A/cm2]	0,6	2	1.5	1
Active cell area	[m2]	2	0,1	0,03	0,02
Degradation rate	[%/1000h]	0,1	0,2	0,5	0,5
Maximum degradation	[%]	10	10	10	10
Lifetime	[1,000 h]	60	80	5	20
Water demand	[kgH_2O/kgH_2]	18-24	18-24	18-24	18-24
H_2 hourly production	[kgH_2/hour]	20,72	19,6	0,045	0,127
Stack capital cost	[€/kW]	270	400	3300	2000

Table 2. Electrolysers technical specifications

Regarding the estimation of BOP, this is carried out as explained in [Bejan et al. 1996]. BOP refers to all the additional equipment required to complete and operate the plant. These can be divided into two categories depending on its nature: direct costs and indirect costs. The first type of cost refers to those expenses dedicated to elements who become a permanent part of the plant, e.g., piping, electrical equipment, civil infrastructure, etc. On the other hand, indirect costs are destined to elements that will not become permanent within the operation lifetime of the plant but that are still paramount for the completion of its construction, such as engineering, construction and contingency costs.

Thus, the breakdown of BOP cost is presented in Table 3 [Bejan et al. 1996]. However, this method is not applied to all four technologies. This estimation of the BOP costs refers to a generic chemical plant and is based on percentages of the purchased equipment. Therefore, for technologies like SOEC and AEMWE, whose capital cost is still too high, this method overestimates the cost of the plant and yields unrealistic results for those two scenarios. The solution to this problem of the methodology is to calculate the BOP for both AWE and PEMWE, which are technologies with a higher level of maturity. This first step provides a value for the BOP in €/kW of installed power. For AEMWE, the value obtained for AWE is employed, since the logistics of both technologies are very similar. In the case of SOEC, PEMWE's BOP cost plus a factor of 5 % is utilized. PEMWE's BOP cost is higher than that of AWE, and SOEC needs additional insulation to cope with the higher temperatures involved in its operation.

Category	Definition
Direct Costs	DC
Onsite Costs	ONC
Installation	0,20*Cost of Stack
Piping	0,10*Cost of Stack
Instrumentation and Control	0,10*Cost of Stack
Electrical Equipment	0,10*Cost of Stack
Offsite Costs	OFC
Civil and Structural Work	0,25*Cost of Stack
Service Facilities	0,25*Cost of Stack
Indirect Costs	IC
Engineering and Supervision	0,10*DC
Construction Costs	0,15*DC
Contingencies	0,05*(DC + rest of IC)

Table 3. Breakdown of BOP cost

4.1.2. Operational Expenses (OPEX)

OPEX refers to the costs associated with the daily production of the plant. These costs are expressed in monetary units per unit of time, in this case per year. For the purpose of this research OPEX is estimated by means of coherent percentages relative to the number of workers and the BOP for the various cost categories involved. In order to facilitate the comprehension of the elements involved in OPEX these are divided into three main categories [Turton et al. 2012]:

- Direct costs: these are directly related with the production rate of the plant. If the hydrogen production increases, so does the quantity of these direct costs. If for whatever reason the throughput of the plant needs to be reduced, this reduction is also noticeable in the amount of direct costs. However, within this category several cost classes are included, each with a different sensitivity to changes in the production rate. Among these expenditures are the cost of fuel (in this case water), the cost of energy, the cost of labor…

- Fixed costs: these are costs which do not depend on the production rate. This means that the operator of the plant incurs these expenditures regardless the produced amount of hydrogen. Within this category lie costs such as plant overhead expenditures, which include any additional costs that are not contemplated in the design of the plant itself. Moreover, maintenance costs are also included, which are estimated as a percentage of BOP.

- General expenditures: these are expenses which are not directly related to the production rate but can be affected by it if a long period of no production occurs. These costs are related to the management structure, the selling and distribution of the produced hydrogen, and the research and development activities. Moreover, administrative costs are also included in this category. Therefore, these expenses can be thought of as an overhead effort required to carry out the business activities that come with the project.

In [Turton et al. 2012] a range is provided for each of the aforementioned cost categories. In the following Table 4 the percentages employed in the calculation of each of the costs is provided:

Category	Subcategory	Definition
Direct	Operating labour	C_L = h*€/h*N_L
	Water	C_W
	Energy	C_E
	Supervisory labour	0,10*C_L
	Laboratory charges	0,10*C_L
Fixed	Overhead costs	0,50*C_L

	Maintenance	0,02*BOP
General	Distribution & selling	0,02*C_L
	R&D	0,05*C_L
	Administrative	0,15*C_L

Table 4. Breakdown of manufacturing costs

For the calculation of the number of workers, the following equation for [Turton et al. 2012] is retrieved:

$$N_L = (6{,}29 + 31{,}7 * P^2 + 0{,}23 * N_{np})^{0{,}5} \qquad (22)$$

In equation 22 P refers to devices in the plant that process materials with solid particles. For the case of a hydrogen production plant, P is considered to be zero. N_{np} refers to devices dedicated to the processing of non-solid particles. For the purpose of this research, this number is estimated to be 11, estimation underpinned by the schematic of a hydrogen production plant presented in [Taibi et al. 2020]. The elements considered in this assessment are the following: two gas separators, two condensers, one electrolyser stack, two compressors, one rectifier, one dryer, one gas reservoir and one high pressure vessel. Thus, the estimated number of workers for the plant is 2.

Regarding the cost of energy, its specifics have already been discussed in Chapter 4.1, making the difference between the wind and PV scenarios, where the LCOE is employed, and the grid scenario, where a certain cost of energy is projected into the future by means of the methodology explained later on the study. On the other hand, water is assigned a value of 0.0015 €/kg. By means of the water demand provided in Table 2. Electrolysers technical specifications its contribution can be calculated and projected into the future.

