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**Techno-economic analysis on the
case study for hydrogen mobility of
German fuel cell electric buses**

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Abstract

The energy transition has already begun and it is essential that all possible ecological paths must be followed, in order to make our planet more sustainable and achieve the different targets set.

In this dissertation is carried out a techno-economic analysis on the case study for hydrogen mobility of German fuel cell electric buses. The German context has been taken as example, due to an already established know-how on hydrogen power supply for people transport. A global fleet of 47 buses has been selected, for the cities of Cologne and Wuppertal in the North Rhine-Westphalia.

In this analysis all the capital expenditures, operation and maintenance costs have been assessed, concerning the overall systems, in order to get a final price of hydrogen in terms of levelized cost of hydrogen (LCOH). The idea is to produce the sustainable gas on-site, by means of an electrolyser that can be an alkaline, a proton exchange membrane (PEMEC) or a solid oxide (SOEC) water electrolysis machine. Furthermore, in order to clearly understand the techno-economic input parameters for these electrolysers, a review and some new development trends have been presented, for all the three machines.

Unlike some works already present in the literature, this thesis has two main purposes. The first one is to carry out a techno-economic analysis of the current state of the technologies (2020). The next goal is to propose a further future temporal scenario, in particular 2030, in which the impact of the expected technological development could have on the final sale price of hydrogen to the consumer is assessed. Therefore a comparison is made between different technologies and in different time periods in which they operate, verifying if perhaps a technology that is expensive today may not be in the future.

For the 2020 context, the LCOH obtained is equal to 12.56 €/kg, 13.16 €/kg, 15.09 €/kg, for alkaline, PEMEC and SOEC, respectively. Instead, for the 2030 context, the LCOH calculated is equal to 10.45 €/kg, 10.90 €/kg, 9.40 €/kg, for alkaline, PEMEC and SOEC, respectively. For both the scenarios, the results have been obtained considering an average German electricity price of 160 €/MWh. In order to become competitive or even completely replace traditional diesel fuel, the electricity price must be reduced. Therefore, to verify when and if the hydrogen for mobility purpose can be identified as an alternative and sustainable fuel, a sensitivity analysis on the electricity price has been carried out.

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List of acronyms

AE	Alkaline Electrolyser
AEC	Alkaline Electrolyte Cell
AEM	Anion Exchange Membrane
AWEC	Alkaline Water Electrolyte Cell
BEV	Battery Electric Vehicle
BoP	Balance of Plant
CAPEX	CApital EXpenditure
CF	Capacity Factor
CHIC	Clean Hydrogen in European Cities
CTE	Coefficient of Thermal Expansion
FC	Fuel Cell
FCEB	Fuel Cell Electric Bus
FCEV	Fuel Cell Electric Vehicle
FCH JU	The Fuel Cells and Hydrogen Joint Undertaking
GHG	Green House Gases
GrInHy	Green Industrial Hydrogen
HRS	Hydrogen Refuelling Station
HT O-SOEC	High Temperature Oxygen-Solid Oxide Electrolyte Cell
IEA	International Energy Agency
IPCC	Intergovernmental Panel on Climate Change
IT SOEC	Intermediate Temperature Solid Oxide Electrolyte Cell
JIVE	Joint Initiative for Hydrogen Vehicle across Europe
JRC	Joint Research Centre
LCOH	Levelized Cost Of Hydrogen
LHV	Lower Heating Value
MEA	Membrane Electrode Assembly
OPEX	OPerating Expense
PEM	Proton Exchange Membrane
PEMEC	Proton Exchange Membrane Electrolyte Cell

PTFE	Polytetrafluoroethylene
PtG	Power-to-Gas
P2P	Power-to-Power
RES	Renewable Energy Sources
RVK	Regionalverkehr Köln GmbH
SMR	Steam Methane Reforming
SOE	Solid Oxide Electrolyser
SOEC	Solid Oxide Electrolyte Cell
SOFC	Solid Oxide Fuel Cell
SRU	Single Repeated Unit
TRL	Technology Readiness Level
TSO	Transmission System Operator
WACC	Weighted Average Cost of Capital
WE	Water Electrolysis

1. Introduction

Starting from the Industrial Revolution of the 18th century, mankind has burned massive amounts of fossil fuels and emitted greenhouse gases (GHGs), which have caused enormous environmental problems, such as global warming, ozone layer depletion, and ecosystem destruction.

The IPCC (Intergovernmental Panel on Climate Change) recommended that net GHG emissions should reach zero by 2050 to achieve a goal that suppresses the temperature increase of the ambient air to be below 1.5 °C [1]. Therefore, the energy transition towards low-carbon technologies has become a key political objective for the European Union, which has defined a strategy to progressively decrease CO₂ equivalent content throughout all relevant power generation and distribution, industrial, transport and buildings sectors [2].

Thus, the crucial point is how to achieve this final goal. Renewable energies have had an incredible development in the last decades.

However, a massive penetration of Renewable Energy Sources (RES) can affect adversely to the grid stability due to its variability and unpredictability that can lead to an imbalance between supply and demand. Therefore, various methods of converting energy into different forms have been studied, and several major electrical energy storage, starting from the most widespread method as pumped hydroelectric storage, flywheel, battery and compressed air storage, have been proposed [3]. Nevertheless a final solution has not yet been found as each of these technologies have advantages and drawbacks.

In this context, hydrogen could play an important role as it has significant potential benefits to enable this transition to low-carbon energy systems, but not only.

Hydrogen, in fact, is considered as the ultimate cleaner-energy carrier as it has no CO₂ emissions when burned, but above all, it is very versatile and it could be used in several number of industrial applications. First of all as feedstock in the ammonia industries, but also for refineries and fuel transportation sector, as shown in the Figure 1 [4].

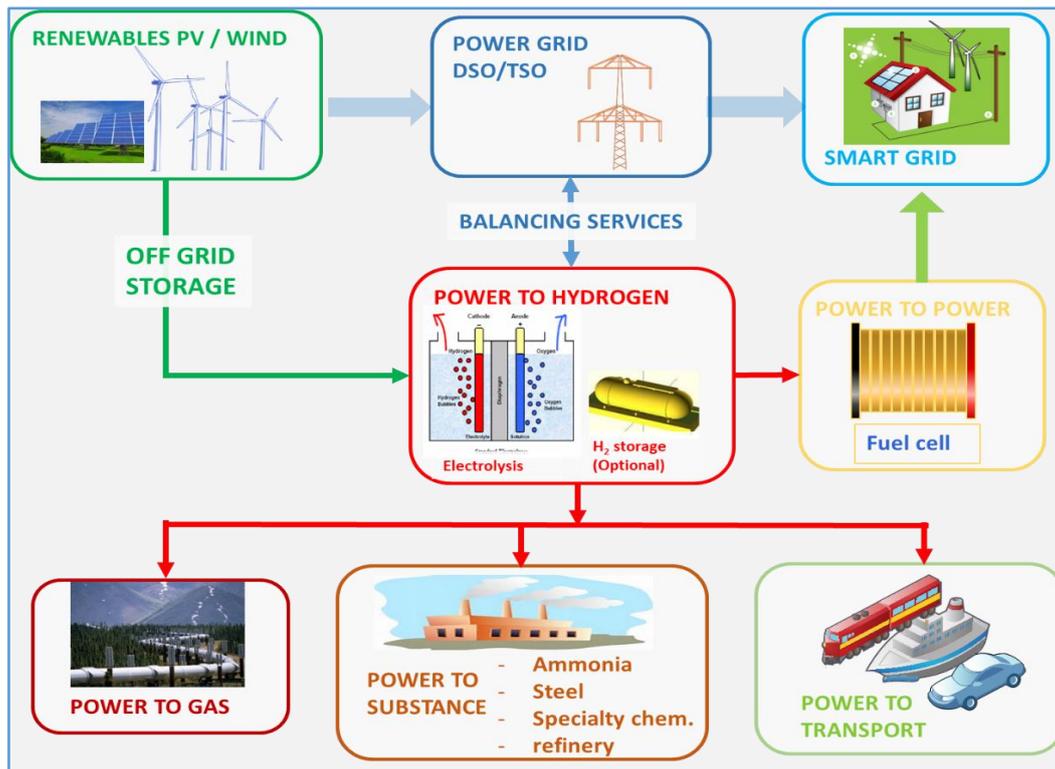


Figure 1. Electrolyser system grid integration [4]

The hydrogen production can take place in several ways, but is still largely based on steam reforming of natural gas for the 85%, obtaining the so called “grey hydrogen”. Such a type of production cannot be classified “renewable”, as it is linked to a fossil fuel feedstock. A further possibility could be the “blue H₂“ production, always by means of the reforming of natural gas, but with total carbon capture of the carbon dioxide, even if the latter technology is yet at low readiness level.

Therefore, the idea is to move towards a more sustainable process, producing H₂ from surplus of the RES to get the “green hydrogen”, even if the estimated price of about $5.0 \div 10.0 \frac{\text{€}}{\text{kg}}$ is too high to reach the parity with the grey hydrogen, that is $1.5 \frac{\text{€}}{\text{kg}}$. This is due to the need of a large buffer of storage to temporarily store the excess of energy from renewables, that at present is too much expensive [5].

In this scenario long term electrochemical energy storage in terms of water electrolysis has been receiving new industrial attention as a possible relevant player in the emerging sustainable energy storage field. This is due to the fact that electrolyzers can operate when electricity generation is available at very low prices or when there is an excess of demand due to the introduction of renewable energy sources. Therefore, the Power-to-Gas concept, that is, the ability to produce a crucial gas energy carrier, exploiting off grid storage or power of the grid, is increasingly becoming

a promising solution for the future, opening up new scenarios, for instance in the hydrogen mobility sector.

1.1 Power-to-Gas

The use of hydrogen can help solve some environmental and social problems, such as air pollution, global warming and hence climate change, since hydrogen does not produce harmful emissions when burned due to its carbon-free nature as a fuel. Studies and promising developments indicate how much hydrogen is a potential energy carrier.

This in particular, for the higher energy density compared to the other energy storage options, such as battery-based electrochemical energy storage, pumped hydro and compressed air.

However, detailed research and analysis are required to use hydrogen as an alternative carrier of energy and also to be fully commercialized as fuel. This is due to the fact that hydrogen is not a freely available energy resource, and it should be obtained using various methods and sources; thus, nowadays, it is more costly to obtain hydrogen than to get fossil fuels.

Hydrogen generated by electrolysis of water, with renewable-based electricity utilization, is an effective option for environmentally and carbonless production [6].

The latter concept finds its application in the Power-to-Gas (PtG) process. It's a solution that converts electricity into gaseous fuels (hydrogen and/or methane) and oxygen, which can then be stored and effectively used. Redundant electricity from RES can be used to produce hydrogen, which, by subsequent reaction with carbon dioxide, thanks to the methanation process, provides storable synthetic methane. This one can be injected into the existing gas distribution network or into underground gas storage facilities without negatively affecting the combustion properties of natural gas.

An alternative is direct injection of hydrogen into the gas network, but its quantity in the gas system is limited by national standards and regulations to the maximum of 0–12 vol% [7].

Therefore, H_2 can be produced exploiting the accumulation of electricity from solar and wind power plants during their peak production period, when there is an excess of energy, mitigating fluctuations and imbalance of the grid.

There are several projects that are working on the possibility to implement a system in which the surplus of RES can be stored, used as an input for the water electrolysis and, finally, taking advantage of the produced hydrogen, obtain again electrical energy, by means of the fuel cell technology. This concept is one of the possible following step of the Power to Hydrogen and takes the name of Power to Power process (or P2P).

A possible example is the EU-funded Green Industrial Hydrogen (GrInHy) which aim is to demonstrate the technological and economic value of high-temperature electrolysis as a highly efficient machine for hydrogen production, and which can be operated in reverse mode as a fuel cell, to produce electricity [8].

Located in a German steel production plant, to capture and exploit the waste heat from this energy-intensive process, the concept assesses the system’s flexibility to produce either hydrogen or electricity. In the first case it shall be used on-site in annealing processes substituting hydrogen based on fossil hydrocarbons. The idea behind this project can be exemplified by the following scheme [9].

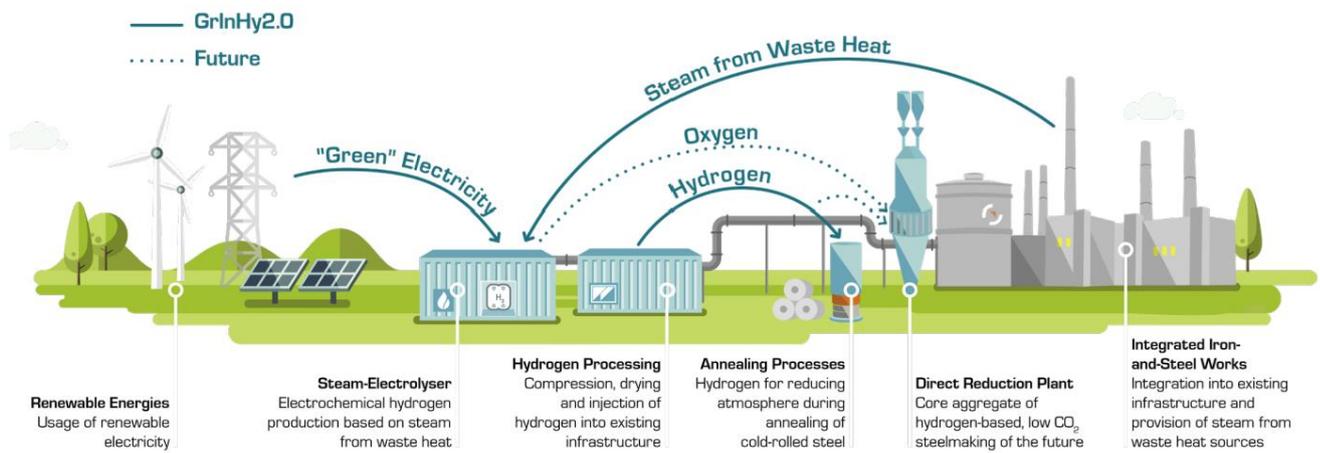


Figure 2. GrInHy2.0 - GREEN INDUSTRIAL HYDROGEN [10]

Thus, the main component of a power-to-gas plant is the electrolyser. The electrolysis process can be performed with three main technologies: Proton Exchange Membrane (PEM), Alkaline Electrolyser (AE) and Solid Oxide Electrolyser (SOE).

AE and PEM can be grouped under low-temperature electrolysis, instead SOE performs a high-temperature electrolysis. The three electrolysis technologies differ in their individual characteristics, like energy input in terms of electricity and heat but also operating temperature, pressure and others performance features.

The AE and PEM electrolyser technologies are crucial for the short-term perspective, while SOE has the best long-term development potential.

1.2 Water electrolysis technology

Water Electrolysis (WE) powered by renewable sources is one of the options to produce sustainable hydrogen, which is generated by passing an electric current through a conductive substance (electrolyte) to force a non-spontaneous reaction. The reaction of interest is the decomposition of water into hydrogen and oxygen, which is endothermic and requires energy input to be carried out. Precisely, a water electrolyser consists of a series of electrochemical cells composed of:

- electrolyte (ionic conductor);
- electrodes (anode and cathode) where oxidation and reduction reactions occur;
- electricity supply system and auxiliary systems for supply and collection of reagents and products [11].

1.2.1 Basics of electrochemistry

Electrolytic water dissociation is an endothermic process, requiring input of heat, in addition to electricity, over the zero to 1,000 °C temperature range. The step change in the required amount of heat and hence, in the total energy need (electricity + heat) at 100 °C, is due to the water phase transition from liquid to gas. The heat demand ΔQ ($T \cdot \Delta S$) linearly increases with temperature T because the entropy change ΔS is assumed constant. Consequently, the electrical energy demand (or Gibbs free energy ΔG) change, decreasing with temperature. Whereas the total energy need corresponding to the enthalpy change is equal to:

$$\Delta H = \Delta G + T \cdot \Delta S \quad (1.1)$$

These behaviours, previously explained, can be observed in the Figure 3, where the different energy demand are represented as a function of the temperature. ΔH only weakly depends on temperature both below and above 100 °C [12].

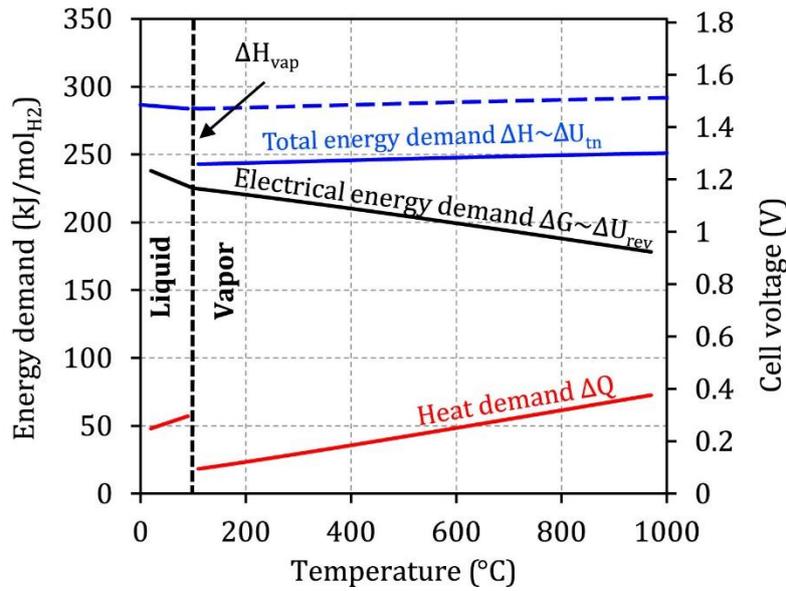


Figure 3. Energy demand as function of temperature [12]

According to Faraday's law, the change in Gibbs free energy for an electrochemical system in equilibrium is expressed as

$$\Delta G = n \cdot F \cdot U_{\text{rev}} \quad (1.2)$$

where

- $F = 96,485$ coulomb/mole is the Faraday constant;
- n the number of electrons involved in the electrochemical reaction;
- U_{rev} the reversible cell voltage, which is the minimum voltage needed to drive the reaction.

Therefore for water electrolysis, U_{rev} is the minimum voltage needed for water splitting. At lower cell voltage, water electrolysis does not occur, whereas at higher cell voltage, electrolysis is performed and heat is consumed in the reaction. Isothermal cell operation, that means, reactant and reaction products at the same temperature, requires additional heat input from the environment. However, cell operation generates heat by internal resistance as electric and ionic currents flow through the cell (Joule heating). This internally generated heat reduces the amount of heat to be supplied from the environment to the cell, for maintaining thermal equilibrium. With increasing cell voltage, the internal heat generation by the Joule effect increases and at the

thermoneutral voltage the internally generated heat equals the amount of heat $T \cdot \Delta S$ required for maintaining the reaction in thermal equilibrium [13].

According to the above statement, the thermoneutral cell voltage U_{tn} can be obtained from:

$$\Delta H = n \cdot F \cdot U_{tn} \quad (1.3)$$

thus, U_{tn} is the voltage required for electrolysis without withdrawing heat from the surroundings. In this case, ΔH represents the amount of electric energy required for electrolysis in the absence of external heat supply [14].