4.2.Levelized Cost of Hydrogen (LCOH)

The first economic parameter employed to compare the performance of the assessed technologies is the LCOH. This parameter considers the time value of money, e.g., the variation in the value of money across time. The cost categories considered in this indicator are the CAPEX and the OPEX, which are normalized to express them in the same time frame and, thus, allowing for its combination. The procedure followed for the estimation of both LCOH and later on NPV is extracted from a combination of [Turton et al. 2012] and [Bejan et al. 1996].

First, the investment costs are considered. The investment is made in the first year of the project and its contribution to the normalized cost of the commodity is spread along the duration of the project. This contribution is called amortization or CAPEX, and it is reflected on an annual constant payment equivalent to the necessary quantity to return both the investment and its interest. The time breakdown of the investment cost is explained in Figure 25:

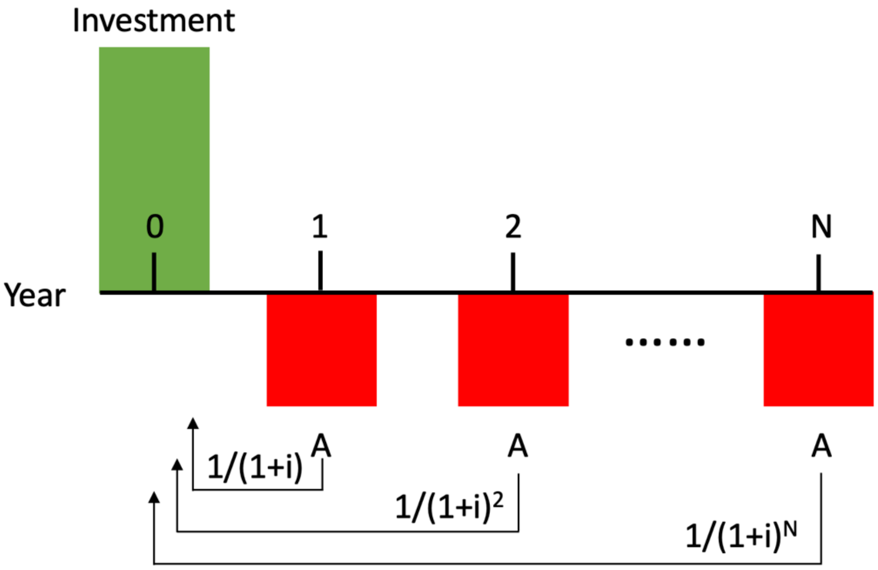

Figure 25. Time breakdown of CAPEX

Therefore, CAPEX is obtained by means of the following equation:

$$Investment = \sum_{j=1}^{N} \frac{A}{(1+i)^j} = A * \frac{(1+i)^N - 1}{i * (1+i)^N} \tag{23}$$

$$A = CAPEX = Investment * \frac{i * (1+i)^N}{(1+i)^N - 1} \tag{24}$$

The parameter i refers to the interest rate required by the investment. For the purpose of energy projects, the index employed is the Weighted Average Capital Cost (WACC), which considers the contribution and the expected return of both debt and equity. In the case of debt, the exemption of taxes is also considered. Thus, WACC can be calculated by means of the following equation:

$$WACC = C_d * \alpha_d * (1 - T) + C_e * (1 - \alpha_d) \tag{25}$$

$$CAPEX = Investment * \frac{WACC * (1 + WACC)^N}{(1 + WACC)^N - 1} = Investment * f_a \tag{26}$$

Regarding the OPEX, these are calculated by performing a similar calculation to CAPEX. OPEX is calculated by estimating the one-time costs in year 0 (fuel, maintenance, manufacturing) and projecting them into the future. This projection takes into account the potential increase in price of these costs with a nominal rate (r_x), which depends on two factors: real factors and inflationary factors. For the purpose of this research, inflationary effects are neglected since their inclusion for long-term projects leads to an overestimation of the costs. Moreover, the costs estimated in year 0 are assumed to be placed in a fund that yields an annual return of i, therefore its future value has to be discounted in order to express it in present units. Thus, for any type x of operating cost in year j, its expression in the year 0 of the project is as follows:

$$C_{x,0j} = C_{x,0} * \left[\frac{1 + r_x}{1 + i}\right]^j = C_{x,0} * k_x^j \tag{27}$$

The costs of every year j must be added and expressed in present units. Therefore, similar to the equation of CAPEX, the summation of all these terms is performed as follows:

$$C_x = C_{x,0} * \sum_{j=1}^{N} k_x^j = C_{x,0} * \frac{k_x * (1 - k_x^N)}{1 - k_x} = C_{x,0} * f_{\Sigma,x} \tag{28}$$

C_x contains the summation of all operational costs incurred throughout the lifespan of the project. Similar to the distribution performed with CAPEX, this C_x is distributed equally for every year of the project by means of the distribution factor f_a already clarified in the explanation of the amortization of the investment. Thus, the contribution of any operation cost “x” to the normalized cost is expressed by the following equation:

$$C_{Nx} = C_{x,0} * f_{\Sigma,x} * f_a \tag{29}$$

For the calculation of LCOH is necessary to express this normalized costs relative to the production of H_2. Therefore, the equation that yields the final LCOH is expressed as follows:

$$LCOH = CAPEX + OPEX = \frac{Investment * f_a}{H_2\ Production} + \frac{C_{x,0} * f_{\Sigma,x} * f_a}{H_2\ Production} \tag{30}$$

Moreover, the economic assessment also requires for the values of WACC and i [Kost et al. 2021], and the selling price of green and non-renewable hydrogen.

Parameter		
WACC	%	7
i	%	2
Price of green hydrogen	€/kg	6
Price of non-renewable hydrogen	€/kg	3

Table 5. Economic parameters of the analysis

4.3.Net Present Value (NPV)

Net present value is a well-extended method employed to determine whether a certain project is profitable. It consists of discounting the future cashflows generated by the project to express them in present units and compare them with the required investment. If NPV is positive, the project is profitable; otherwise, the project will generate losses in the future, and it should not be carried out at the required WACC. In order to calculate the project's cashflows it is necessary to know at which price the product can be sold. In this case, a price for hydrogen in year 0 (P_0) can be set and then projected into the future by mean of a rate, similar to what has already been explained in the normalized cost section. Moreover, this income can be normalized employing the same distribution factor presented in the LCOH chapter.

$$Price_N = P_0 * f_{\Sigma,I} * f_a \tag{31}$$

$$Income_N = Price_N * Production \tag{32}$$

Thus, NPV is defined as the difference between the normalized income and the normalized costs, but without considering the amortization factor.

$$NPV = \frac{Income_N - Cost_N}{f_a} = (Price_N - LCOH) * \frac{Production}{f_a} \tag{33}$$

The meaning of NPV is determined by its sign. If NPV equals 0, that means the project will generate enough cashflow to fulfill the return requirements of both lenders and shareholders. If NPV is positive, the project will provide with additional profits which can be then utilized for further investments. And last, if NPV is lower than 0, shareholders, or lenders, or both, will incur in losses if they decide to carry out the project.

4.4.Internal Rate of Return (IRR)

The IRR is a relative indicator that sheds light on the profitability of the project. In contrast with NPV, which is dependent on the magnitude of the project, IRR yields a percentage that allows for the comparison of different sized plants. IRR is the WACC that results in a NPV of zero, meaning the maximum profitability that could be potentially required by the stakeholders. Its calculation is derived from equation (33) by equaling NPV to zero and solving the interest rate. Thus, expressed in terms of prices and cost in year 0, IRR results from solving equation (34):

$$P_0 * Production * f_\Sigma - Costs_0 * f_\Sigma = Investment \tag{34}$$

4.5.Sensitivity Analysis and Monte Carlo Simulations

In addition to the calculation of LCOH and NPV this study includes a sensitivity and variability analysis. These two additional assessments are key to understand the key factors that drive the cost of this technology. Moreover, for projects like green hydrogen production, which are not yet applied in a significant large-scale, it is paramount to account for this unpredictability by including the potential variability of the input parameters.

Regarding the sensitivity analysis, this is dedicated to determining which of the input variables contribute the most to the final cost of the produced hydrogen. This achieved by introducing variations to the base case, changing a single variable each time while maintaining the other unchanged. This variation consists of a ±15% variation in the input value of the assessed variable, which sheds light on the specific impact of the analyzed parameter.

On the other hand, Monte Carlo simulations are included to provide with broader insight on the potential future cost of the technology. Predictions [Clean Hydrogen JU 2020] have been made on the expected performance of the various technologies in 2030, as presented in Table 6. Estimations of electrolysers performances by 2030. However, this predictions might not be fulfilled; therefore, it is paramount to account for this uncertainty.

Technology		**AWE**	**PEMWE**	**SOEC**	**AEMWE**
Capital cost	€/kW	270	400	520	300
Energy consumption	kWh/kg	48	48	37	48
Degradation	%/1000h	0,1	0,12	0,5	0,5

Table 6. Estimations of electrolysers performances by 2030

Each of the contributing factors is assigned a certain justified variation, which is used to generate 1500 random cases. Then, the same calculations performed for the obtention of LCOH, NPV and IRR are carried out, but this time considering the variation of the input variables. Thus, the obtained economic parameters show a statistical deviation as well which is the result of the variation of the input parameters' value. Thus, the 1500 size sample is plotted to show the statistical distribution of LCOH under all the assessed operating scenarios. Below presented is Table 7. Variation of input variables for Monte Carlo simulations with the assigned deviation to each of the input variables, with the corresponding justification, that yield the randomized sample.

Input Variable	**Assigned variation**	**Justification**
Capital cost	30%	High uncertainty of the estimations
BOP	10%	Additional elements costs are not expected to have a great variation
Manufacturing costs	5%	Very small variation expected
Cost of energy	30%	Depends on both the energy consumption and its price. High uncertainty
Cost of water	5%	Very small variation expected

Table 7. Variation of input variables for Monte Carlo simulations

5. Results Presentation

This section is dedicated to the presentation of the obtained results. First, the results corresponding to the current performance of the four technologies is presented. Beyond the presentation of the economic indicators, a breakdown of LCOH is provided so as to analyze the main factors driving the cost of the technology. Then, the sensitivity analysis is presented to set the basis of the comparison of the cost reduction potential of each of the variables involved.

Second, the section focuses on the presentation of the results for the analysis of the performance of the technology in 2030 based on the provided estimations. In addition to the economic parameters, this section includes the results of the Monte Carlo simulations so as to provide with a range that considers the uncertainty of such predictions.

5.1. Current State of the Technology

First, the current performance of the technology is assessed, so as to analyze the viability of the today available devices for the deployment of a green hydrogen production plant. It is worth referring to some of the assumptions involved in the calculation of the following economic parameters: Table 1 gathers the information relative to the price of the energy and the utilization factor of each of the scenarios; Table 2 contains all the technical specifications of the assessed devices; and Table 5 outlines the economic parameters and the selling price of the produced hydrogen. The results are presented in Table 8:

		Power Scenario		
Indicator	**Technology**	**Wind**	**PV**	**Grid**
LCOH (€/kg)	AWE	4,35	6,87	3,29
	PEMWE	5,51	8,93	3,45
	SOEC	11,70	13,66	10,85
	AEMWE	79,93	81,60	74,98