When the cell is operated at higher voltage than U_{tn} , the reaction becomes exothermic and heat needs to be removed for maintaining thermal equilibrium. In practice excess heat is generated because electrolyzers are operated above the thermoneutral voltage to overcome losses incurred by inefficiencies of the electrochemical reactions and by electrical and ionic resistance, as the current flows through the cell. On the contrary, an electrolysis cell operated at voltage lower than thermoneutral is endothermic and heat needs to be provided to the cell in order to sustain the reaction and keep the cell in the operating temperature range. This is why thermoneutral voltage at cell and stack level is so important.

Considering the values for ΔG , $T\Delta S$ and ΔH apply for a perfect cell operating in a thermodynamically reversible manner at standard conditions of temperature (25° C) and pressure (1 bar), with $n = 2$ for hydrogen, is possible to state [4] :

$$U_{rev}^{HHV} = \frac{\Delta_{G_{H_2O(l)}}}{(n \cdot F)} = \mathbf{1.229 \text{ V}} \quad (1.4)$$

$$U_{tn}^{HHV} = \frac{\Delta H_{H_2O(l)}}{(n \cdot F)} = \mathbf{1.481 \text{ V}} \quad (1.5)$$

1.2.2 State of the art

As previously mentioned, in literature are present configurations of electrolysers at different research and development levels. Nowadays, however the main technologies are Solid Oxide Electrolyte Cell (SOEC), Alkaline Electrolyte Cell (AEC or AWEC) and Proton Exchange Membrane Electrolyte Cell (PEMEC). The PEMEC and AEC operate at temperature from ambient to 90 °C, while solid oxide electrolyser are able to operate at a temperatures range of 500 °C to 1000 °C. Solid oxide electrolysers are one of the water electrolysis technologies under development, currently showing very high values of capital expenditure, both for the stack replacement and for the global system, even if in the future it would appear to be the best solution, considering a scenario in which large amount of H_2 will be produced, thus requiring a technology able to spend the least possible amount of energy.

PEM electrolysers are the units that split water by electrolysis utilizing an acidic electrolyte and produce hydrogen with high purity above 99.999% [15]. The maturity of the PEM electrolysis technology is less than alkaline electrolysis and is mostly utilized for small-scale applications. It's characterized by high membrane cost of fluorinated type, high complexity of the system due to the requirement of high operating pressure and pure water, and shorter lifetime than alkaline electrolyser. Thus, further research and development are required to reduce the cost of hydrogen produced by PEMEC [16].

Alkaline water electrolysers have mature technology and widely utilized for applications of large scale since the 1920 [17]. This electrolyser system is easily available, stable and holds lower capital cost because of the absence of noble metals and presenting mature components of the stack [18].

Nowadays, it's worth to point out that the hydrogen production technologies have different Technology Readiness Levels (TRL) [19]:

- PEM TRL 8: first of a kind commercial, that is, commercial demonstration, full scale deployment in final form;
- alkaline TRL 9: early adoption, solution is commercially available which needs evolutionary improvements to stay competitive;
- highly efficient SOE 6-7: large prototype and full prototype at scale stage [6].

1.2.3 Structure and goals of the dissertation

In a world where more and more people of different nations are realizing the urgency to move towards a more sustainable way of thinking about the planet, this dissertation proposes a further way to contribute to the so-called energy transition. In fact, being the mobility sector one of the main actor in global CO_2 emissions, the possibility to create new carbon-free vehicles, in particular for the heavy transport category, must be implemented as soon as possible. The idea is to replace the traditional diesel fuel, with a sustainable hydrogen gas, that can be produced on-site by different technologies of water electrolyzers, such as alkaline (AEC), proton exchange membrane (PEMEC) and solid oxide (SOEC) water electrolysis machines. Therefore, to evaluate the feasibility of implementation of the new “green” fuel, a techno-economic analysis has been carried out, evaluating all the costs associated to its production.

Starting from the cost of electricity, that is the input of the electrolyser, up to the capital expenditure related to the hydrogen refuelling station with the different operation and maintenance costs taken into account, a final cost of hydrogen in terms of Levelized Cost of Hydrogen (LCOH) has been assessed.

Therefore, the thesis work can be divided into these different sections:

- Section 1: introduction to the context, basics of electrochemistry essential to understand the operating principles of the water electrolysis technology; then for the latter a brief introduction with some examples of applications, as Power-to-Gas concept;
- Section 2: focused on the low temperature water electrolysis in terms of proton exchange membrane and alkaline technologies, with also an example of a global system implementation, with the required balance of plant;
- Section 3: focal point on the high temperature water electrolysis SOEC, with a final summary table of the pros and cons of the shown technologies;
- Section 4: hydrogen trend in the various market, from the common production for industrial applications up to the electrolyzers adoptions, to cover new markets, such as grid ancillary services and mobility purposes;
- Section 5: presentation of the case study on fuel cell electric buses for the German context, showing and justifying the various input parameters used;
- Section 6: results of the techno-economic analysis with the following discussion;
- Section 7: final considerations.

2. Low temperature water electrolysis

Focusing in a deeper analysis on the low temperature water electrolysis, three different technologies are currently available as commercial products or under development, namely:

- Proton Exchange Membrane (PEM) that uses an acidic polymer membrane sheet as solid electrolyte;
- Alkaline Electrolyser (AE) that uses a diaphragm and a liquid electrolyte, usually an aqueous solution of an alkaline product such as potassium hydroxide;
- Anion Exchange Membrane (AEM), more recent, that uses a hydroxyl-ion conducting polymer membrane sheet as solid electrolyte.

Relevant state of the art data for these three technologies are summarized in the following Table 1 [4]:

Table 1. State of the art low temperature water electrolysis technologies [4]

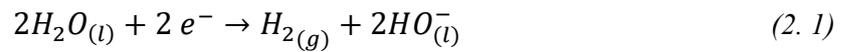
ELECTROLYSIS TYPE	PEMEC Proton Exchange Membrane	AWEC Alkaline	AEMWE Anion Exchange Membrane
Charge carrier	H ⁺	OH ⁻	OH ⁻
Reactant	Liquid Water	Liquid Water	Liquid Water
Electrolyte	Proton exchange membrane	NaOH or KOH 20-40 wt.% /water	Anion exchange membrane
Anode Electrode	IrO ₂ IrO ₂ /Ti ₄ O ₇ Ir _x Ru _y Ta _z O ₂ , Ir black	Co ₃ O ₄ , Fe, Co, Mn Mo, P, S, NiFe(OH) ₂ , Fe(Ni)OOH, oxides, hydroxides, borides, nitrides, carbides based catalyst	IrO _x Pb ₂ Ru ₂ O _{6.5} , Bi _{2.4} Ru _{1.6} O ₇ NiO _x , Li _x Co _{3-x} O ₄ , Cu _{0.6} Mn _{0.3} Co _{0.21} O ₄ , CuCoO _x
Cathode electrode	Pt/C	Raney Ni, Co, Cu, NiCu, NiCuCo, Ni- Co-W, Ni-Cu-Zn-B, Ni-Co, Ni-Fe, Ni-Co- Mo, NiCoZn, Raney Co, Ni-Mo, Ni-S, Ni- rare earth alloys	Raney Ni, NiO, Co based catalystNi/(CeO ₂ - La ₂ O ₃)/C

Due to the fact that the AEM is yet at the early stage of development, in the following sections, for the low temperature water electrolysis, is proposed an overview on the commercialized AEC and PEMEC.

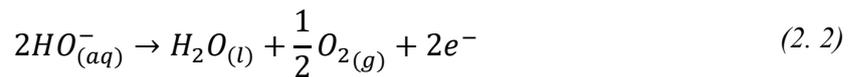
2.1 Alkaline Water Electrolyte Cell (AWEC)

In an alkaline water electrolyser, water molecules are electrochemically split by a DC current, at the cathode, to hydrogen molecules and hydroxide ions. The latter is able to diffuse through the alkaline electrolyte and then through a diaphragm, finally discharge at the anode releasing oxygen molecules. Therefore the following reaction occur:

- Cathode reaction:



- Anode reaction:



for a total reaction of:

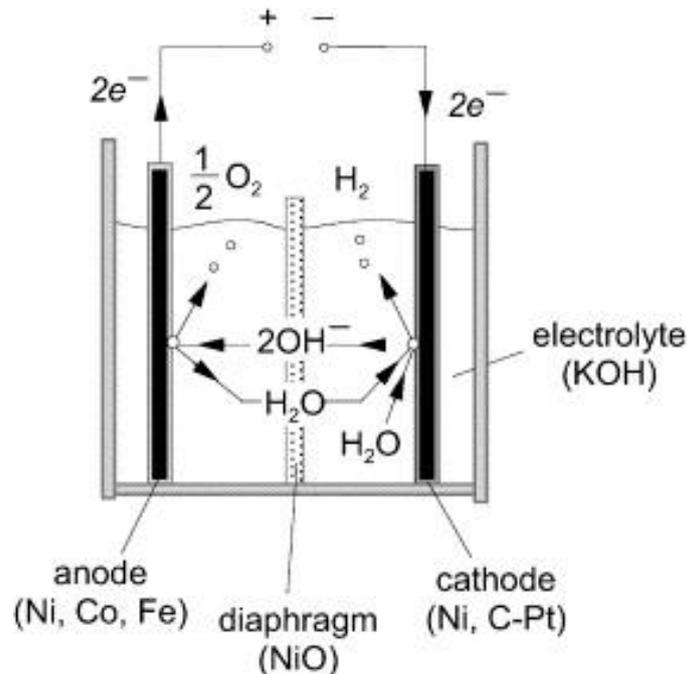


Figure 4. Internal structure of an alkaline electrolyser [20]

As it is possible to see from the Figure 4, the major components of the single cell are the two electrodes and the diaphragm. The latter has a microporous structure, having an high ionic conductivity with so low resistance, which is why nickel oxide (*NiO*) is used as diaphragm element.

Regarding the two electrodes, anode is made of cobalt, nickel and iron, while cathode is made of nickel and platinum activated carbon catalyst (C-Pt), used instead of a normal electrode to guarantee a protection against corrosion phenomena in the alkaline solution and having good electric conductivity [21].

The electrolyte is an aqueous solution containing either sodium hydroxide (NaOH) or potassium hydroxide (KOH). The latter is usually preferred for its higher OH⁻ conductivity for the same molarities. The typical optimum concentration of 20-40 wt.% corresponds to the highest conductivity due to the fact that at higher concentrations the conductivity decreases due to Coulombic force interactions [4].

The research and development on the AEC is focused on the possibility to increase the value of the current density, which is strictly related to the amount of hydrogen produced. However, higher current densities results in a higher value of ohmic losses. Therefore, to achieve this goal modification in the electrodes and diaphragm configurations and new materials adoption become necessary.

Starting from the latter, a wide range of new materials has been investigated, including nickel oxide, PTFE and different types of polysulphone. One of the materials that has been commercialized is Zirfon[®] Perl UTP 500 (Zirfon), which consists of a combination of zirconium oxide and polysulphone and combines good conductivity and wettability, with an high bubble point, giving it the right properties to act as a gas separation diaphragm. The thickness of Zirfon is 0.5 mm and its resistance in 30 wt.% KOH has been reported to be 0.3 Ω cm² at 20 °C and 0.13 Ω cm² at 80 °C [22].

As for electrode instead, the cathode catalyst typically can be a high-area nickel foam or nickel supported on stainless steel. Alternatives are Ni-Mo on a ZrO₂-TiO₂ support. The anode catalyst is usually made of Ni₂CoO₄, La – Sr – CoO₃ or Co₃O₄ [4].

The last pre-requisite for a high current density alkaline electrolyser is a good “zero gap” configuration. “Zero gap” means that the electrodes are pushed against the diaphragm to minimize the area resistance through the solution [22]. Gases evolve at the rear of both electrodes leading to a reduction of ohmic losses caused by the gaps previously present [4].

Therefore the thickness of commercial diaphragms Zirfon® becomes equal to the distance between two electrodes and further development are involved in the integration of the electrodes and the diaphragm into a single component to achieve a true zero gap.

The following Table 2 is reported in order to point out the main features of the alkaline electrolyser. The data are taken from several scientific journals, especially regarding operating and economic parameters but also flexibility, durability and efficiency of this technology. The goal is to have a clear picture of the main figure of merits of AEC.

Table 2. Main characteristics of alkaline electrolyser technology

		AEC
Operating parameters		
Cell pressure	<30 bar [23]	
	10-30 bar [12]	
	1-30 bar [24]	
Operating temperature	70-90°C [23]	
	60-90°C [12]	
	60-80°C [25]	
Nominal current density	0.2-0.8 A/cm^2 [23]	
	0.25-0.45 A/cm^2 [12]	
	0.2-0.5 A/cm^2 [25]	
	0.2-0.4 A/cm^2 [25]	
Voltage range	1.4-3 V [23]	
	1.8-2.4 V [26]	
Efficiency		
Power consumption	50-78 kWh/kg (1MW) for the system [24]	
	56-66 kWh/kg for the system [12]	
	51-60% LHV for the system [12]	
	63-70% LHV for the system [25]	
	4.5-6.6 kWh/ $Nm^3_{H_2}$ for the system [26]	
	4.2-4.8 kWh/ $Nm^3_{H_2}$ for the system [27]	
	52 kWh/kg for the system [28]	

Flexibility	
Load range	15%-100% [24]
	20%-100% [12]
	10%-110% [25]
Cold start up	<50 min [24]
	1-2 h [12]
	<60 min [26]
	15 min [27]
Warm start up	1-5 min [12]
Durability	
Lifetime (stack)	60,000 h [24]
	55,000-120,000 h [12]
	60,000-90,000 h [25]
System degradation	0.25-1.5%.a [12]
System lifetime	20-30 y [27]
	20 y [7]
Capacity	
Electrode area	1-3 m ² [24]
Cell area	<3.6 m ² [12]
	<4 m ² [26]
	3-3.6 m ² [27]
Plant footprint	0.095 m ² /kW _e [25]
Production rate	1-500 $\frac{Nm^3}{h}$ [25]
	<760 $\frac{Nm^3}{h}$ [26]
	<1400 $\frac{Nm^3}{h}$ per stack [27]
Economic parameters	
CAPEX stack replacement	USD 270/kW (minimum 1 MW) [24]
	339 €/kW _e [26] (obtained by linear interpolation)
	340 €/kW _e [27]
CAPEX system	USD 500-1,000/kW (minimum 10 MW) [24]
	800-1,500 €/kW _e [12]
	USD 500-1,400/kW _e [25]

	1,000-1,200 €/kW _e [12] 744 €/kW _e [28] 786 €/kW _e for a mild scenario [28] 800 €/kW _e [27]
OPEX(% CAPEX per year)	2-3% [12] 3% [27] 2% [27]
H₂ purity	99.9%-99.99998% [24] >99.5% [26] >99.8% [27]
Maturity	Mature [26] Widespread commercialization [27]

2.2 Alkaline water electrolysis plant

In order to produce large amount of hydrogen, cells are interconnected into a stack by means of bipolar plates. The idea is to join series of single cells with the aim of increasing the voltage rate. The interconnectors, or bipolar plates, contain channels in order to feed each cell with reagents and let out the gases produced.

In order to verify a good operation of the reactor, several functions are required and cannot be fulfilled by the stack on its own. That is why an electrolysis system must include auxiliary components, namely, the so called Balance of Plant (BoP) in order to carry out [29]:

- temperature and pressure regulation of the stacks;
- fluid flow rate regulations in terms of composition/concentration;
- separation and purity regulation of the gases produced;
- back-pressure valve regulation at the outlet of the gases produced;
- recirculation of the electrolyte into the stack, verifying the right input value of pressure;
- control of the input power to the stack current voltage characteristics.

Thus, a typical AEC configuration represented in the JRC technical report [30] is shown in this dissertation. This is because in a techno-economic analysis, which is the real purpose of this work, it is important to understand what the different components are, due to the fact they will have a certain capital expenditure that will influence on the overall cost of the plant.

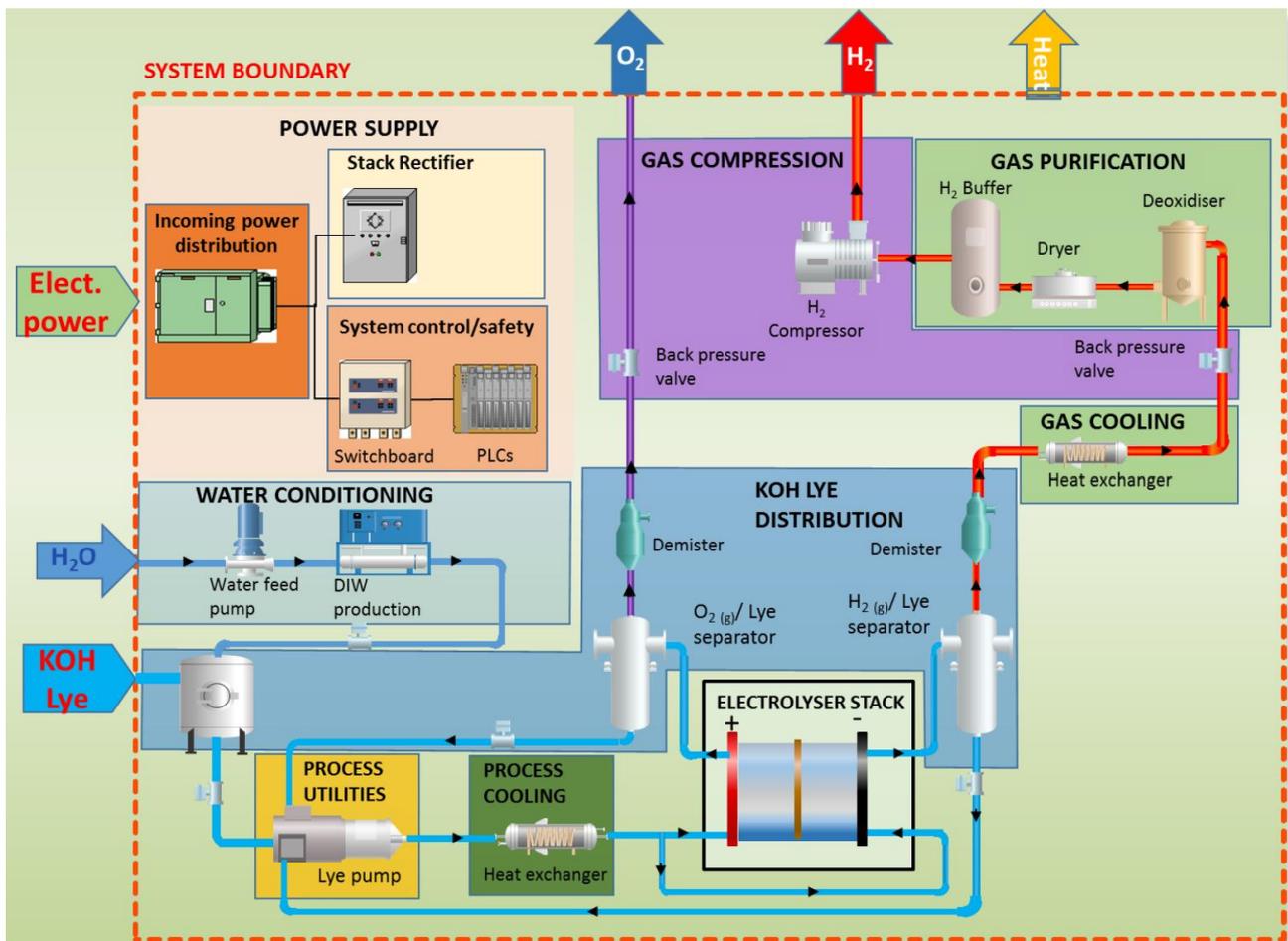


Figure 5. Schematic representation of the AWE system and the BoP [30]

Therefore, as it is possible to see from the schematic representation in Figure 5, different blocks can be highlighted :

- the power supply with rectifier and system control safety to provide DC current to the electrolyser;
- the water conditioning with the water pump and water demineralizer;
- a lye supply/recirculation system used to provide a continuous electrolyte flow, with the heat exchanger, lye pump as main components to feed the stack and separator;
- a demister unit to remove residual liquid and lye aerosols from the gas outlet stream;
- cooling and purification system of the H_2 produced, mainly thanks to deoxidiser and dryer to respectively recombine catalytically residual traces of oxygen that could be present due to crossover effects and remove residual moisture;
- gas compression station, required as in the case of hydrogen produced for mobility purpose to reach the target pressure of the hydrogen refuelling station.

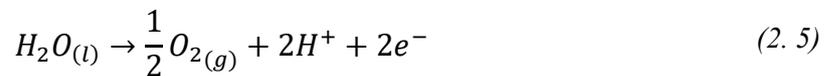
2.3 Proton Exchange Membrane Electrolyte Cell (PEMEC)

In PEM electrolyser, water is introduced at the anode, where it is split into protons H^+ and oxygen. The protons travel through the cell and, after crossing the proton conducting membrane, are able to reach the cathode, where they are recombined into hydrogen $H_{2(g)}$. On the contrary the oxygen gas produced remains at the cathode, where is also present the unreacted water. Therefore the following reaction occur:

- Cathode reaction:



- Anode reaction:



for an overall reaction which is the same as for alkaline electrolyzers:

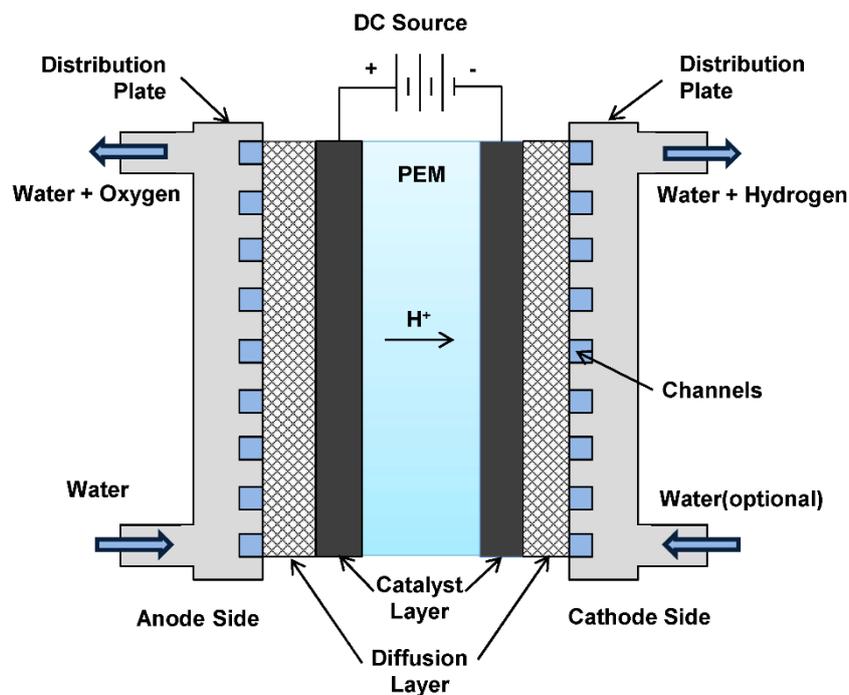
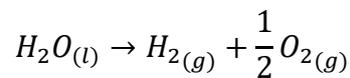


Figure 6. Schematic representation of PEMEC [31]

Observing the schematic representation, the reactions take place at the catalyst layer coated on each electrode. The latter is made of graphite material, instead, regarding the catalyst, iridium at the anode and platinum at the cathode are basically adopted. The core of the system is the electrolyte membrane, a polymeric material with Nafion as commercial name. It's chemical structure is composed by PTFE, polytetrafluoroethylene $(CF)_n$, what is called Teflon, which is modified adding lateral chains containing HSO_3^- . The membrane, if dry, has a movements of ions H^+ which is very limited, but when is hydrated with water it starts to increase a lot the ionic conductivity. In fact the movement of the ions H^+ is a hopping mechanism enhanced by the water, that is improved by rising the number of lateral chain of hydrogen sulphite. The diffusion layer on each side helps a proper current distribution, molecular diffusion and also connects the Membrane Electrode Assembly (MEA) to the bipolar plates, as it is possible to see from the Figure 7, which represents the different components. Distribution bipolar plates contribute to the structural integrity of the cell and also separate one cell from the other, when they are assembled together in the form of a stack to deliver the required hydrogen flow rate [31].

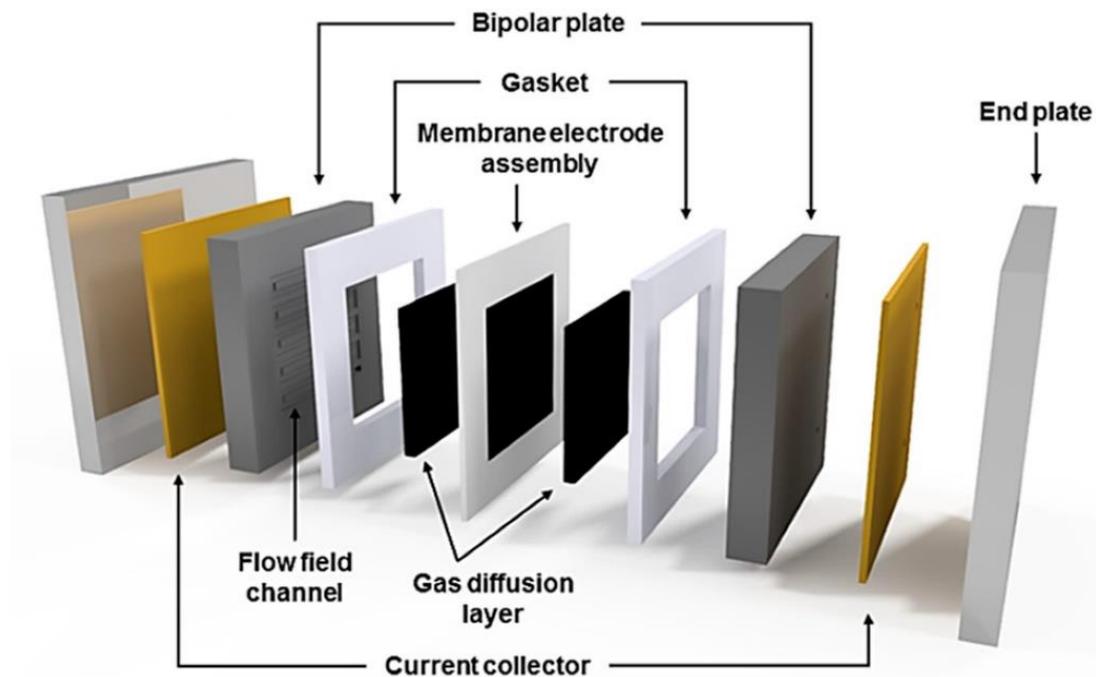


Figure 7. Main components of a polymer electrolyte membrane cell [32]

The single repeated unit (SRU), that is, anode, cathode, electrolyte with the interconnector, has a thickness of about 2 mm. PEM electrolyzers have low ionic resistances and therefore high currents, even values higher than $1.6 A/cm^2$ can be achieved, while maintaining an high efficiencies of 55–70%. Industrial PEM electrolyzers have a typical hydrogen discharge pressure of 10-30 bar. High pressure operation is possible with anode and cathode at the same pressure, “equibar” condition, or in differential mode with the hydrogen compartment at higher pressure. In the latter case, the BoP of the oxygen compartment is simpler, but with the drawback of the additional stress on the MEA. Hydrogen and oxygen produced have a very low level of contaminants: in the gases is possible to find some residual percentage of water that can be easily removed and some oxygen due to gas crossover, easily remove with catalytic conversion. The final hydrogen purity can reach 99.99% [4].

The power of PEM electrolyzers ranges from a few kilowatts to several megawatts. In addition to the cell/stack, an electrolyser has auxiliary components to ensure the proper functioning of the stack, as in the previous case of the alkaline. For the two technologies, the overall plant presents many similarities having both a drier that may be used, for purity requirements, to remove residual water after a gas/liquid separations unit. What can be highlighted is that at the same level of power input, the footprint of PEM with respect to the alkaline is one third.

In the following Table 3, as in the previous case for alkaline technology, is reported the main features of the PEM electrolyser. Even for this one, data are taken from several scientific journals, especially regarding operating and economic parameters. Furthermore, unlike the alkaline cell, for PEM systems flexibility assumes an important feature. In fact, observing the above-mentioned Table 3, it is worth to point out how they present very good dynamic behaviour. Durability, efficiency and maturity of this technology is also highlighted.

Table 3. Main characteristics of PEMEC technology

PEMEC	
Operating parameters	
Cell pressure	20-50 bar [12]
	<30 bar [23]
	30-80 bar [24]
	< 200 bar [25]
	15-30 bar [26]

Operating temperature	50-80°C [23]
Nominal current density	1-2 A/cm^2 [23] 0-3 A/cm^2 (up to 20) [24] 0.6-2.0 A/cm^2 [25] 1-2 A/cm^2 (up to 20 A/cm^2 at lab experiment)[33]
Voltage range	1.4-2.5 V [23] 1.8-2.2 V [33]
Efficiency	
Power consumption	48 kWh/kg [7] 46-60 (% LHV) including aux. and heat supply [12] 5.0-6.5 kWh/Nm^3 [12] 50-83 kWh/kg (1MW) for the system [24] 56-60 (% LHV) [24] 4.2-6.6 $kWh/Nm_{H_2}^3$ for the system [25] 4.2-5.5 $kWh/Nm_{H_2}^3$ for the stack [25] 4.4-5 kWh/Nm^3 [33] 61 kWh/kg [26] 58% (LHV) for a mild scenario [30]
Flexibility	
Load range	0-100% [12] 5%-120% [24] 0%-160% [24]
Cold start up	5-10 min [12] <20 min [24] <15 min [33] <5 min [26]
Warm start up	<10 s [12]
Durability	
Lifetime (stack)	50,000-80,000 h [23] 10,000-50,000 h [24] 20,000-60,000 h [25] 60,000-100,000 h [33] 50,000 h [26]

System degradation	0.5-2.5 %/a [12]
System lifetime	10-20 y [33] 20 y [26]
Capacity	
Electrode area	0.15 m ² [24]
Cell area	<0.3 m ² [25] < 0.13 m ² [33]
Plant footprint	0.048 m ² /kW _e [24]
Production rate	400 Nm ³ /h (per stack) [12] 1-250 Nm ³ /h [24] < 40 Nm ³ /h [25] <400 Nm ³ /h [33]
Economic parameters	
CAPEX stack replacement	USD 400/kW (minimum 1 MW) [24] 470 €/kW _e [26] 420 €/kW _e [27]
CAPEX system	USD 700-1,400/kW (minimum 10MW) [24] 1,100-1,800 €/kW _e [24] 1,860-2,320 €/kW _e [25] 1,400-2,100 €/kW _e [33] 1,300 €/kW _e [26] 1,000 €/kW _e [27] 1,209 €/kW _e for a mild scenario [28]
OPEX(% CAPEX per year)	3-5% [12] 3% [26] 2% [27]
H₂ purity	99.9%-99.9999% [24] 99.99% [25] 99.999 % [33]
Maturity	Commercial [25] Commercialization [33]

3. High temperature water electrolysis

There are several reasons that drive researchers to move towards higher temperatures, for electrolysis technology. First of all, as it has been explained in the Section “Basics of electrochemistry” of this dissertation, electrolytic water dissociation is an endothermic process, that requires heat input, in addition to electricity. However, the total amount of energy ΔH required by the reaction remains almost constant varying the temperature, unlike the heat demand $\Delta Q (T \cdot \Delta S)$ that linearly increases with temperature. Therefore being ΔH given by the sum of the thermal demand and the electrical one (ΔG), the latter has to decrease to keep constant ΔH . Hence, increasing the operating temperature, decrease the amount of electrical energy that has to be provided, leading to an increase of electrical efficiency of the process. On the contrary the increase of thermal demand can be satisfied by the heat generated by the internal irreversibility, so called activation, ohmic and diffusion overvoltage. In fact, operating at the thermoneutral point or above, it is possible to completely cover the heat demand. Furthermore, another solution is to exploit the waste heat from industrial plants or from different processes. Thus, it's also allows an economic advantage in terms of power consumption, reaching very high level of efficiency. For instance, the waste heat can be utilized to generate vapour and rising the temperature of the reagent to reach the operating point.

In addition working at higher temperature allows to reduce the losses for irreversibility, previously mentioned. This is due to the fact that, the higher temperature provided to the stack improves the kinetic of reaction and diffusion process, leading to a further reduction of the input electrical energy.

Instead, regarding the material, there are some advantages but also drawbacks. With respect to the PEM technology, for instance at temperature of 700-800°C, there is no need of precious catalyst, as the platinum group metal. This is possible thanks to these operating conditions that makes the catalytic activity already sufficient, considering the current use of the material at the electrode. The direct consequence is a larger flexibility in terms of reactants and so fuels that can be exploited, with catalyst that are more tolerant to molecules containing carbon. However, high temperature means to consider a cell and a balance of plant able to withstand at this set-up, leading to higher cost and problems for materials and fabrication. Moreover, lower long-term stability of the cell has to be considered. The dynamic behaviour of the system is worse due to difficulties related to the thermal management that leads less promptness in operational transients.

Nowadays, the high temperature water electrolysis is implemented by the solid oxide electrolyte cell, with a temperature range of 700-1000°C with the electrolyte that exploits the conduction of oxygen ions (HT O-SOEC). Nevertheless, the trend seems to be to raise the temperature of the AEC and PEMEC and to decrease that of SOEC. The idea is to reach an intermediate value for the system, concept which is receiving more and more attention [34]. This technology can be implemented either with conducting ions of O^{2-} , or with conducting ions of H^+ . The latter, however, for intermediate temperature, shows a better ionic conductivity, good compatibility with nickel and negligible electric conductivity: the main figure of merits for a good electrolyte [35]. This operating condition will allow a better long term-stability, less cost for the material used, and a larger possibility to exploit different sources of waste heat, required at lower value of temperature.

It is worth highlighting how this technology at intermediate temperatures is still very immature and therefore will not be the subject of further discussion in this thesis work.

3.1 Solid Oxide Electrolyte Cell (SOEC)

In an solid oxide electrolyte cell, water molecules are electrochemically split, by a DC current, at the cathode, to hydrogen molecules and oxygen ions O^{2-} . The latter is able to diffuse through the solid oxide electrolyte and finally discharge at the anode releasing oxygen molecules, as in the case of alkaline cell. Therefore, the following reactions occur:

- Cathode reaction:



- Anode reaction:



for a total reaction as for AEC and PEM:



The electrolyte is made of a ceramic material: yttria stabilized zirconia, that is, Z_nO_2 doped with Y_2O_3 . It is the most used in market application. This electrolyte contains O^{2-} ions, therefore they are the transported ions, that, being negative, migrate from cathode to anode. The temperature of the cell is mainly in the range 650-800°C, precisely due to the fact that the ionic resistivity starts to decrease significantly for values greater than 620°C, obtaining a good parameter of ionic conductivity. For the anode electrode a solution implemented is the Cermet, a mix of ceramic and metallic material: nickel and yttria stabilized zirconia, with a global porosity of about 30% allowing a good trade-off between stability and diffusion phenomena. Nickel allows to satisfy catalytic activity and electron conductivity and the ceramic material guarantee the capability to conduct ions, that has to arrive from the electrolyte. Regarding the cathode side, characteristic similar to the anode are required, with good thermo-mechanical compatibility with the adjacent layers. Thus a possibility is the Lanthanum doped Strontium Manganese oxide. It is a perovskite material: family of ceramic materials with structure ABO_3 , with A rare earth material, B as a transition metal and oxygens distributed on the faces of the cubic lattice. Hence, the cathode is ceramic defined as MIEC material (mixed electronic and ionic conductor) because it manages to conduct both in a good way.

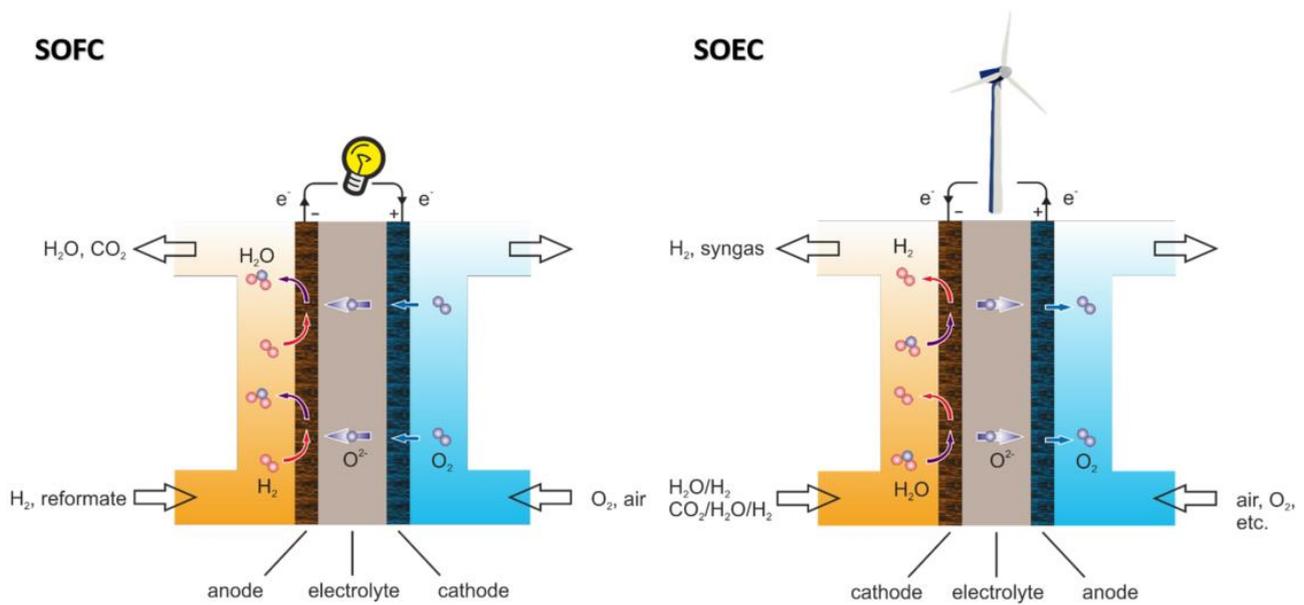


Figure 8. Working principle of SOEC [36]

As it is possible to see from the Figure 8, the SOEC is exactly the same machine but in the reverse condition of the Solid Oxide Fuel Cell (SOFC), which aims is instead to produce electrical energy starting from an input of hydrogen.