NPV (million €)	AWE	10,693	0,930	6,549
	PEMWE	6,201	-6,997	5,938
	SOEC	-17,720	-25,293	-22,679
	AEMWE	-281,561	-288,004	-270,678
IRR (%)	AWE	21,57	6,04	24,93
	PEMWE	12,14	0,6	21,65
	SOEC	-0,57	-3,49	-3,49
	AEMWE	-16,24	-18,46	-18,88

Table 8. Economic indicators for the current state of the technology

Table 8 serves as the starting point of the analysis. Based on this initial results, the assessed technologies can be divided into two groups. On the one hand, AWE and PEMWE have demonstrated to be profitable under most of the operating scenarios and conditions. Among these, the PV scenario is the one under which the profits are the lowest, due to lower availability of such resource in the assessed region, which could be solved by combining this power source with other alternative back up energy sources. Between the two, AWE is the one that appears to be more robust in its profitability, while PEMWE struggles to provide with benefits under the PV scenario. On the other hand, SOEC and AEMWE reveal themselves to be unready to be employed in a project of this characteristics. Neither of the technologies is able to reach profitability under any of the considered scenarios, which means the rollout of this project based on any of these two technologies is not to be carried out yet. However, it is evidenced by the results that SOEC is closer to profitability than AEMWE, whose LCOH is still around 20 times higher than a competitive hydrogen cost.

Having established the conditions and scenarios that divide the technologies into profitable and non-profitable, it is paramount to analyze the structure of the LCOH, so as to analyze which are the main driving factors of the cost of the technology.

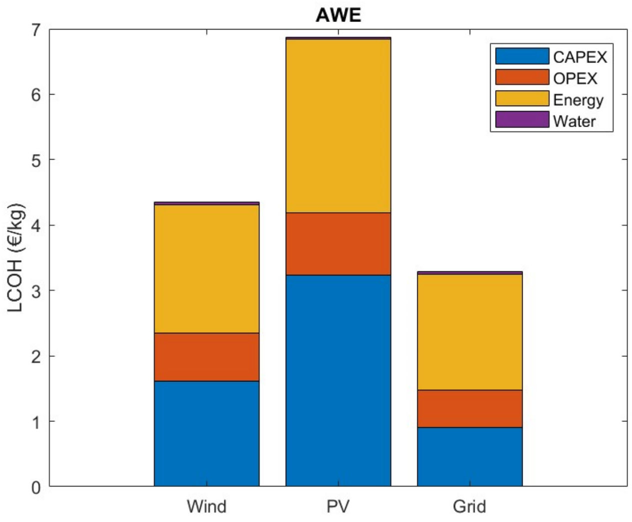

Figure 26. AWE breakdown of LCOH

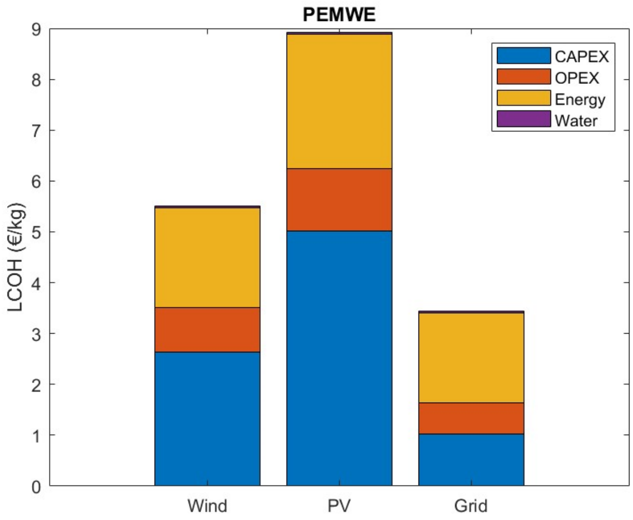

Figure 27. PEMWE breakdown of LCOH

In Figure 26 and Figure 27 the breakdown of AWE and PEMWE LCOH is presented, respectively. The distribution of the different categories of costs is very similar for both technologies. CAPEX is the main driver of the cost; however, for the scenario in which the plant is powered by the grid this cost is significantly reduced. This is caused by the higher utilization factor of this scenario which translates into a smaller plant for the production of the same amount of hydrogen. Alongside with CAPEX, energy is the other main driver of the cost. This shows the importance of improving the efficiency of the technology in terms of energy consumption to further enhance the cost of the produced hydrogen. However, the contribution of energy to the final cost also depends on the price of the consumed energy, and improvements in that area are independent of the subject of this study. Regarding the other two cost categories, water consumption is negligible and OPEX is in the order of one third the amount of the main cost driver. Therefore, the efforts in these two cases should be focused in improving the capital cost and reducing the energy consumption of the cells.