Different structure of the cell can be implemented: anode, cathode electrolyte, interconnect or metal substrate supported cell. Nowadays, the state of the art is the mechanic support of the anode, due to the fact that it guarantees a larger room for catalyst, with respect to the cathode layout which also has the problem of increasing the path of an already large molecule like oxygen. Instead the electrolyte and interconnect configuration are not respectively chosen due to an excessive ohmic drop for its thickness, and corrosion problem [37]. In fact, regarding the interconnection plate, called Crofer 22 APU, being made of stainless steel with 22% of chromium, that in contact with O_2 in the cathode atmosphere generates chromia Cr_2O_3 , which in turn causes a degradative phenomenon, that lead to the de-activation of the cathode. A possible solution could be a dual layer coating on the surface: first a thick chromium blocking layer, then, above it a spinel of $M_nCo_2O_4$, that is, a protected layer to avoid evaporation of chromium and it has to be deposited on the face of the cathode side. Between the two layers, however, there is a thin active anti-corrosion layer based on yttria to slowdown the oxide scale growth [38].

Another issue related to the SOEC high temperature operating condition, is the necessity of a sealing border. In fact, molecules thanks to the temperature activation, are able to diffuse, escape, above all hydrogen, that is very small. The only packing of the electrode and interconnector is not

sufficient at these conditions of working. A glass-ceramic material is required as a solution to seal the cell. However, the insertion of the sealing material is difficult because it has to withstand at very high temperature, compared to the time when is placed (at 20°C) and it has to join two different materials. For this last issue, the Coefficient of Thermal Expansion (CTE) of the materials plays a crucial role, due to the fact that it has to be matched with the ones of the surrounding components to guarantee thermo-mechanical stability. Therefore, considering that electrolyte has a CTE of $10.5 \cdot 10^{-6} K^{-1}$, cathode has $12.4 \cdot 10^{-6} K^{-1}$, anode has a value in the range $10-14 \cdot 10^{-6} K^{-1}$, interconnector has $11-13 \cdot 10^{-6} K^{-1}$, the sealing material has to show a CTE in the middle of these values [39].

In the following Table 4, as previously done for the other two technologies, the main features of the SOEC electrolyser are reported. In this case, data are taken from scientific journals, but with an high level of uncertainty, especially regarding operating and economic parameters. The reason is because the technology is still at its early stage of lab-scale, R&D demonstration.

As it is possible to see from the Table 4, in case of SOEC, it assumes an important feature the possibility to achieve very high level of efficiency (%LHV), reducing the power consumption and trying to reach the 100%. On the contrary, the issue related to the thermal management leads to require a very long time for the cold and warm start-up.

It is worth to point out that the capital expenditure, especially for the stack replacement, is a parameter that, due to the low level of maturity, seems to be very difficult to be found and defined in literature, except with the assumption of a wide range.

Table 4. Main characteristics of SOEC technology

		SOEC
Operating parameters		
Cell pressure	1-15 bar [12]	
	1 bar [23]	
	1-5 bar [24]	
	< 25 bar [25]	
	<30 bar [33]	
	1-20 bar [40]	
Operating temperature	700-900°C [12]	
	700-850°C [23]	

	900-1,000°C [33] 650-1,000°C [24]
Nominal current density	0.3-1 A/cm^2 [23] 0-2 A/cm^2 [24] 0.3-2 A/cm^2 [25] 0.2-1.0 A/cm^2 [40]
Voltage range	1.0-1.5 V [23] 0.7-1.5 V [25] 0.95-1.3 V [33] 0.9-1.6 V [40]
Efficiency	
Power consumption	76-81 (% LHV) including aux. and heat supply [12] 3.7-3.9 kWh/Nm^3 [12] 40-50 kWh/kg (1MW) for the system [24] 74-81 (%LHV) [24] > 3.7 $kWh/Nm_{H_2}^3$ for the system [25] > 3.2 $kWh/Nm_{H_2}^3$ for the stack [25] 2.5-3.5 kWh/Nm^3 [33] 77.5 (%LHV) for a mild scenario [30] > 80 (%LHV) electrical efficiency [40] 77-90 (%LHV) for total system efficiency [40]
Flexibility	
Load range	-100% - +100% [12] 30% - 125% [24] 20% - 100% [24] 0% - 100% [40]
Cold start up	Hours [12] >600 min (to nominal load) [24] > 60 min [33] > 4 h [40]
Warm start up	15 min [12] > 1 h [40]
Durability	

Lifetime (stack)	<20,000 h [24] 500-30,000 h [24] < 10,000 h [25] 8,000-20,000 h [33]
System degradation	3-50 %/a [12]
System lifetime	Up to 10ys continuous operation reported by industries [40]
Capacity	
Electrode area	0.02 m ² [24]
Cell area	< 0.01 m ² [25] < 0.06 m ² [33]
Plant footprint	0.1 m ² /kW _e [41]
Production rate	< 10 Nm ³ /h per stack [12] <40 Nm ³ /h [25] < 10 Nm ³ /h [33]
Economic parameters	
CAPEX stack replacement	> USD 2,000/kW (minimum 1 MW) [23]
CAPEX system	Unknown [23] USD 2,800-5,600/kW [24] > 2,000 €/kW _e [25] > 2,000 €/kW _e [33] 3,400 €/kW _e for a mild scenario [28]
OPEX(% CAPEX per year)	3% [42]
H₂ purity	99.9%-99.9999% [23] 99.9% [25]
Maturity	Lab-scale, R&D [24] Demonstration [25] Research &Development [33]

3.2 Pros and cons of water electrolysis technologies

After have explained and listed the characteristics of the three main configurations of electrolyzers AEC, PEMEC and SOEC, in this section a comparison among them is reported, highlighting their pros and cons, in order to establish in which case is better to select one or the other.

Alkaline water electrolyzers have a widespread commercialization and as it is possible to understand by observing the AEC parameter Table 2, it presents the lower capital cost both in terms of stack replacement and global system. It also shows good values of production rates which makes it a cost-effective solution. In spite of this, it presents a number of drawbacks:

- due to the inertia of the liquid electrolyte, they react less readily than PEMEC technology to changes in input power, thus possibility of dynamic operation is limited, adversely affecting gas purity and system efficiency [43];
- the degree of purity of the hydrogen produced is lower than that achieved with the PEMEC and SOEC electrolyzers due to the diffusion of the products through the diaphragm;
- the current density is reduced to try to limit the ohmic losses through the liquid electrolyte and the diaphragm;
- in order to avoid the crossover of gaseous products through the diaphragm, they show a more limited load range.

Therefore, design improvements are ongoing so that it can operate dynamically, for instance in the scenario of connection with the intermittent nature of renewable sources.

PEMEC provides some well-established advantages with respect to other water electrolysis technologies. First of all, they are more compact, which is relevant for the future scale-up of the technology. MEA is thin, flexible and easily handled, that is not the case for oxide ions conducting ceramics used in solid oxide technology. The electrolyzers can be operated at significantly elevated current densities, in the multi-A/cm² range, with good energy efficiencies. They accept highly transient power loads, such as those resulting from the use of intermittent energy resources of electricity via PV panels or wind turbines, and can operate over the quasi-entire load range within seconds with no significant operational constraints. Operation of pressurized PEM electrolyzers is safer in the sense that potential leakage of hot water is more manageable than leakage of hot alkaline solutions [44].

In order to reduce the investment cost, the challenge is the substitution of electrocatalysts consisting of platinum group metals by non-noble metals. In fact, platinum is currently implemented in the technology together with highly corrosion-resistant materials to limit the negative effect related to the presence of the polymer membrane [16]. Therefore, various improvements are required to reduce the electrolytic hydrogen cost.

Unlike conventional proton exchange membrane or alkaline-based electrolysis, solid oxide electrolyte cell presents the possibility to provide co-electrolysis of CO_2 and steam with a special form of SOEC [45]. This is possible due to the fact that, working at high temperature, it does not need to exploit precious catalyst like platinum group metals. Thus, it's sufficient to use nickel, the most classical and cheap industrial catalyst, that is more tolerant to molecules containing carbon, giving to the cell a fuel flexibility, opening the door at very different species that can be oxidized.

Therefore, due to the increasing demand of hydrogen and the low amount of electrical energy utilized by this water electrolysis technology, compared to the traditional ones, there is recently increasing interest in SOE technology. In addition to reducing the consumption of electricity, another advantage is the thermodynamic and kinetic restrictions related to the electrochemical reaction and reactant/product transportation that becomes small, at high temperatures. Furthermore, nearly 100% efficiencies can be achieved at current densities of approximately 1 A/cm^2 [46]. The advantage is also maintained at the system level, although it is necessary to preheat the reagents to high temperatures. The main challenge is the higher degradation rates of material than competing alternatives, as a consequence of the higher operating temperatures. The transient operation of the SOEC is also more difficult due to the temperature and the complex thermal management of the system. High temperatures also create problems regarding the materials to be used for the stack and its BoP.

Therefore, many researchers are focused on stabilizing the current materials, decreasing the operating temperature to an intermediate level and developing new materials to enable the commercialisation of this type of electrolyser [47].

A conclusive summary of the previously listed pros and cons of the three technologies is reported in the following Table 5 to highlight the main figure of merits at the current state of art.

Table 5. Pros and cons of AWEC, PEMEC and SOEC

Technology	Advantages	Disadvantages
Alkaline Electrolysis	<ul style="list-style-type: none"> Oldest and well established Cheapest and effective Long term durability Stack in the MW range Non noble catalyst 	<ul style="list-style-type: none"> Low current density Crossover of gases Low degree of purity Corrosive liquid electrolyte Low dynamic operation Low load range Low operational pressure Not compact system structure
PEM Electrolysis	<ul style="list-style-type: none"> High current density High voltage efficiency Good partial load range Compact system structure High degree of gas purity High dynamic operation Rapid system response Reversible operation 	<ul style="list-style-type: none"> Limited and costly membrane High cost of components Precious catalyst Acid medium Lower durability Stack below the MW range Partially established Commercialization in near term
SOEC Electrolysis	<ul style="list-style-type: none"> Lower energy need High current density No precious catalyst High pressure operation Fuel flexibility Reversible operation High degree of gas purity Lowest overpotential losses Highest global efficiency 	<ul style="list-style-type: none"> Unsuitable sealing Delamination of electrodes Bulk system design Instability of electrodes Early stage (low TRL) Fabrication and material issues Difficult transient operation Thermal management issue Lower durability

4. Hydrogen trend in the various market sectors

First of all, a clear distinction of the different types of hydrogen has to be pointed out. This gas does not exist in nature in the pure form and thus it has to be produced. Nowadays, the most commonly used method to make hydrogen is by means of the Steam Methane Reforming (SMR). High temperature water steam reacting with methane CH_4 , can produce H_2 and carbon monoxide CO , or carbon dioxide CO_2 . Another possibility consists of using electrolysis, in which electricity is used to split water H_2O into hydrogen H_2 and oxygen O_2 . Both production techniques exploit different types of energy: gas in case of SMR and electricity in case of electrolysis.

SMR typically uses natural gas and also bio-methane, which is CH_4 produced either from thermal gasification of dry organic residues or from the anaerobic digestion of waste wet organic material. The carbon emissions associated to the production of hydrogen can be treated in different ways. If the carbon emitted in the SMR process is not captured and stored, the hydrogen is called 'grey'. If the carbon is removed and stored, the hydrogen is called 'blue'. This technique is increasingly considered as an option to produce hydrogen without carbon emissions. If bio-methane is used as input in SMR, then there would be no net carbon emissions while with carbon capture even negative emissions would occur. Electrolysis uses power, which can be generated in different ways. When the electricity is generated through renewable sources, as in the case of wind turbines or solar panels, the hydrogen is made in a pure sustainable way and it is called 'green'. Hydrogen made through electrolysis does not have direct carbon emissions, but the electricity which is used may be generated by fossil-fuel power plants which indirectly results in carbon emissions [48].

Hydrogen already play a fundamental role in established markets but also in new and future sectors at the basis of the decarbonization process:

- through its direct use in the steel, chemical, and refining industrial sectors as a raw material;
- in the energy-intensive industry that requires heating at very high temperatures even over $1000^\circ C$;
- as fuel in mobility, primarily for heavy long-range;
- indirectly, especially when it will be more abundant and cheap, for the production of electrical and thermal energy through the injection of hydrogen into the gas network mixed with natural or in a pure gas configuration.

Hydrogen, hydrogenated biofuels and synthetic fuels produced from it, will contribute to the relaunch of the automotive supply chain, after the health emergency due to COVID-19 virus. Hydrogen is a storage medium with high energy density and can also play a crucial role in the integration of renewable sources in energy systems: suitable for large storage, thousands of tons of hydrogen storable, for an accumulation load capacity of GWh and for long periods. It is a solution that makes possible to connect seasonal grids and energy transfers from the excess production of renewable energy to other sectors [49].

Nowadays, the consumption of hydrogen in Italy is almost entirely limited to industrial uses in refining and chemistry, for instance ammonia and is mainly of the 'grey' type, so we could start from these uses to replace that colour of hydrogen with the sustainable 'green' one.

Production takes place on site in large natural gas steam reforming plants, and directly feeds the chemical processes. The current final consumption of hydrogen in Italy is approximately 16 TWh, roughly equal to 1% of final energy consumption at national level (1,436 TWh) and corresponding to approximately 480,000 t/year, of which approximately 8,500 t/year are marketed in cylinders and in special pipes [49].

4.1 Production of H_2 for industrial applications

Nevertheless, the greatest demand for hydrogen over time, which ensures a consolidated market potential, is represented by the different industrial applications. It is possible to split into large and light industry, based on the hydrogen consumption volume. Typically, large industries, such as refineries, chemical plants and potentially steel manufacture, consumes very large amount of hydrogen, thousands of Nm^3/h . Hydrogen is produced centrally or on-site and can also be intended for sale to a final consumer either through pipeline distribution, pressurized tanks or through trucks carrying hydrogen cylinders. The latter is the typical solution to supply light industries if on-site production is not considered.

Refineries produce hydrogen as a by-product of catalytic reforming, and it is mainly used for desulphurisation of crude oil. They are expected to use more hydrogen due to the restrictive fuel quality regulation and lower crude oil quality. Power to Hydrogen could be an opportunity to supply this increasing hydrogen need in the short-to-mid-term, if favourable regulation to lower carbon intensity of produced fuel can be put in place. The emergence of a business case in large industries such as refineries, can lead to a large volume deployment of electrolyzers [41]. Even if the hydrogen currently produced in refineries via SMR is obtained at very low cost of 1-2 €/kg [5].

Focusing the attention on the chemical industry, it is possible to say that, it is the largest producer and consumer of hydrogen, due to the several number of applications in this field for which it can be exploited. Among them, most important dominant processes are the production of ethanol and ammonia, which is a precursor of fertilizers. Nevertheless, up to now, electrolytic production of hydrogen plays a minor role due to the fact it is not competitive with steam reforming and is only applied where relatively small amounts of pure hydrogen are required. Therefore, developments of the European ammonia and methanol market are at the basis for the chemical industry to become sustainable, thanks to the integration of a large-scale production of renewable hydrogen [50]. An emerging market is the one related to the possibility to perform by means of the methanation reactor a catalytic hydrogenation of the CO_2 , recovered from the carbon capture technology or a collected source from power stations. The overall process is shown in the Figure 9 and the most probably pathway in the short-term is to exploit an alkaline water electrolyser to produce the H_2 to send to the reactor.

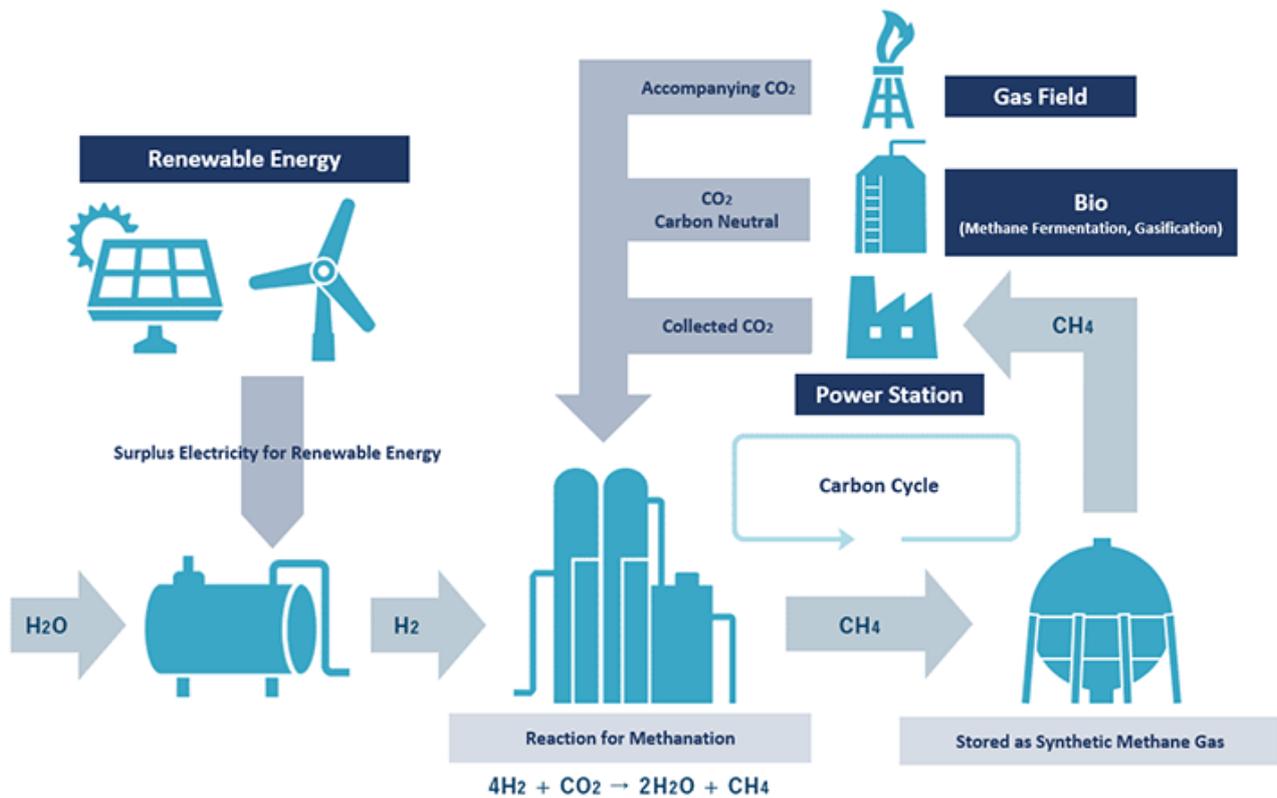
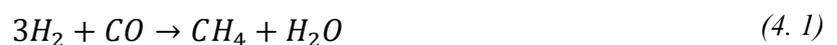


Figure 9. Production of the synthetic methane through PtG pathway [51]

The proposed configuration takes advantage of RES as input to electrolyser system. A further solution in the long-term prospective is to perform the same process but exploiting an high temperature SOEC which can split both water and carbon dioxide molecules. In this case at the methanation reactor occurs the directly hydrogenation of the CO , with the consequent production of synthetic natural gas, with the following chemical reaction:



This leads to an increase of the global efficiency, for instance, given by the ratio between the enthalpy content of the produced CH_4 and the total Δh of reaction, reaching efficiency values of about 86%.

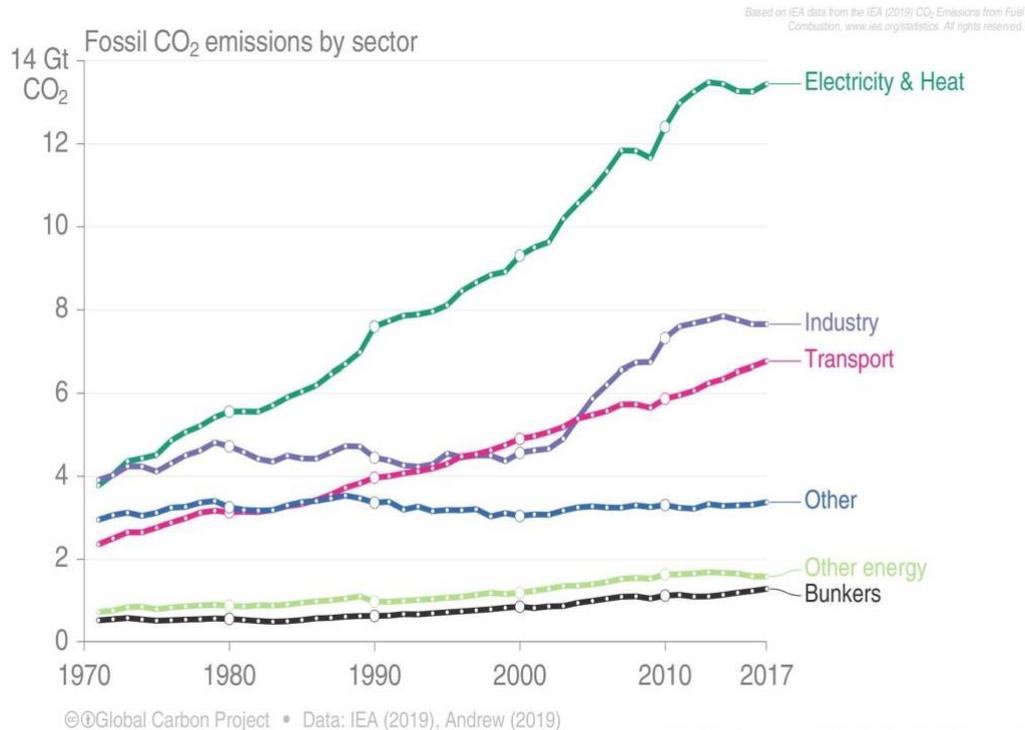


Figure 10. Fossil carbon dioxide emissions by sector [52]

Finally, as highlighted by the above graph's evolution over the years, extracted by IEA energy outlook, industry provides the second highest contribution in terms of fossil CO₂ emission, almost reached by the transport sector. Thus, the use of hydrogen could mainly provide the opportunity to exploit low-carbon hydrogen to decarbonise the metallurgical industry, in particular the annealing processes of steel, and also the reduction of iron ores with H₂, being this one together with nitrogen, the common reducing atmospheres for the production of carbon steel.

4.2 Electrolysers application for green hydrogen production

Following the discussion of the Section 3 of this dissertation, about the main technologies of water electrolysis, the next step is to focus the attention on their applications and the way to exploit the sustainable, carbon-free produced hydrogen.

Electrolysers used for industrial applications are generally weakly affected by the requirement of dynamic performance due to the fact that they work for most of the operating hours at the nominal point conditions. This is possible because, as in the case of the chemical industry or steel industry previously explained, there is a constant and predictable demand for hydrogen over time. This observation could be also extended to the mobility sector, especially the related one to public transport, where the request of H_2 for the refuelling station may occur during the night. On the contrary, only if the electrolyser has been assigned the task of providing ancillary services to the grid, a more specific dynamic behaviour of the machine becomes important and it has to be established and evaluated by the Transmission System Operators (TSOs).

For some years now, new market applications for green hydrogen produced by electrolysers have emerged, creating a good opportunity of investment, even if some at the early stages:

- long-term grid energy storage and integration of variable RES such as wind and solar energy;
- capability of provision of ancillary services to the grid such as frequency and voltage regulation;
- injection of hydrogen into the natural gas network, in a blended configuration or in a own pipeline;
- stand-alone off-grid energy systems mainly for back-up power and microgrid applications;
- production of sustainable, carbon-free fuel for different types of Fuel Cell Electric Vehicles (FCEVs), considering the example of cars, and above all buses.

4.2.1 Grid ancillary services

Electrolysers can act as a variable electrical loads for a flexible demand condition, thanks to their capacity to be connected or not, and regulated when is requested by the grid operators. Thus, they are able to satisfy several grid balancing services, which are necessary for the correct functioning of the electricity system whose goal is to always provide a balance between supply and demand, maintaining a stability of frequency and grid voltage within a certain fixed range. They have to ensure that the available capacity is sufficient to satisfy peak demand over time even in extreme conditions. These ancillary services could be associated, for example, with the primary production of hydrogen for industrial plant, going to constitute a further business for the electrolysers market. However, mainly PEM electrolysers currently appear to be suitable to better respond to the market for network balancing services. SOEC technology are the most disadvantaged, precisely because of the high temperature which places stricter limits on their dynamic operability. In fact, there are many issues related to the heat management and the thermo-mechanical fatigue that it will be induced by the cyclic thermal load and for the fast changing in operation to follow the load.

Their ability to carry out certain network services while withstanding even very severe dynamic performance parameters is a point of attention that must be assessed in detail for each individual electrolytic technology. However by far, the implementation of frequency control and the formulation of the requirements to establish the performance of the electrolysers for load flexibility and response time, is not yet univocally defined. In the different member states of the European Union, load versus time profiles included in the pre-qualification requirement of each transmission system operators diverge, for what concern the three grid balancing services identified in Regulation EU (2017) 1485 [4].

The Joint Research Centre, in the “EU Harmonised Protocols for testing of low temperature water electrolysers” [4], in order to harmonise the different profiles it suggests an agreement on a set of representative load versus time profiles to be adopted in the pre-qualification process. The different severe load profiles are reported in the following Table 6, at which corresponds a set of test protocols to be carried out on the machine.

Table 6. Load profiles for grid balancing

Load Profile for Grid Balancing	
1	Frequency containment reserve (FCR)
2	Automated frequency restoration reserve (aFRR) <ul style="list-style-type: none">• aFRR Negative Control Power• aFRR Positive Control Power
3	Manual frequency restoration reserve (mFRR) <ul style="list-style-type: none">• mFRR Negative Control Power• mFRR Positive Control Power
4	Replacement reserves (RR) <ul style="list-style-type: none">• RR Negative (upward) Control Power• RR Positive (downward) Control Power

Thus, performing the abovementioned protocols to assess the dynamic behaviour of the electrolyser, certain operating characteristics in transient regime are acquired, such as:

- the initial system response to positive and negative power steps, determining the characteristic duration time;
- the ramp-up;
- the ramp-down duration.

Further legislations, still in strong evolution also at EU level, are necessary to make this market an opportunity of business.

4.2.2 Hydrogen mobility

Observing the previously proposed Figure 10, not only industry represents an issue for what concern fossil CO_2 emission, but even the transport sector is increasingly going to constitute a main actor in greenhouse gas emissions. The different trends in the use of the produced hydrogen are illustrated in the Figure 11, where some of which have already been described, with now the addition of the mobility pathway, highlighted with green circles.

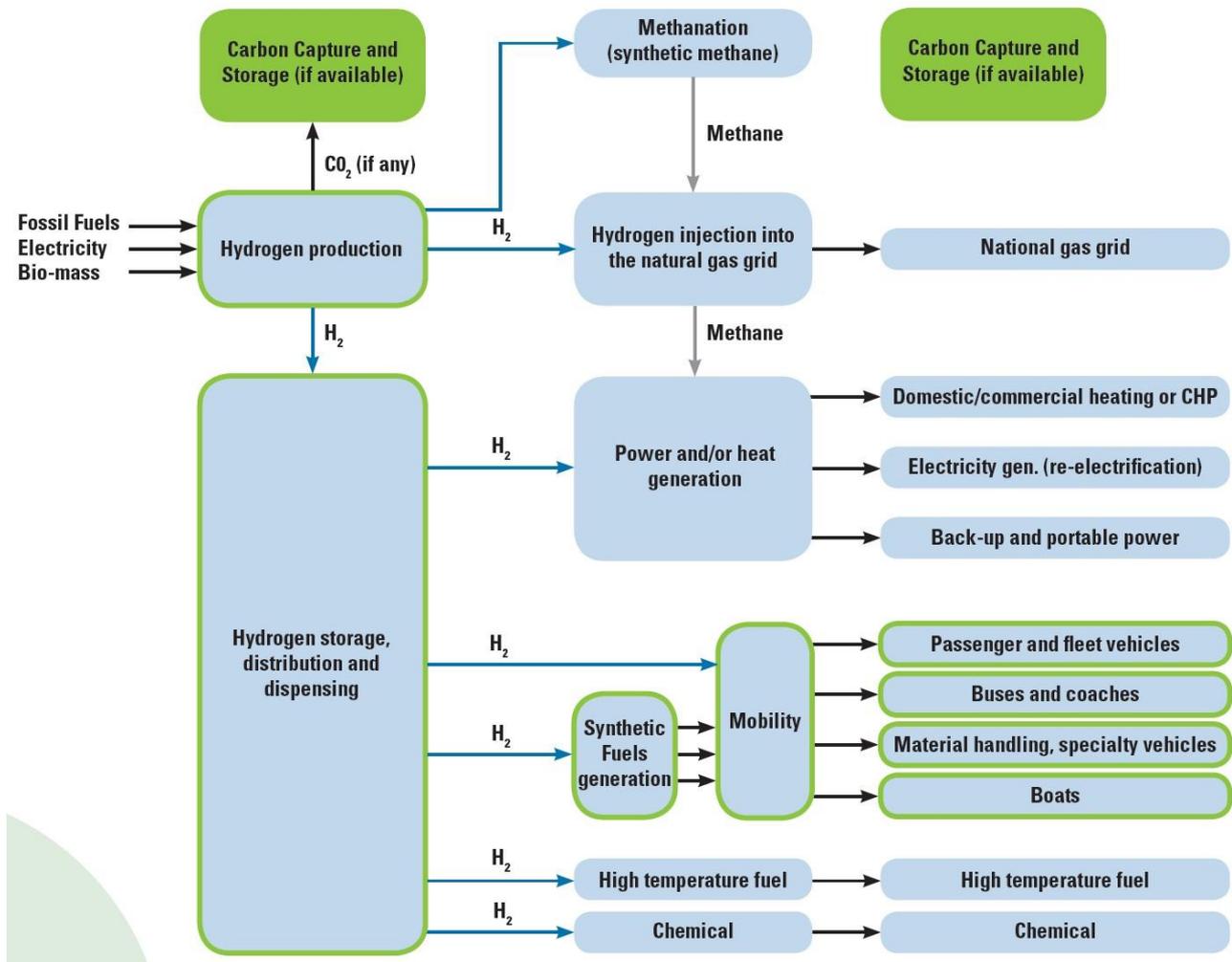


Figure 11. Hydrogen as a versatile energy carrier for several markets [53]

As shown, synthetic fuels or directly H_2 can represent a low-carbon or even zero-emissions fuel for vehicles, becoming a key market for achieving sustainable mobility in the near future, for different types of final users. Regarding the hydrogen infrastructure a possibility is to exploit the

already existing refuelling stations, in terms of current network of road fuel dealers, even if new decentralized supply options have been made available, such as hydrogen filling stations built in the depots of the public buses. Nevertheless, nowadays, the decarbonisation of light commercial vehicles used for the logistics and mobility of urban people seems to be more feasible through electrification. Mainly it is due to the fact that these solutions are already widely widespread on the market and with a charging network under development [49].

It becomes necessary to make a first comparison between what is the main features of hydrogen and full electric mobility, to better understand if they are only two competitors or whether in the short-term they can be complementary.

Table 7. Pros and cons of Battery and Fuel Cell Electric Vehicles [53]

Technology	Battery electric vehicles (BEVs)	Fuel cell electric vehicles (FCEVs)
Advantages	<ul style="list-style-type: none"> Existing recharging infrastructure largely in place (electricity grid) Well suited to smaller vehicles and shorter trips High grid-to-wheel efficiency low price/km fuel cost 	<ul style="list-style-type: none"> Long range possible (more than 400 km) Refuel in 3 minutes (or for instance in case of buses no more than 10 minutes) Wide range of primary sources of energy for hydrogen fuel
Disadvantages	<ul style="list-style-type: none"> Limited range based on existing battery technology Long recharge times (6-8 hours standard (3kw), 30 minutes fast charge (50kw)) Generally required off-street parking for home charging 	<ul style="list-style-type: none"> Need national network of refuelling stations Lower grid-to-wheel efficiency compared to BEVs when using hydrogen produced from renewable electricity

In the Table 7 two types of electric vehicles are analysed: a fully electric system powered by battery (BEV), and one powered by a fuel cell (FCEV). The state of the art of the two technologies allows to understand where the immediate use of hydrogen can play a crucial role in the decarbonization of the transport sector. In fact, heavy transport of goods and people vehicles will be responsible for an increasing share of greenhouse gas emissions, with a 98% diesel transport fleet [49]. They could be replaced with propulsion systems consisting of fuel cells, an advantageous solution even compared to the hypothesis of using plug-in battery electric vehicles, both in terms of payload and consumption. In fact, up to now, with the same total mass of the vehicle, in order to guarantee the same distance, battery electric vehicles would have a very limited payload [54]. On the contrary FCEVs show comparable values to those of today's diesel vehicles. This is of great interest considering the fact that the freight transport sector has a very significant weight in terms of energy consumption, accounting for over 40% of the total consumption of all liquid fuels for road use in the EU-25 [55]. In addition to an acceptable payload, heavy hydrogen vehicles have the advantage of extremely fast refuelling times when compared to purely electric vehicles. FCEVs do not emit CO_2 or other pollutants generated in combustion, such as NO_2 and fine dust, that are harmful to human health. To these important benefits is added an effect, although minor, of purification of the air sucked in by fuel cell systems [49].

Several global initiatives have been undertaken in the last years to support the diffusion and scale-up of the hydrogen technologies and implementations with the main development occurring in Japan, China, UK, USA especially California, home to FCEV's largest road fleet in the world.

For what concerns the European context, several countries already have H_2 mobility programs that include political and financial incentives, with a significantly expected growth after 2020. In particular, linking to the topic of this dissertation, hydrogen buses are widespread throughout Europe, with vehicles in operation and many others which are planned.

As far as Italy is concerned, it is worth highlighting the presence of a fleet of Fuel Cell Electric Buses (FCEBs), especially in Bolzano, within the CHIC project, as demonstration of the readiness of fuel cell electric buses for a widespread commercialization. The trial involves 23 partners from 9 cities of 8 European Countries, with 60 buses in operation of which 26 are co-funded by the Fuel Cells and Hydrogen Joint Undertaking (FCH JU) and 9 hydrogen refuelling stations (350 bar) relying on €25.8 million of FCH JU co-funding, for a total budget of €81.8 million [56].

This is only an example of the different activities which have covered the last decade and which will develop with increasing vigour starting from 2020.

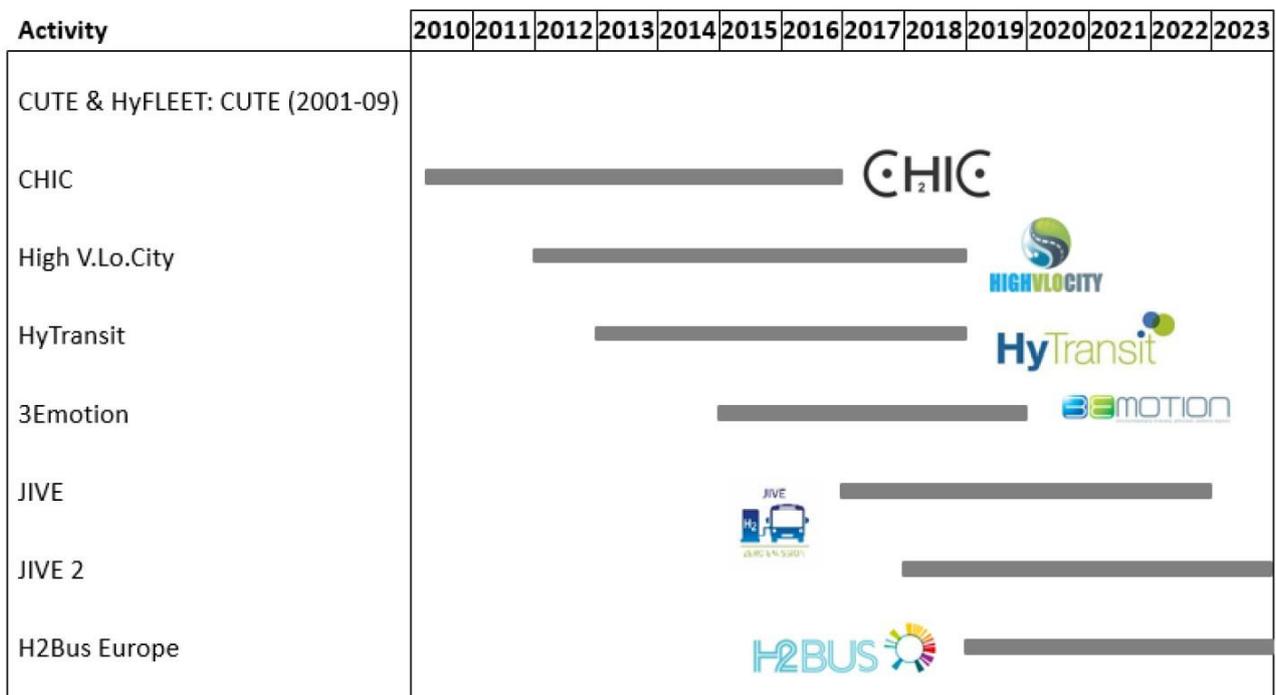


Figure 12. Timeline of European demonstration projects [57]

In Figure 12 the name of the different projects are reported and, in particular thanks to the Joint Initiative for Hydrogen Vehicles across Europe (JIVE) and H2BUS campaigns, a further deployment of a consistent fleet of hydrogen buses all over the Europe, is also expected in the next decade.

However the path has just been traced: further efforts are needed in order to allow an economy of scale of this new way of thinking the mobility, overcoming the issue related to the price at which hydrogen is sold at refuelling stations, compared to the use of traditional fuels.

Therefore, the goal of this master thesis' work is to carry out a techno-economic analysis on the price of H_2 , produced by the water electrolysis systems and delivered to the final users through the dispenser at the hydrogen refuelling station (HRS). The study has to be carried out making a sensitivity analysis of the different parameters involve in the overall system, with the aim of verifying whether a final price is in the range of currently available fuels.

In case of steam methane reforming, hydrogen costs depend mainly on the price of natural gas and thus, H_2 is produced on a large scale, in large plants, with the following prices:

- 0.65 €/kg in the US;
- 1.60 €/kg in Europe;
- 2.32 €/kg in Japan [54].

These values are based on IEA calculations that consider the following natural gas prices: 9.43€/MWh in the United States, 26.83 €/MWh in Europe and 40.61 €/MWh in Japan [54].

However, considering that the final use is for mobility purpose, at this €/kg must be added those for distribution, compression at higher pressure and for the HRSs. Therefore, this particular application can in principle tolerate a higher cost of hydrogen per kg delivered to end users. Thus, considering a not stable current price of gasoline and diesel of about 1.6 €/L, up to 1.9 €/L, and taking into account a suppose average car fuel consumption of 8 L/100 km for gasoline, final costs of 12.8 € up to 15.2 € every 100 km are derived [58]. Hence, on the basis of this, for hydrogen can be estimated that the €/kg for the final user may be in this price range since, as highlighted in “Piano Nazionale di Sviluppo–Mobilità Idrogeno, Italia”, with 1 kg of H_2 there is the same mileage in kilometres for the cars, as with slightly over 7 litres of gasoline [54].