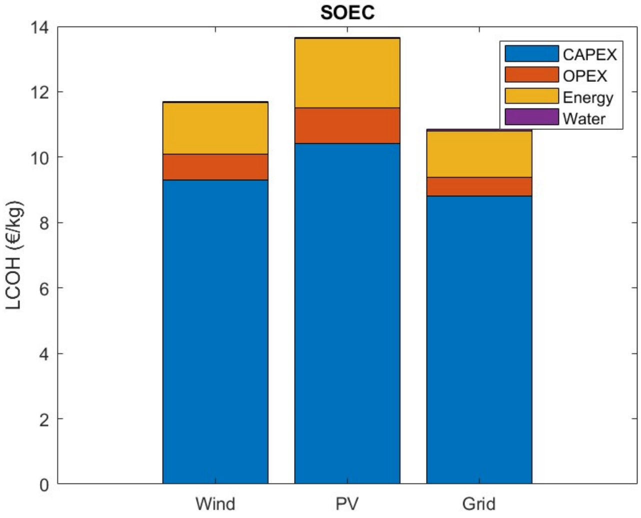

Figure 28. SOEC breakdown of LCOH

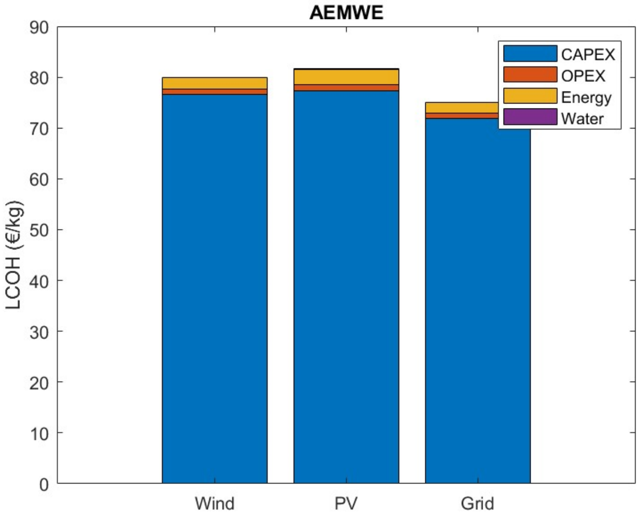

Figure 29. AEMWE breakdown of LCOH

Figure 28 and Figure 29 are the evidence of the different cost structure characterizing the profitable and the non-profitable technologies. In the breakdown of both SOEC and AEMWE a strong dependence on CAPEX can be observed, which is a sign of lack of maturity of the technology. Although SOEC shows a closer cost structure to that of the first two technologies, it is still far from achieving the same cost performance in terms of investment. These two graphs justify the need of further researching these techniques before considering their deployment as large-scale hydrogen production alternatives.

Once the cost structure of the LCOH for the different technologies has been explained, a sensitivity analysis is carried out in order to further broaden the comprehension of the potential cost reduction the improvement of each of the factors could yield. Also, the worsening of each of the factors is analyzed. This analysis is developed under the wind scenario conditions and considers the cost categories gathered in the following Table 9:

		LCOH (€/kg); Variation (%)			
	Variation	**AWE**	**PEMWE**	**SOEC**	**AEMWE**
Utilization factor	+15%	4,17;(-4,1%)	4,97;(-9,8%)	13,99;(+19,6%)	78,12;(-2,3%)
	-15%	4,72;(+8,5%)	5,79;(+5,1%)	13,34;(+14,1%)	82,38;(+3,1%)
Capital cost of the stack	+15%	4,62;(+6,2%)	5,96;(+8,2%)	12,87;(+10%)	91,28;(+14,2%)
	-15%	4,07;(-6,4%)	5,06;(-8,2%)	10,44;(-10,8%)	68,59;(-14,2%)
Energy consumption	+15%	4,65;(+6,9%)	5,81;(+5,4%)	11,89;(+1,6%)	80,27;(+0,4%)
	-15%	4,06;(-6,7%)	5,22;(-5,3%)	11,42;(-2,4%)	79,60;(-0,4%)
Price of energy	+15%	4,65;(+6,9%)	5,81;(+5,4%)	11,89;(+1,6%)	80,27;(+0,4%)
	-15%	4,06;(-6,7%)	5,22;(-5,3%)	11,42;(-2,4%)	79,60;(-0,4%)
OPEX	+15%	4,46;(+2,5%)	5,64;(+2,36%)	11,77;(+0,6%)	80,08;(+0,2%)
	-15%	4,24;(-2,5%)	5,38;(-2,36%)	11,54;(-1,4%)	79,78;(-0,2%)

Table 9. Sensitivity analysis for the wind scenario

Table 9 shows where the cost reduction potential lies. For the already profitable technologies, namely AWE und PEMWE, both the reduction of the energy cost or the capital cost yields a reduction of the LCOH. However, the impact of the reduction of the OPEX is not as significant. On the other hand, the non-profitable technologies are only affected by reduction in the capital cost. As mentioned before, these are technologies that are not yet ready for a large-scale deployment; therefore, the cost reduction efforts must be dedicated to the reduction of its manufacturing costs.

Regarding the impact of the utilization factor, additional comments are required to understand the obtained results. This factor, which represents the availability of the energy resources that power the electrolysis, directly impacts the size of the plant and the number of stack replacements needed in the lifetime of the plant. Since the amortization period is fixed to 20 years, it can happen that at the end of the amortization period there are still stacks that have not been fully used, thus, incrementing the contribution of CAPEX to the LCOH without completely harnessing all the potential of the technology. This is the case of the improvement of the utilization factor under the SOEC scenario. In this example, the size of the plant is reduced; however, the stacks will have to be replaced an additional time. At the end of the amortization period, the last set of stacks will not be fully harnessed, which leads to the unexpected increase of the LCOH.

This chapter provides a comprehensive analysis of the cost of the hydrogen produced by the four assessed alternatives, considering its structure and the cost reduction potential depending on the contributing factors.

5.2. 2030 Estimations and Monte Carlo Simulations

The second section of the results discussion is focused on the analysis of the future cost of the technology based on the estimations of their future technical specifications. Improvements in the technology itself, combined with a reduction in its manufacturing due to economies of scale, will deliver a cost reduction that can further improve the competitiveness of the production of green hydrogen. These estimates are presented in Table 6. Estimations of electrolysers performances by 2030.

First, the same economic indicators are calculated, similar to the methodology followed for the base case. These are shown in Table 10, Table 11 and Table 12.

		Power Scenario		
Indicator	**Technology**	**Wind**	**PV**	**Grid**
LCOH (€/kg)	AWE	4,27 (-1,8%)	6,77 (-1,5%)	2,89 (-12,1%)
	PEMWE	5,08 (-7,8%)	8,33 (-6,7%)	3,13 (-9,3%)
	SOEC	5,26 (-55,1%)	7,08 (-48,2%)	3,39 (-68,8%)
	AEMWE	6,98 (-91,3%)	8,78 (-89,2%)	5,98 (-92,1%)

Table 10. LCOH for 2030 estimations

Regarding the LCOH it can be observed that the technologies that were not profitable under the current conditions are the ones that experience the greater reduction in their cost. Regarding AWE, it is not expected that the cost of the technology will significantly be reduced in the next five years.