On the other hand, for what concerns the bus fuel consumption, a value of 38.04 L/100km can be assumed, leading to obtain around €66.19, up to €72.28 every 100km for diesel buses, derived using the previously reported prices [54]. However, a value slightly lower than 10 kg of hydrogen, to cover 100 km, are required for a bus, unlike the car case [54]. Hence, this means that in order to be competitive with diesel, prices must show a range to the end user between 6 and 8 €/kg of hydrogen produced.

5. Case study on FCEB for hydrogen mobility

The FCEBs performance has been recently tested and validated in Europe through several demonstration projects, but more actions are still required to allow their commercialisation:

- FCEBs must satisfy the high availability levels requested by public transport sector;
- capability to cope with the high ownership costs relative to conventional buses;
- a well-established HRS to provide reliable and low-cost hydrogen;
- increase understanding of the potential of FC buses for zero emission public transport.

Among the various European initiatives mentioned in the previous sections, the activity carried out by JIVE is tracing the path to commercialization by addressing the above listed issues through the deployment of 142 FCEBs across 9 locations, more than doubling the pre-existing number of operating buses in EU. JIVE, adopting coordinated procurement activities, is trying to unlock the economies of scale which are required to reduce the cost of the public transport. The task is to reduce the overhead costs per bus, allowing more efficient supply chains and maintenance operations, compared to previous deployments, adopting single fleets of 10-30 buses. JIVE will also test new hydrogen refuelling stations with the required capacity to satisfy the demand of more than 20 buses. All this is an attempt, not only to reduce the costs of hydrogen and increase the availability of equipment, but also to test the capability to guarantee very high reliability, more than 99%, which is fundamental for the commercialisation of FCEBs [59].

In particular for the case study that will be presented, the successor of the JIVE initiative will be taken into account. The second Joint Initiative for hydrogen Vehicles across Europe (JIVE 2) started in January 2018 will ended in the 2022 with the aim of deploying, 152 FCEBs across 14 European cities in different countries such as France, Germany, Iceland, Norway, Sweden Netherlands and the UK. Among them, Auxerre in France, Gavleborg in Sweden are only some examples of cities that are at the first experience and are trying to build their know-how by demonstrating small fleets of FCEBs. Thus, considering the previous contribution given by the JIVE demonstration, it will deploy nearly 300 fuel cell buses in 22 cities and regions across Europe [60].

The new realities will be supported by the several industrial partners in regions where the experience of the technology scaling up their FCEBs fleets is already consolidated, as in the case of Cologne and Wuppertal in Germany.

The latter is precisely the reference situation that has been chosen for the case study of this dissertation. The German regional transit agencies Regionalverkehr Köln GmbH (RVK) in Cologne and WSW Wuppertaler Stadttwerke GmbH in Wuppertal through the project “Zero Emission” have set an ambitious goal to replace the entire diesel bus fleet with alternative powertrains, by 2030. In order to reach the goal of zero emissions there were only two choices that could be made: hydrogen or full electric mobility. Therefore an accurate analysis of the best possible solution to be adopted was carried out, considering three main factors:

- the buses, especially in the Cologne region, travel no less than 250-300 kilometres a day;
- a fixed and rigid operation schedule has to be respected;
- the instability of the electricity grid.

In fact considering the charging of the battery electric buses during the day, it would not have been possible to do it on route or even in the return to the depot. In light of all this to meet the requirements for range, flexibility and refuelling time, FCEBs seem to be the best solution to implement [61].

Belgian bus builder Van Hool has signed an ambitious contract with RVK in Cologne and Wuppertal to provide 40 new generation FCEBs. After which they submitted a purchase order to their Canadian-based Ballard Power Systems partner, for 40 FCveloCity®-HD fuel cell modules to power buses in the two German cities [62]. As it is possible to see from Figure 13, Ballard fuel cell products are increasingly present all over the world and it is a Europe’s leading fuel cell company with more than 100 employees in Denmark, Germany, UK, Norway and France, mainly focused on R&D, engineering, manufacturing, and sales [63].



Figure 13. Hydrogen buses all over the world [63]

The order required by RVK consists of 30 FC buses for Cologne and 10 for Wuppertal, both major cities in the North Rhine-Westphalia. The bus is designed for 29 seats plus 49 (Wuppertal) and 46 (Cologne) standing passengers [60]. The bus procurement is supported under the previously cited JIVE 2 funding program financed by the EU’s Horizon 2020 programme “H2020-EU.3.4.” and “H2020-EU.3.4.6.1.” coordinated by Element Energy Limited (UK) [64].

5.1 Hydrogen bus technology

The buses for Cologne and Wuppertal are Van Hool A330 hybrid fuel cell-battery vehicles, 12 m long with dual axles, equipped with the latest FCveloCity-HD85 fuel cell from Ballard, and with a 210 kW Siemens electric traction motor [60]. However, for a better understanding of the technology used, a briefly overview on the different types of buses and operation has to be carried out.

A fuel cell electric bus is an electric bus that presents both hydrogen fuel cell and batteries or capacitors. The hybrid configuration allows to optimize in the best way the size of each components for a given route. A compressed hydrogen is used as fuel, instead of storing energy in large batteries. The H_2 is sent to the FC power module onboard the bus, which through an electro-chemical process, generates electricity, which then is exploited to power the hybrid electric motors, providing electric traction and charging the energy storage system. Water and heat are the only by-products of the reaction, thus there are no local emissions. Moreover, the heat by-product is stored on the brake resistors and is used to maintain heating passenger comfort and considerably increase the fuel economy and energy efficiency. The batteries are able to provide peak power to the motors to meet rapid acceleration and gradients [65]. All the energy for the bus, required to operate is provided by hydrogen stored on board. In fact, high pressure tanks located on the roof of the bus store hydrogen fuel, providing sufficient range for almost a full day of operation. This long range is possible thanks to the fact that this gas shows a higher energy density compared to electrical storage systems such as batteries [61].

Although most of the hydrogen is produced by steam reforming of natural gas, the majority of hydrogen refuelling stations are based on hydrogen for low and zero carbon sources. Thus, taking advantage of renewable electricity, biomass, including carbon capture and storage and on-site production of H_2 by means of water electrolyzers, FCEBs guarantee a completely zero carbon solution to public transport.

Furthermore, as reported on the website of Ballard company, refuelling time for FC buses only up to 7-10 minutes are required, that is a strongly advantage with respect the long time needed in case of electric battery.

There are standard or articulated buses. The former differ from each other according to which component prevails more over the other. They are long 12-13 metres and can have a small battery and a large FC, or a large battery and a fuel cell as a range extender to increase the overall

performance. Another possibility is to replace the battery with a supercapacitor which then works together with FC. Instead, for what concern, the articulated buses, they are long 18 metres and show a large battery and a fuel cell used as a range extender [65].

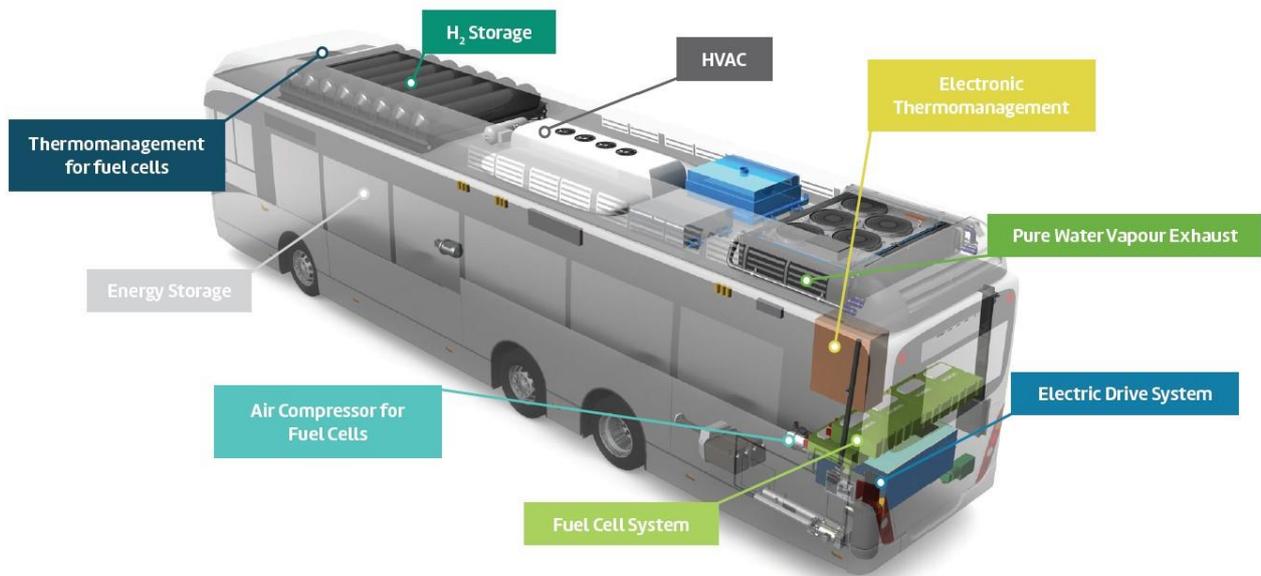


Figure 14. Main components of a fuel cell electric bus (FCEB) [61]

From the above Figure 14, extracted by the report of Ballard about the case study on “Fuel Cell Zero-Emission Buses for Cologne Region, Germany”, the main components of the bus are highlighted. High purity standards are a must for this application, as specified in ISO 14687, as well as a high supply pressure of 350 or 700 bar, depending on the type of vehicle, with the latter pressure which can be reached by external recompression.

The FCEBs is an all-electric zero emission solution that offers an operation close to that of a diesel buses, a promising solution for the sustainable transport sector.

5.2 Techno-economic input data for the mobility case study

The aim of this techno-economic analysis is the evaluation of the entire manufacturing and exploitation chain of hydrogen, starting from on-site production by means of an electrolyser, up to release to the dispenser of the refuelling station, taking into consideration all the costs that can be encountered.

The case study is carried out considering the introduction of a fleet of hydrogen-powered buses, in a context of urban mobility. In particular, it has been chosen, as a reference scenario, two fleets of FCEBs. The first one is located in Wuppertal:

- 10 buses in operation;
- 10 buses planned;
- size of 12 metres;
- project: JIVE and JIVE2 ;
- Van Hool and Solaris as bus supplier [65].

The second, on the other hand, is one of the largest in Europe and is deployed in the Cologne region:

- 37 buses in operation;
- 13 buses planned;
- size of 12 metres;
- project: JIVE and JIVE2 ;
- Van Hool and Solaris as bus supplier [65].

In the case study, the two fleets of FCEBs are analysed together, as they are managed by the same regional operator RVK. Compared to the purchase order to Van Hool, Solaris and Ballard, executed by RVK in 2018 previously mentioned, recently a further request for hydrogen buses has been carried out. This is the reason why between the ones in operation and those planned there is a total number of 70 buses.

It is necessary to point out the main characteristic of these fleets of FCEBs in order to make use of it for the economic and technical analysis.

Table 8. FCEBs data input

Input Parameters	
Number of units:	47 [65]
Bus availability [day/y]:	365
Daily distance covered (per bus) [km/day]:	350 [60]
Fuel consumption [kg/100 km] 2020:	8.88 [63]
Fuel consumption [kg/100 km] 2030:	7.3 [54]
Delivery pressure [bar]:	350 bar [63]
Hydrogen tank capacity [kg/day bus]:	38.2 [60]
Refuelling time [min]:	7-10 [63]

The Table 8 above lists the different input data, also extracted by the Ballard's webpage, in which a bus consumption of 11.26 km for 1 kg_{H₂} is reported, thus the value is referred to a distance of 100 km. Furthermore, for the 2030 scenario, taking into account an improve in FCEBs technology a value of 7.3kg of H₂ is adopted to cover 100 km.

Regarding the bus availability an hypothesis is proposed: it is supposed to be extended for all the year, capacity factor $CF_{year} = 100\%$, with the possibility of recharging vehicles during the night $CF_{day} = 50\%$.

The idea is to make the process as sustainable as possible, thus the hydrogen is assumed to be produced by an on-site water electrolyser, therefore not considering the transport to the point of use. A possible relevant source of CO₂ can be represented by the generation of electricity that is extracted by the grid to feed-up the electrolyser. However for example by using a photovoltaic system this type of issue can be overcome by making the system even more carbon-neutral.

For the electrolyser the three main technologies previously described and compared in this thesis have been considered: AEC, PEMEC, SOEC.

This dissertation has two main purposes. The first is to carry out a techno-economic analysis of the current state of the technologies. The consequent idea is to propose a further future temporal scenario, in particular 2030, in which the impact that the expected technological development could have on the final sale price of hydrogen to the consumer is assessed. Therefore a comparison is made between different technologies and in different time periods in which they operate, verifying if perhaps a technology that is cheaper today may not be in the future.

Nowadays, even if some multi-MW-scale of alkaline and PEM are implemented, in this work, as starting case, a size of 1 MW is selected for both the technologies. This decision is supported by the fact that in several European projects a size of this type is chosen for the mobility purpose [66].

Moreover, in the “Store&Go analysis” of the future technology options and on the techno-economic optimization [67] an average maximum size of 1.2 MW and 0.5 MW, respectively for PEMEC and SOEC, are indicated, in the case of 2020 scenario.

Table 9. Techno-economic input data to the AEC

AEC	2020	2030
Operating pressure:	1 bar [24]	30 bar [24]
Power consumption (system):	52 kWh/Kg [7]	50 kWh/Kg [7]
Stack degradation:	0.12 %/1000 h	0.097%/1000 h
Stack lifetime:	81111 h	102564 h
CAPEX system:	1088 €/kW	713 €/kW
CAPEX stack replacement:	381 €/kW	249 €/kW
OPEX system:	3% [26]	3% [26]

In Table 9 are listed the data input to the case study for AEC. For the 2030 scenario, the goal is to further improve efficiency and reduce costs, thanks to an economy of scale and technological development. Among the parameters that may be most affected by a technical improvement there is certainly the degradation rate. In particular, 1.1% per year and 0.85% per year, respectively for 2020 and 2030, are the values of stack degradation chosen. These are selected taking into consideration the range proposed in the literature, 0.25 – 1.5 %/y, reported in Table 2. However, precisely those data are used because they are also validated by the similar ones obtained exploiting a linear interpolation between the 2017 and 2025 stack degradation values reported in reference [41]. At the base of the calculation of all these degradative parameters, there is the assumption of stack replacement when a percentage degradation level of 10% is reached, leading to obtain the final values of stack lifetime proposed [41].

For what concerns the capital expenditure, the final choice is to make use of the capital expenditure for system and stack replacement obtained by the linear interpolation of the values provided by the FCH JU in its hydrogen business case [41].

Many other CAPEX have been taken into account or evaluated as possible alternatives. In the “Cost reduction potential for electrolyser technology” [66], alkalines’ price are provided in the kW scale, precisely 312kW, for 2015 and 2030. Therefore, in order to get the right value for a size of 1 MW, the following relationship is a common method of estimating costs by scaling:

$$C = C_0 \cdot \left(\frac{S_0}{S_{ref}} \right)^f \quad (5.1)$$

Where

- C is the questioned equipment cost at the appropriate scale;
- S_0 the size, capacity or nominal power of the questioned component;
- C_0 and S_{ref} represent the cost and scale of the known reference component, respectively;
- f is the scale factor applied to the technology in question, assumed equal to an average value of 0.75 [67].

This procedure allows to compute a CAPEX system of 1335 €/kW for 2030 and a final result of 1600 €/kW is reached for 2020 year, after have also carried out the linear interpolation in this last case. Further values present in the literature were observed to understand which could be the most correct value to use, as examples for the 2020 year:

- CAPEX system 1500 €/kW , CAPEX stack replacement 450 €/kW [67];
- CAPEX system 800 – 1400 €/kW , CAPEX stack replacement 550 €/kW [68];
- CAPEX system 744 €/kW , CAPEX stack replacement 339 €/kW [26];
- CAPEX system 1000 €/kW , CAPEX stack replacement 630 €/kW [7].

Hence, comparing the different investment costs required for system and stack, the ones reported in Table 9 have been selected, in order to carry out a techno-economic analysis in a mild scenario. This data is also validated being the same reported in the “Piano Nazionale di Sviluppo – Mobilità Idrogeno, Italia” for 2020 scenario [54].

The same approach is adopted for the remaining two technologies, even if in the case of SOEC a reduction of the size investigated has been considered, due to the limitations of the device, being yet at the early stage. In this case, as previously introduced, a size of 0.5 MW is adopted as reference configuration and supported by the state of the art of the technology [67].

Table 10. Techno-economic input data to the PEMEC

PEMEC	2020	2030
Operating pressure:	30 bar [24]	80 bar [24]
Power consumption (system):	57 kWh/Kg [28]	51 kWh/Kg [28]
Stack degradation:	0.17 %/1000 h	0.11 %/1000 h
Stack lifetime:	60000 h [24]	75000 h [24]
CAPEX system:	1333 €/kW	1000 €/kW [66]
CAPEX stack replacement:	533 €/kW	400 €/kW [66]
OPEX system:	3% [26]	3% [26]

For what concerns the PEMEC, in Table 10 the two extreme limits of the pressure range are considered for the working operation of the years selected. Instead, regarding the power consumption, the values are assessed, starting from an efficiency of 58% and 65.5%, referred to the LHV, respectively for the 2020 and 2030 scenario. Unlike the AEC evaluation, due to the lack or inhomogeneity of data regarding the annual percentage degradation of the stack, this time it is computed imposing the lifetime, as the average of the ranges proposed in Table 3, for the two time periods.

The capital expenditure of the system is obtained by linear interpolation, consequently the CAPEX stack replacement is computed taking into account a value equal to the 40% of the CAPEX system [66]. Regarding the 2020, 1333 €/kW for the global system is perfectly in line with the other prices previously shown in Table 3, while for the stack component 533 €/kW can be chosen as a precaution, being slightly higher than the values found. Instead in the case of 2030, the CAPEX system is assumed equal to 1000 €/kW and for the stack replacement 400 €/kW. For what concerns the first value, carrying out a careful analysis on the values found in the literature, 918 €/kW or 650-1500 €/kW are some alternatives [28] [24]. In the long-term it would seem that proton exchange membrane technology may have lower cost than alkaline, especially regarding the stack

component, although this would appear to occur for years beyond 2030 in most of the scientific journals analysed [69] [7].

Therefore, in order to continue to carry out a techno-economic case study that is however precautionary, and as realistic as possible to current perspective, the fairest value to use seemed to be that of 1000 €/kW, also to be coherent with the other selections.

Table 11. Techno-economic input data to the SOEC

SOEC	2020	2030
Operating pressure:	1 bar [23]	30 bar [23]
Power consumption (system):	43 kWh/Kg [28]	37 kWh/Kg [70]
Stack degradation:	0.50 %/1000 h [24]	0.20 %/1000 h [24]
Stack lifetime:	20000 h [24]	50000 h [24]
CAPEX system:	3154 €/kW	1800 €/kW
CAPEX stack replacement:	788 €/kW	270 €/kW
OPEX system:	3% [42]	3% [42]

For the latest technology, numerous problems and issues have been encountered in the choice of input data due to the still early stage of the solid oxide electrolyte system. In fact, in the literature there are very few studies, compared to AEC and PEMEC, on future forecasts both as regards operational and economic parameters and there is also a strong divergence on these values. Therefore, unlike the other two cases, a new path has been undertaken: for the 2020 a more conservative scenario is adopted as for AEC and PEMEC, instead for the 2030 year a more aggressive, but always in line with the literature, is selected. This approach is validated by the strong reduction of cost expected for the SOEC technology, showing the highest learning rate among the water electrolysis technologies [67].