		Power Scenario		
Indicator	**Technology**	**Wind**	**PV**	**Grid**
NPV (million €)	AWE	10,998	1,339	8,077
	PEMWE	7,859	-4,706	7,144
	SOEC	7,199	0,125	6,161
	AEMWE	0,515	-6,418	-3,864

Table 11. NPV for 2030 estimations

With regards to the NPV of the project, it can be observed that for the selected WACC of 7% almost all the operating scenarios yield positive returns. The results obtained under the PV conditions show the importance of combining the electrolysis technology with an adequate power source that provides greater utilization factors.

		Power Scenario		
Indicator	**Technology**	**Wind**	**PV**	**Grid**
IRR (%)	AWE	22,08	6,52	38,19
	PEMWE	13,81	2,53	24,27
	SOEC	12,28	6,08	16,71
	AEMWE	6,40	1,68	3,43

Table 12. IRR for 2030 estimations

The last of the indicators is the IRR. While with the current available technology it is unfeasible to profit from the deployment of SOEC and AEMWE, by the end of this decade both of these two alternatives will provide profitability under all the operating scenarios.

All in all, it is worth discussing the results obtained under the grid operating conditions. In this scenario a utilization factor of 0,8 is assumed, which implies a higher availability of the energy sources and, therefore, a better utilization of the electrolyser. Thus, if the utilization factor of both the PV and the wind resources were to be incremented, the overall performance of the technology under these scenarios could be significantly improved. This could be achieved mainly by a strategic selection of the location in which the plant will be installed, i.e., is gifted with strong and stable winds or is located in a region where the sun availability is high. Furthermore, it could be studied the combination of both these power sources, and how its coordination could help enhance the overall utilization factor of the plant.

The same analysis of the cost structure of each of the technologies is made for the 2030 estimates. These are shown in the following Figure 30, Figure 31, Figure 32 and Figure 33.

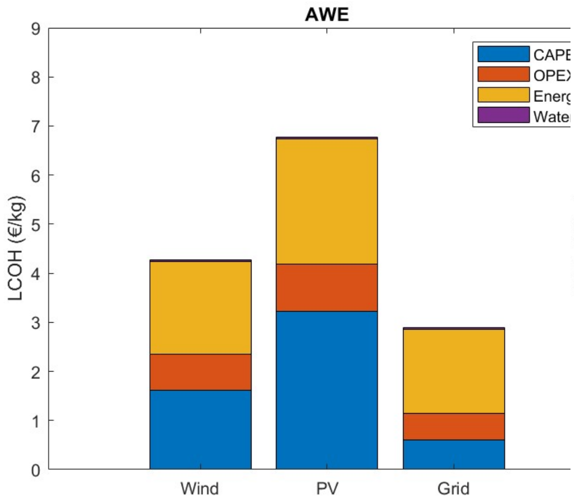

Figure 30. LCOH of AWE in 2030

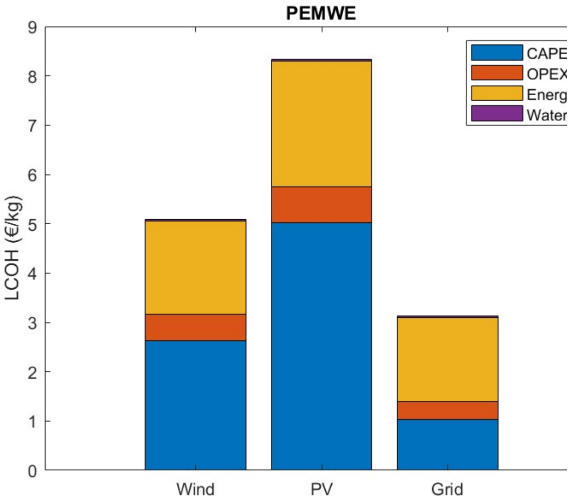

Figure 31. LCOH of PEMWE in 2030

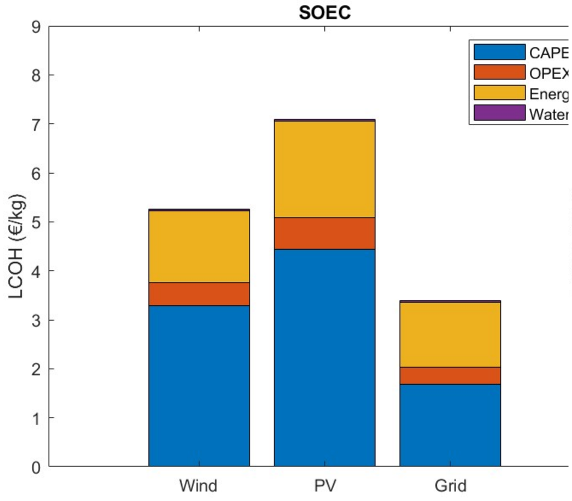

Figure 32. LCOH of SOEC in 2030

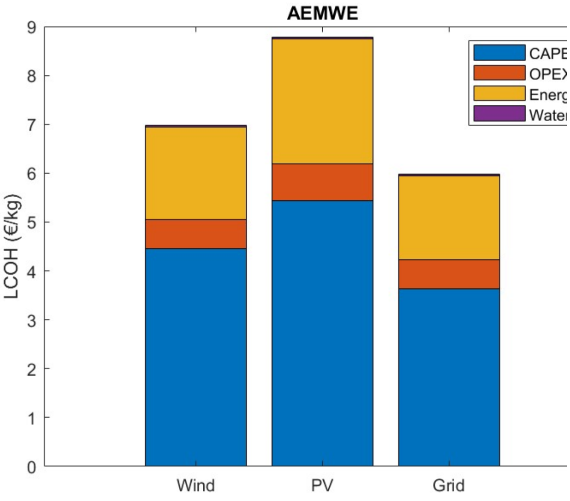

Figure 33. LCOH of AEMWE in 2030

In contrast to the results obtained for the base case, which showed two different types of technologies depending on the relative weight of CAPEX in the final cost, in this case all four technologies present a very similar structure. By 2030, it is expected that the production costs of SOEC and AEMWE cells will drop to levels that allow them to be competitive with the other two alternatives. However, CAPEX relative weight on AEMWE is still high compared to the other three alternatives and further research will be required to further enhance the performance of this technique.

As it has previouly been mentioned, these results are derived from predictions whose accuracy could be biased by optimism. Thus, this research includes an analysis of this potential variability of the future calculated cost of the produced hydrogen. This is achieved by means of Monte Carlo simulations, supported by the assigned variabilities of the contributing factor as shown in Table 7. Variation of input variables for Monte Carlo simulations

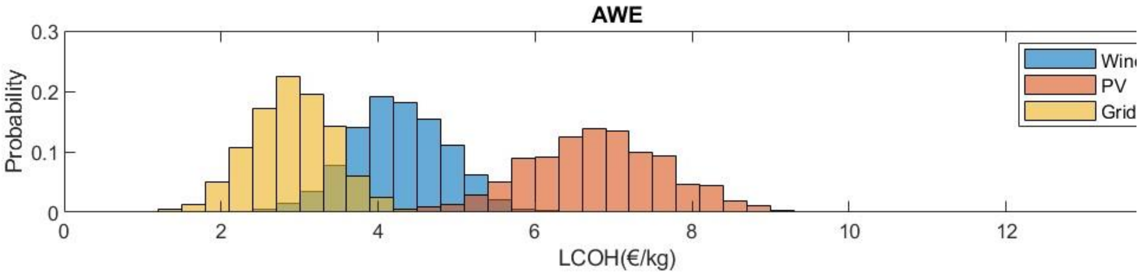

Figure 34. Results of MC simulations for AWE

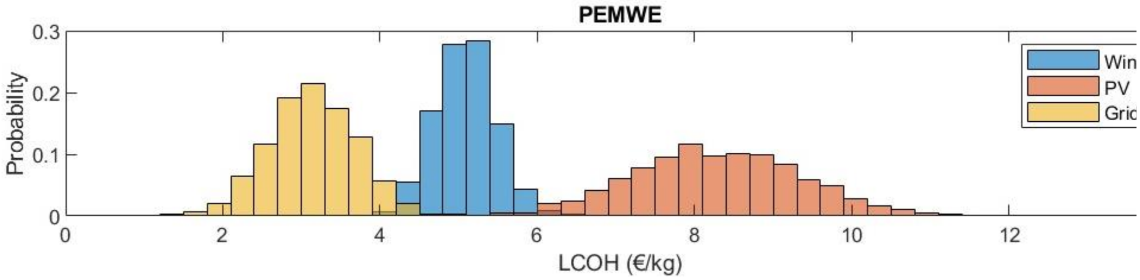

Figure 35. Results of MC simulations for PEMWE

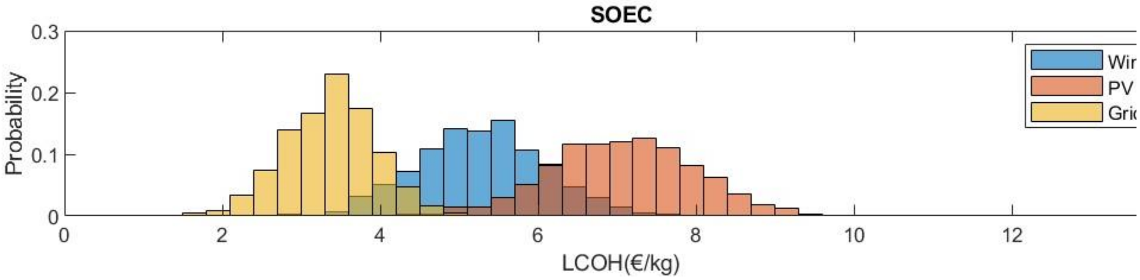

Figure 36. Results of MC simulations for SOEC

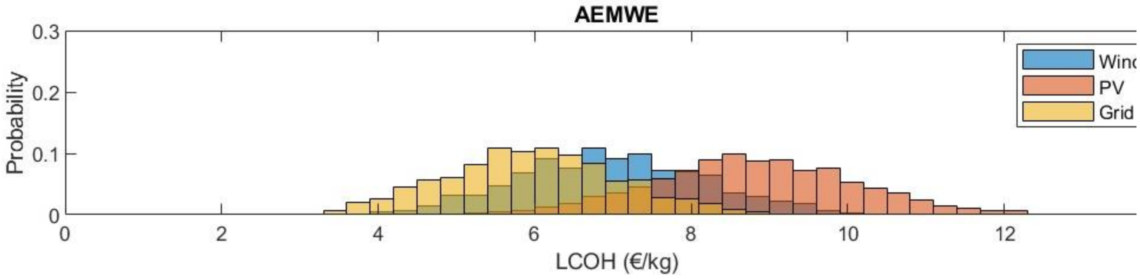

Figure 37. Results of MC simulations for AEMWE

Figure 34, Figure 35, Figure 36 and Figure 37 show the distribution of the results obtained in the Monte Carlo simulations of the different assessed scenarios. Moreover, the following Table 13 gathers the average and the standard deviation in €/kg of the LCOH distributions above presented.