First of all regarding the pressure for the second temporal scenario, a precautionary value is used, even if the forecast in the long-run is for an increase of more than 30 bar. Regarding the power consumptions, they are selected in two different ways. For the year 2020, the value is computed starting from an efficiency of 77,5%, with respect to the LHV; instead a further reduction is expected towards the 2030, with the proposed parameter. This is possible, with respect to the AEC and PEMEC, thanks to the high working temperature, as explained in the previous sections.

One of the main problems is the evaluation of the stack degradation and consequently the stack lifetime of the SOEC. In fact, this parameter is hardly provided among the different scientific papers, if not in a very approximative range such as 3-50 %/a. This span can be identified with values starting from 1750 hours up to a maximum of 30000 hours. For this reason, an hypothesis has been done, considering a mean value for the stack lifetime of 2020 and 2030, respectively from 10,000-30,000 hours and 40,000-60,000 hours [24]. After that, the stack degradation is evaluated as in the case of AEC and PEMEC, considering that its end of life occurs when the 10% degradation value is reached.

A further difficulty is highlighted by the assesment of the investment costs for the system. Several values present in the literature have been observed to understand which could be the most correct one to use. For instance, the following CAPEX system are suggested, respectively for the case of the 2020 and 2030:

- CAPEX system 3294€/kW, CAPEX system 2374 €/kW, obtained by linear interpolation of the proposed values for 2017 and 2050 scenarios [69];
- CAPEX system 2250 €/kW, CAPEX system 1250 €/kW, where the last value is deduced by the graph in the reference [68];
- CAPEX system 1990 €/kW, CAPEX system 1060 €/kW [67];
- CAPEX system 3400 €/kW, CAPEX system 1537 €/kW [28];

The last two values are of a more recent study and it is reported for a mild scenario, even if, for the 2020, compared to the other results, the investment cost 3400 €/kW appears to be the highest. Instead the CAPEX system equal to 1990 €/kW for 2020, and 1060 €/kW for 2030 are so low with respect to the others, since they have been evaluated referring to a size of 5 MW. Therefore starting from them, a cost function has been implemented to obtain the new values of CAPEX for the size of the SOEC investigated in this study, that is equal to 500kW:

$$\frac{c_a}{c_b} = \left(\frac{S_a}{S_b}\right)^{n_2} \quad (5. 2)$$

Where:

- c_a and c_b are the specific costs (€/kW) investigated and taken as a reference, respectively;

- S_a and S_b are the sizes expressed in kW, 500 kW and 5000 kW, respectively;
- $n_2 = n_1 - 1$, being n_1 the average scaling factor for SOEC, assuming different values according to the temporal scenario: $n_1 = 0.8$ for 2020 and $n_1 = 0.77$ for 2030 year [67].

From the above cost function the following values are assessed:

- CAPEX system 3154 €/kW for the 2020 scenario;
- CAPEX system 1800 €/kW for the 2030 scenario.

Hence, observing all the proposed values, they have been chosen to be consistent with the hypotheses previously made: a more aggressive learning rate over the year with respect to the AEC and PEMEC, thus a more optimistic prospect for SOEC, but always taking as a reference a realistic scenario to be achieved by 2030.

If with regard to the investment costs of the system some information could be found in the literature or evaluated, this cannot be said for the cost of the stack replacement. In order to proceed with the analysis an hypothesis on the ratio between the investigated value and the overall system cost is performed. Unlike the AEC and PEMEC, the cost percentage of the stack with respect to the auxiliary components, forming the global system is lower. The reason is explained in the previous section on SOEC, but can be resume with two main points:

- higher cost of the balance of plant in terms of resistance of the material used, due to the higher temperature;
- lower request of precious stack material, in particular for catalytic activity and conduction in the electrolyte, thanks to the higher kinetic imposed by the elevated values of temperature.

Therefore a value of 25% and 15% of impact of the stack on the global system cost is considered for the years 2020-2030, respectively [67].

5.3 Methodology

The techno-economic data highlighted in the previous section in Tables 9, 10 and 11 regarding the three electrolysis technologies, alkaline, PEM, and SOEC, are the inputs for the study developed, for both the two temporal scenarios: 2020 and 2030 years.

The economic analysis for the investigated mobility case study is carried out by reporting the calculations for the cost of hydrogen production as Levelized Cost Of Hydrogen (LCOH). The LCOH is intended as the current minimum average price at which the green hydrogen generated by the electrolyser must be sold to offset the total production costs over its lifetime. The following formulation is the one used to compute this metric:

$$\frac{\sum_{t=1}^n (CAPEX_{stack} + CAPEX_{no-stack} + OPEX + Electricity + Water + Steam - Salvage Cost)_t \cdot (1+r)^{-t}}{\sum_{t=1}^n (Produced\ hydrogen \cdot (1+r)^{-t})} \quad (5.3)$$

As it is possible to understand from the above-reported formula, all costs incurred during the useful lifetime of the plant are included in:

- CAPEX investment costs;
- operation and maintenance costs (OPEX);
- costs associated with mass flow entering the plant, in terms of water, steam or electrolytic solution, as in the case of AEC;
- costs associated with energy flow entering the plant, in terms of electricity.

all is discounted using a fixed interest rate (r) at 5%, that is, assumed equal to the weighted average cost of capital (WACC) [41].

Furthermore, in order to make the techno-economic analysis more precise a salvage cost has been taken into account for the evaluation of the LCOH. It represents the economic value of a component at the end of the analysed period of the global system (called L_{PR} equal to 20 years) and it is supposed to be directly proportional to its remaining life. This term is considered for components that are potentially subjected to replacement, as in this study in the cases of the stack replacement and HRS lifetime.

The salvage cost has been assessed in the following way:

$$C_{sal,i} = C_{rep,i} \cdot \frac{L_{rem,i}}{L_i} \quad (5.4)$$

where L_i is the component lifetime in years; $C_{rep,i}$ is the replacement cost of the investigated component; $L_{rem,i}$, also in years, is the remaining lifetime of the component at the end of the project lifetime and is given by (for $L_i \neq L_{PR}$):

$$L_{rem,i} = L_i - \left[L_{PR} - L_i \cdot INT \left(\frac{L_{PR}}{L_i} \right) \right] \quad (5.5)$$

where INT is a function that returns the integer amount of a real number. Obviously, $L_{rem,i}$ is zero in case $L_i = L_{PR}$.

For what concerns the denominator of (5.3), it expresses the quantity of hydrogen in kg produced annually by the electrolyser system in order to satisfy the overall demand.

It is worth to point out a clear subdivision of the global system, in order to understand which components the costs refer to. The capital expenditures regarding the electrolyser provided in the previous Tables 9, 10 and 11 with the name CAPEX system are referred to:

- stack;
- gas conditioning;
- power electronics;
- balance of plant.

The last three terms can be defined as auxiliary equipment of the electrolyser, and therefore their overall cost can be calculated through the difference between the values proposed of CAPEX system and stack replacement for each technologies and temporal scenario.

Therefore, in order to form the total required CAPEX of the global plant, in addition to the CAPEX of the stack replacement, other costs must be highlighted to compose with the auxiliary components the $CAPEX_{no-stack}$:

- civil works;
- engineering;
- control and management system;
- interconnection, commissioning and start-up.

However the hydrogen produced by the electrolyser is not at the proper operational condition to be used. A compression station, and its respective cost, has to be taken into account to deliver the hydrogen at the right pressure equal to 350 bar to the hydrogen refuelling station. Even the capital expenditure of the latter has to be evaluated to carry out the techno-economic analysis.

Furthermore, in order to guarantee a continuous service of the hydrogen mobility of the FCEBs, failures relating to the on-site production of hydrogen must also be managed. Hence, the presence of a storage with a capacity such as to cover the daily hydrogen requirement is considered.

This value of daily requirement is assessed starting from the daily consumption of hydrogen of a bus, that is for instance of about 31.1 kg, for 2020 scenario. At this point, it is possible to calculate the total daily and annual consumption equal to 1,461 kg/day and 533,177 kg/year, respectively, which are referred to the 47 units involved in the study. The cost of storage is assumed to be 470 €/kg, value unchanged between 2020 and 2030, considering the maturity of the pressurized tank storage technology [41].

Therefore the station must be sized in such a way as to supply approximately 1461 kg (or 1201 kg for 2030 scenario) of hydrogen daily to the various buses of the fleet during the night ($CF_{year} = 100\%$, for the buses availability and $CF_{day} = 50\%$, for the electrolyser production).

As regards the costs relating to the compressor, the refuelling station and other contributions to the total CAPEX, the calculation procedure is shown in the Appendix.

Concerning the evaluation of OPEX of the plant, even in this case a subdivision of the contribution has been carried out. A value equal to 3% of the sum of contributions of the auxiliary components costs, capital expenditures of storage and compressor has been assessed. To this, it has been added the OPEX of the HRS, evaluated by means of two fixed values, 0.26 €/kg and 0.19 €/kg for 2020 and 2030, respectively. These results have been assessed exploiting a linear interpolation of the data referred to an OPEX station of 1500 kg/day and 2000 kg/day for 2020, and 1000 kg/day and 1500 kg/day for 2030, being 1615 kg/day and 1440 kg/day, respectively, the hydrogen produced for the investigated HRS [54]. Therefore a final percentage of the station CAPEX equal to 5.5% and 4% have been obtained for 2020 and 2030, respectively.

The main cost assumptions used are summarized in the following Table 12:

Table 12. Techno-economic input parameter

Input Parameters	
Lifetime of the system (L_{PR}):	20 year [41]
Lifetime of the HRS (2020):	12 years [70]
Lifetime of the HRS (2030):	20 years[70]
Discounted rate/WACC (r):	5% [41]
Storage cost:	470 €/kg [41]
Water cost ($C_{H_2O,l}$):	3.8 €/m ³ [41]
Steam cost ($C_{H_2O,v}$):	10 €/ton [71]

As it is possible to see from the table above, a lifetime of the plant is assumed equal to 20 year (L_{PR}). However, there are two exceptions: the stack of the electrolyser and the hydrogen refuelling station. In the first case the duration values shown in Table 9, 10 and 11 have been used, depending on the degradation rate of the technology investigated. Instead for the HRS a lifetime of 12 years has been selected for the 2020 scenario, and 20 years for that of 2030 [70].

Therefore, the different CAPEX_{no-stack} costs, displayed in the LCOH equation, are incurred at the zero year of plant operation, whilst the CAPEX cost attributed to the stack replacement and to the HRS are repeated based on the useful life of them.

As regards the cost of water ($C_{H_2O,l}$), a value of 3.8 €/m³ is assumed considering demineralized liquid water. Instead the term related to the steam refers to the cost of steam production ($C_{H_2O,v}$) assumed to be 10 €/ton, and it is adopted taking as a reference medium pressure industrial steam.

For what concern the cost of electricity (C_{el}), in a first analysis it is considered constant in the calculation procedure of the LCOH. An average German electricity price for industrial final uses equal to 160 €/MWh has been adopted [72]. In a second step the electricity price is exploited as a variable parameter to carry out sensitivity studies on the results obtained.

It is important to underline that this parameter will particularly affect the LCOH value of the less efficient technologies, thus alkaline and proton exchange membrane, whose electricity consumption per unit of hydrogen production is higher, while the more efficient technology such as SOEC is less sensitive to this parameter.

Therefore, the annual costs relating to energy and mass flows have been calculated with the following approaches:

- Electricity = $C_{el} \cdot size_{tot} \cdot CF \cdot 8760$ (5. 6)

where C_{el} is the value of electricity prize previously mentioned, $size_{tot}$ is the overall size of the electrolyser under investigation and CF is the product of the two capacity factors, $CF_{year} = 100\%$ and $CF_{day} = 50\%$;

- Water = $C_{H_2O,l} \cdot \dot{m}_{tot,H_2O} \cdot CF \cdot 8760$ (5. 7)

with $C_{H_2O,l}$ is the water cost reported in Table 12; \dot{m}_{tot,H_2O} is the water flow rate entering the system in nominal conditions for alkaline and PEM, and it has been assessed considering an assumption of 15 L of water per kg_{H_2} [41];

- Steam = $C_{H_2O,v} \cdot \dot{m}_{tot,H_2O} \cdot CF \cdot 8760$ (5. 8)

only taking into account for SOEC technology, working at higher temperature, where a value of about 33 L per kg of hydrogen is assumed [8]. The latter is selected being referred to a size module of the high temperature water electrolyser of about 500 kW.

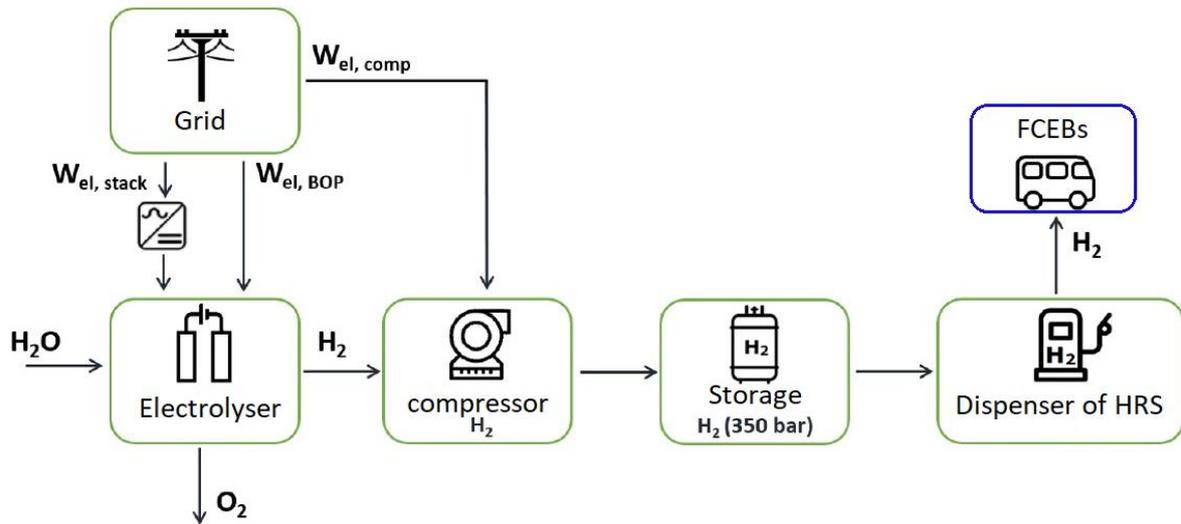


Figure 15. Schematic representation of the plant investigated

In the Figure 15 is shown the schematic representation of the overall investigated plant. It consists of an electrolyser system, for the production of hydrogen, that can be of alkaline, PEMEC or SOEC typology, according to the case selected. It receives, for instance, electrical energy as input from the grid, but the power supply can also be a wind turbine or a photovoltaic system to obtain green hydrogen, with no carbon emission.

Nevertheless in this case, an AC-DC converter is required to feed-up the water electrolysis machine, that works with DC current only. The electrical energy is also necessary to feed-up the compressor, whose consumption has been evaluated by means of the formula of technical work reported in the Appendix, which leads to get different values according to the technologies and temporal scenario selected.

The pressure is raised from the outlet value of the electrolyser, depending on the type, to the set point of 350 bar. After this, the storage system is adopted to cover the daily demand in case of issues related to the HRS, that is the last step of the illustrated chain. The dispensers are able to feed-up the fuel cell electric buses, and then they are ready to fulfil their working day.

6. Results of the techno-economic analysis

The results of the techno-economic analysis, derived from the implementation of the previously explained methodology, are reported in this section of the dissertation.

The electricity price plays a crucial role on the levelized cost of hydrogen trend. The baseline case study shows the average price of electricity for industrial consumption in Germany equal to 160 €/MWh. This value is the highest among the nations of the European area, with reference to a quantity of MWh/year higher than 20 [72]. Consequently, the LCOH increases dramatically, due to the electricity consumption by the compressor and mainly by the electrolyser.

Therefore, it becomes essential to carry out a sensitivity analysis on the cost of electricity. It allows to understand for which values the H_2 price at the HRS dispenser outlet can become competitive, in the completely replacement of the traditional fuels, as for example diesel for transport vehicles.

Figure 16 and Figure 17 show the LCOH trend as a function of the cost of electricity in the range of 20-200 €/MWh.

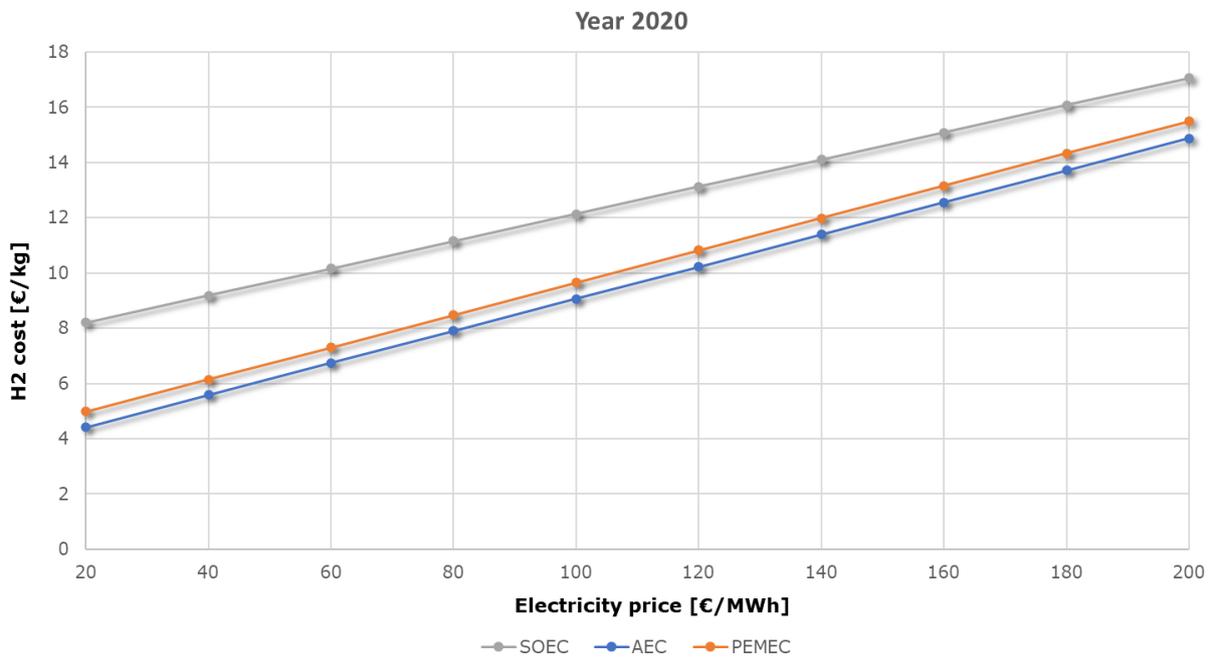


Figure 16. Year 2020: H_2 cost as a function of the price of electricity

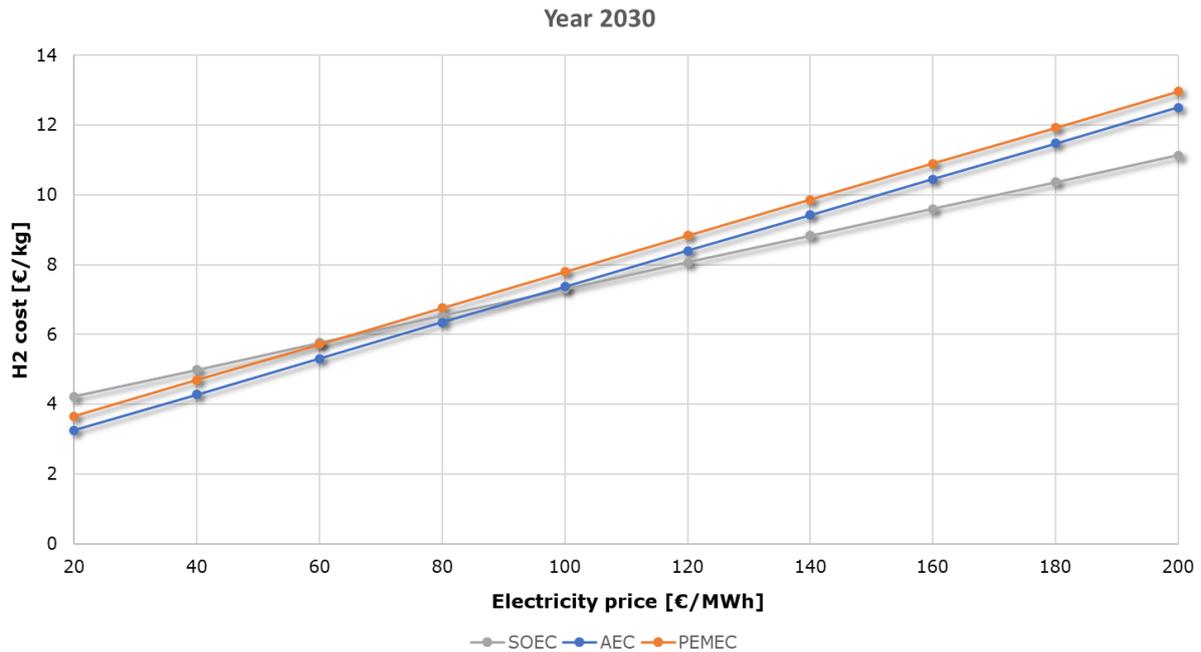


Figure 17. Year 2030: H₂ cost as a function of the price of electricity

As it is possible to see, the wide range of €/MWh has been chosen to verify when and if the price of hydrogen becomes such as to be a competitive value. The lower values as in the case of 20 €/MWh, are extreme scenarios, with very low costs, perhaps in the situation in which there are many RES available and a lot of excess energy to be exploited. In these cases, the hydrogen prices assume very interesting values, sometimes significantly lower than the price of diesel.