	Power Scenario					
	Wind		PV		Grid	
	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Std. Dev.
AWE	4,25	0,63	6,76	0,87	2,90	0,53
PEMWE	5,10	0,38	8,34	1,05	3,14	0,54
SOEC	5,24	0,80	7,11	0,89	3,40	0,56
AEMWE	6,96	1,20	8,79	1,27	6,03	1,11

Table 13. Statistical indicators of the LCOH distributions

The results of the Monte Carlo simulations shed light on the potential variability of the cost of the technology in 2030. As mentioned before, these estimations might or might not be fulfilled, thus, the expected cost of the technology can be different as forecasted. This analysis is paramount in order to assess the risk of the investment decision. This risk is represented by the standard deviation of the LCOH: the higher the value of this indicator, the higher the uncertainty associated with the technology under the specific operating conditions.

AEMWE is the technology showing the greater uncertainty of the four technologies. Moreover, it is the one with the greater overlapping of the results for the three different operating scenarios. This is evidence of the higher dependence on the capital cost of stack over the utilization factor of the power sources employed, which suggests that in 2030 it could still be too soon to invest on a large scale AEMWE hydrogen production plant. On the other hand, the other technologies show a more robust behavior in terms of cost uncertainty. For the high utilization factor scenario, the standard deviation is around 50 cents per kg of hydrogen, which results in a very competitive range of costs for AWE, PEMWE and SOEC.

6. Conclusions and Future Work

Similar to the structure of this study, the conclusions section is divided into two parts. First, conclusions regarding the technical assessment are drawn, in order to shed light on the advantages and disadvantages of the different alternatives, and the main challenges of the technology. Second, the conclusions derived from the results provided in Chapter 4 are presented to summarize the main findings regarding the current and future economic feasibility of the four assessed techniques. Moreover, the methodology employed for the economic analysis is also analyzed, and suggestions to its enhancement are presented as well.

The technical research developed in this study provides a thorough a comprehensive understanding of the hydrogen sector and the electrolysis technology. Hydrogen produced by means of renewable energy will play a main role in the future energy sector, especially for its potential application in energy storage. Amongst the alternatives to carry out this electrochemical decomposition of water, four standout: alkaline water electrolysis, proton exchange membrane water electrolysis, solid oxide electrolysis cell and anion exchange membrane water electrolysis.

AWE and PEMWE are the more mature technologies, however, they present two main drawbacks that complicate their large-scale deployment. On the one hand, AWE is difficult to operate under fast changing conditions, which are typical of renewable energy sources, such as solar and wind energy. On the other, the main disadvantage of PEMWE is the materials required for the electrodes of the cell. These belong to the noble metal group, which hinders the further reduction of its capital cost.

SOEC and AEMWE are technologies that do not reach the same level of maturity compared to the previous two. However, in the long term, by harnessing economies of scale, their price will be competitive with the other two alternatives. Moreover, they present advantages compared to AWE and PEMWE: they are fit for fast changing conditions, and they do not employ noble metals. However, the current devices still struggle with one main issue, which is the degradation of its materials. How to solve these problems and to combine the different alternatives is the main challenge this sector will face.

Regarding the economic analysis, the results provided allow for the following conclusions. First, the decision of building an electrolysis plant today in Germany, in agreement with the new European regulation on renewable hydrogen, should be limited to selection of either AWE or PEMWE. As demonstrated in the analysis, the current state of the SOEC and AEMWE technologies do not allow for their immediate deployment, since the project would incur in losses. However, based on the analysis of the predictions for 2030, this could change thanks to the higher production of such technologies and the harnessing of economies of scale. It is also worth mentioning that AEMWE will still be the riskier choice amongst the four alternatives.

With regards to the methodology employed in this study several comments must be added. First, the results are location dependent, meaning they could be further improved by choosing locations with better characteristics than Germany for the installation of renewable energy plants. Moreover, the results also depend on the amortization period. In this case, it was 20 years, however, this might not be optimal for certain cases in which the electrolysis cells have not been fully used by the end of the period. Also, the amortization period for the BOP could also be considered to be higher, further enhancing the performance of the technology.

All in all, this study shows the potential of this technology to become a key player in the future of the energy sector, while providing insights on the main challenges it will face during its path towards robust profitability.

Appendix A: Contribution to SDGs

As explained in the first section of this study, governments all around the globe have pledged to reduce their emissions as a result of the signing of the Paris Agreement. Furthermore, this agreement was expanded by the addition of commitments regarding other areas of the social activity. These are the Sustainable Development Goals (SDGs).

With regards to green hydrogen, this compound could play a main role in the achievement of several of these goals. The SDGs that could positively be affected by the deployment of a wide hydrogen economy are SDG 7 (Affordable and Clean Energy), SDG 9 (Industry, Innovation, and Infrastructure), and SDG 13 (Climate Action) [United Nations 2015b]. Green hydrogen can provide affordable and clean energy to remote areas and support the development of sustainable infrastructure. Hydrogen can also support the transition to a circular economy by enabling the use of renewable energy to produce green hydrogen, which can be stored and transported to areas with high energy demand.

As demonstrated in the results section, the price of hydrogen is expected to decrease by the end of this decade, becoming then a competitive commodity. Moreover, the development of this technology is also expected to continue its improvement beyond 2030 by harnessing economies of scale and employing new and cheaper materials. Also, the results showed the increased potential this technology can have by combining different sources of power and various electrolysis techniques. This coordination of different production possibilities could enhance the flexibility of the technology and achieve a greater cost reduction.

SDG 7, SDG9 and SDG13 could be deeply benefited from a cheap and clean hydrogen obtained through water electrolysis. The large-scale roll out of green hydrogen could mean the solution of the main issue society is facing in its quest to sustainability: the lack of large-scale energy storage capabilities.

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