The simulation to 2020 shows a higher LCOH for the high temperature SOEC technology, mainly due to the degradation rate, 0.5%/1000h, that leads the stack to be replaced repeatedly after a few years. The gap with respect to the other low temperature technologies seems to be reduced towards even higher values of the price of electricity. Indeed, there is a lower slope of the line relating to high temperature system. This is strictly related to the fact that SOEC technology is characterized by higher efficiency, thus its use becomes more favourable as the cost of electricity increases. This behaviour is even more pronounced in the 2030 scenario, when there are lower values of power consumption (37 kWh/Kg) for the solid oxide electrolysis technology.

Again with regard to 2030 scenario, thanks to the drastic reduction of the degradation rate from 0.5% /1000h to 0.20% /1000h, to the significant reduction of the investment costs and to the greater efficiency, the use of SOEC seems to be cheaper than the AEC and PEMEC, for half of the electricity values analysed (starting from 100 €/MWh).

In order to clearly highlight the comparison between the different technologies, the various contributions to the LCOH for AEC, PEMEC and SOEC, in the current (2020) and future scenario (2030) are specified. The following graphs have been drawn up having set the cost of electricity at 160 €/MWh. This also allows to evaluate the extent of the improvement in terms of LCOH between the two scenarios 2020 and 2030.

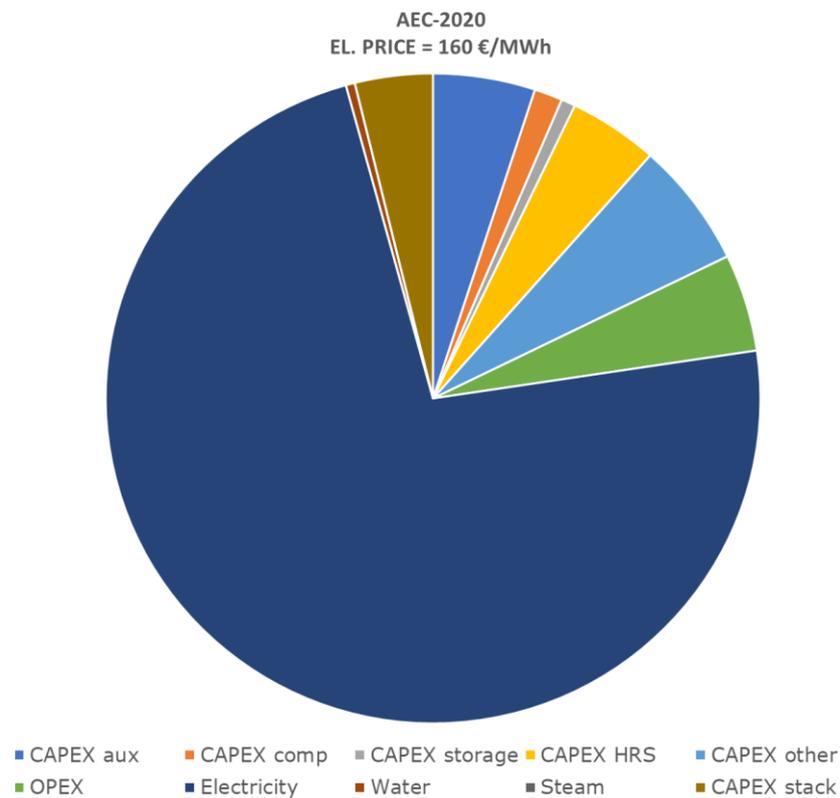


Figure 18. AEC-2020: Contributions to the cost of hydrogen with $C_{el} = 160 \text{ €/MWh}$

Therefore, Figure 18, 19 and 20 show in more detail the breakdown of the cost of hydrogen in the various contributions. They are mainly grouped into Electricity, Water, Steam (equal to zero for AEC and PEMEC), OPEX, $\text{CAPEX}_{\text{stack}}$ and $\text{CAPEX}_{\text{no-stack}}$. However for the latter, due to the complexity of the techno-economic analysis, it is worth to point out the several terms that composes its overall capital expenditure:

- $\text{CAPEX}_{\text{aux}}$, for the gas conditioning, BoP and power electronics;
- $\text{CAPEX}_{\text{comp}}$, for the compressor required by the system;
- $\text{CAPEX}_{\text{storage}}$, for the dimensioned storage;

- $CAPEX_{HRS}$, for the hydrogen refuelling station, with different lifetime according to the temporal scenario;
- $CAPEX_{other}$, to take into account all those costs related to engineering, soil preparation, civil work, control and management systems, interconnection, commissioning and start-up.

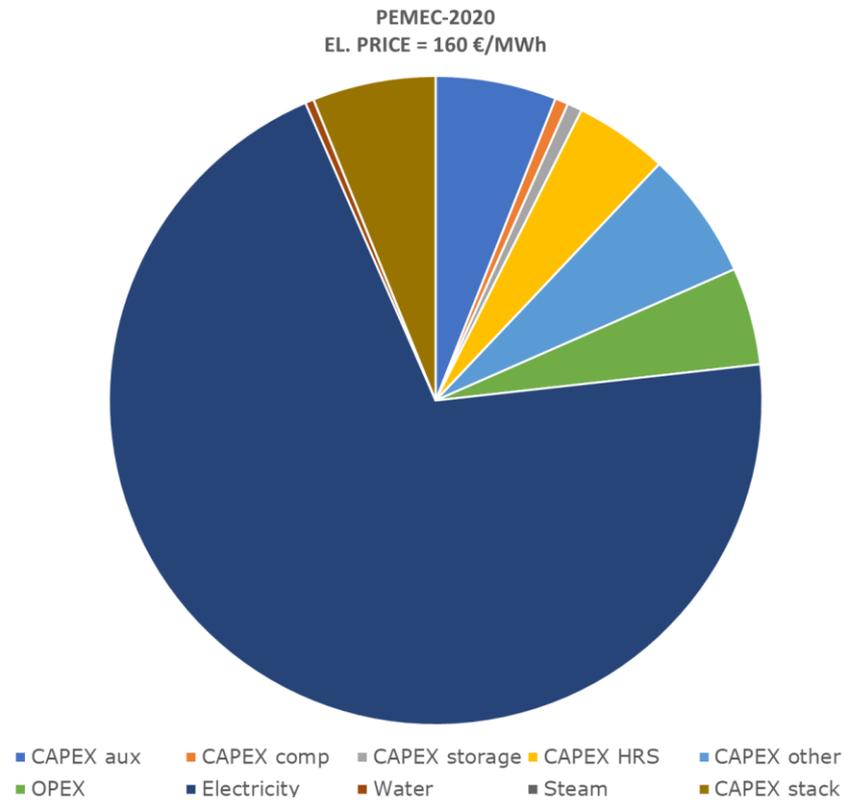


Figure 19. PEMEC-2020: Contributions to the cost of hydrogen with $C_{el} = 160 \text{ €/MWh}$

Observing the figures, it is evident how the main contribution is given by the electricity cost related to the operation of the electrolyser and of the compressor. This is especially true in the case of AEC and PEMEC where the higher power consumption leads to a higher value of electricity in input per kg of hydrogen. Instead, the values related to the $CAPEX_{stack}$, for the low temperature water electrolysis technologies, cover a smaller portion in the overall set of system costs. Especially for the alkaline electrolyser, the capital expenditure for the stack reaches a price that is even lower with respect to other items such as the $CAPEX_{aux}$ and $CAPEX_{other}$ and in the same range of

CAPEX_{HRS}. This phenomenon is closely linked to the frequency with which the replacement of the stack takes place, which already in the 2020 scenario happens at most twice, for AEC and PEMEC.

Furthermore, the substitution may occur near the end of the investigated period (20 years), thus, it has to be taken into account by means of a salvage cost, leading to a reduction of LCOH.

The opposite case occurs for the SOEC technology, as shown in Figure 20, where thanks to the better efficiency, the electricity consumption is reduced. In spite of this, a larger contribution has to be considered for the capital expenditure of the stack, at least as regards the 2020 scenario. This is strictly dependent on the fact that the technology is still at a lower level of technological maturity and the stack replacement occurs five times during the investigated period of 20 years, for the 2020 context.

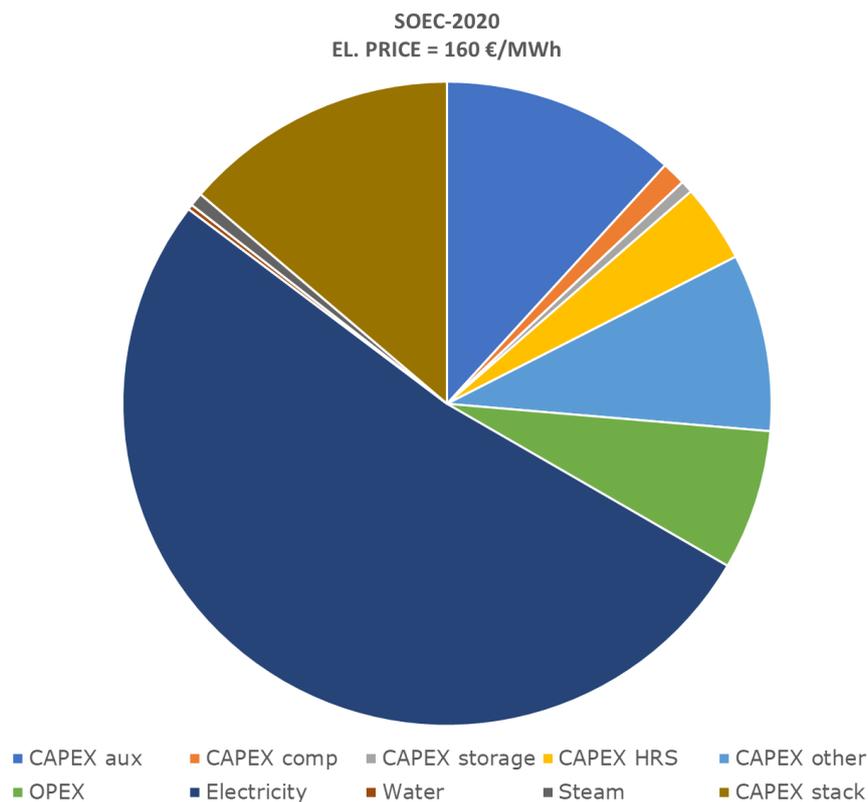


Figure 20. SOEC-2020: Contributions to the cost of hydrogen with $C_{el} = 160 \text{ €/MWh}$

Moreover, for the high temperature water electrolysis a further contribution related to the steam consumption has to be counted. It is also possible to state that working at higher temperature

requires more resistant, anti-corrosion material, with more efforts in their operation and maintenance. This is why for SOEC the CAPEX_{aux} and OPEX contributions are larger than the previous technologies.

The same pie charts are represented for the 2030 temporal scenario and shown below.

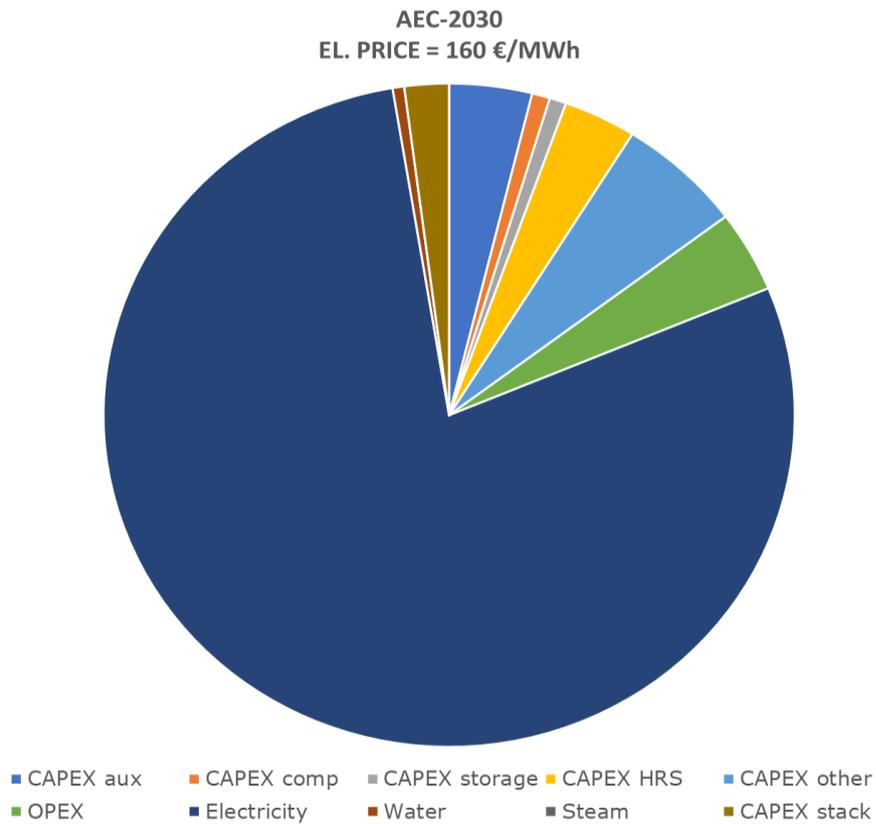


Figure 21. AEC-2030: Contributions to the costs of hydrogen with $C_{el} = 160$ €/MWh

For low temperature machines, the contribution of the cost of electricity will always be predominant with respect to the others even if a better system efficiency will be expected, leading to a reduction of the MWh required per year. Thanks to the learning rate and an economy of scale which is supposed to occur between the two temporal scenarios, a reduction of all the remaining costs is awaited. By 2030, alkaline technology still appears to be better in terms of costs than PEMEC technology, showing lower CAPEX_{stack}.

If as regards the alkaline and PEM technologies from the 2020 to the 2030 context they seem to undergo a quite similar trend, this cannot be said for the high temperature technology.

In fact, SOEC becomes more competitive for some values of electricity prices, compared to the low temperature systems, considering the future scenario.

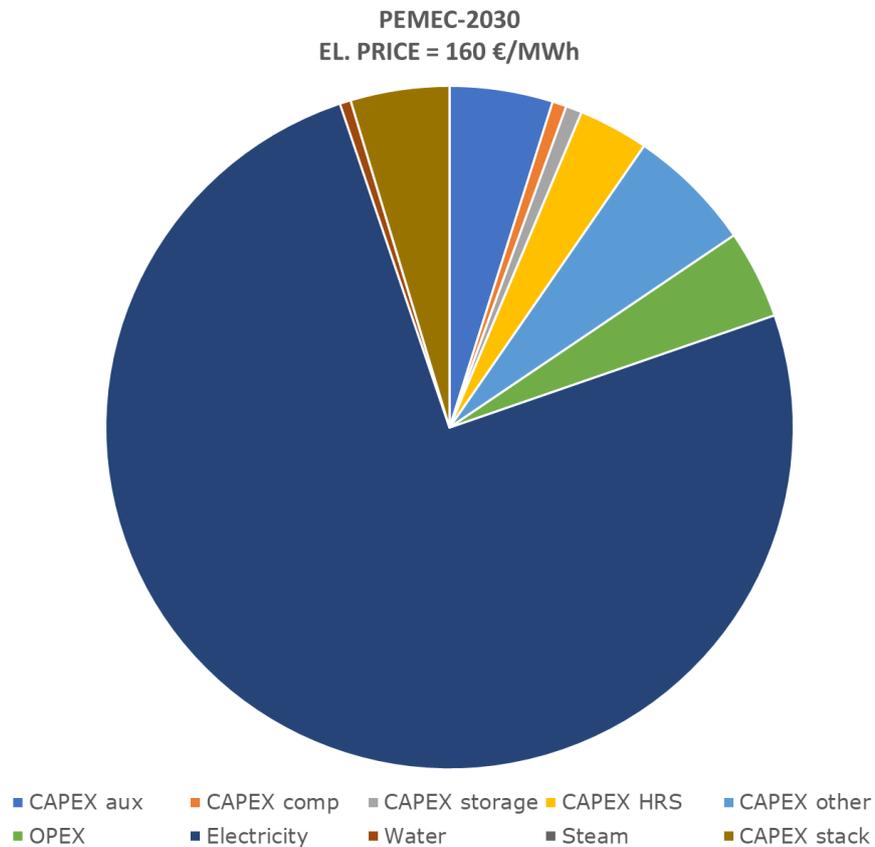


Figure 22. PEMEC-2030: Contributions to the cost of hydrogen with $C_{el} = 160 \text{ €/MWh}$

This, as explained in the previous sections, is due to a combination of various factors:

- greater efficiency with the consequently strong reduction of power consumption and thus a lower contribution to the cost of electricity;
- reduction in degradation rates and therefore lower overall cost relating to the replacement of the stack, that occurs only two times for 2030 with respect to the five times in 2020 context;

In fact, as it is possible to see from Figure 23, by the 2030, the $\text{CAPEX}_{\text{stack}}$ of the SOEC reaches values even lower than the PEM water electrolysis machine, and in the range of the alkaline one, representing only the 3% of the overall costs to build the global high temperature system.

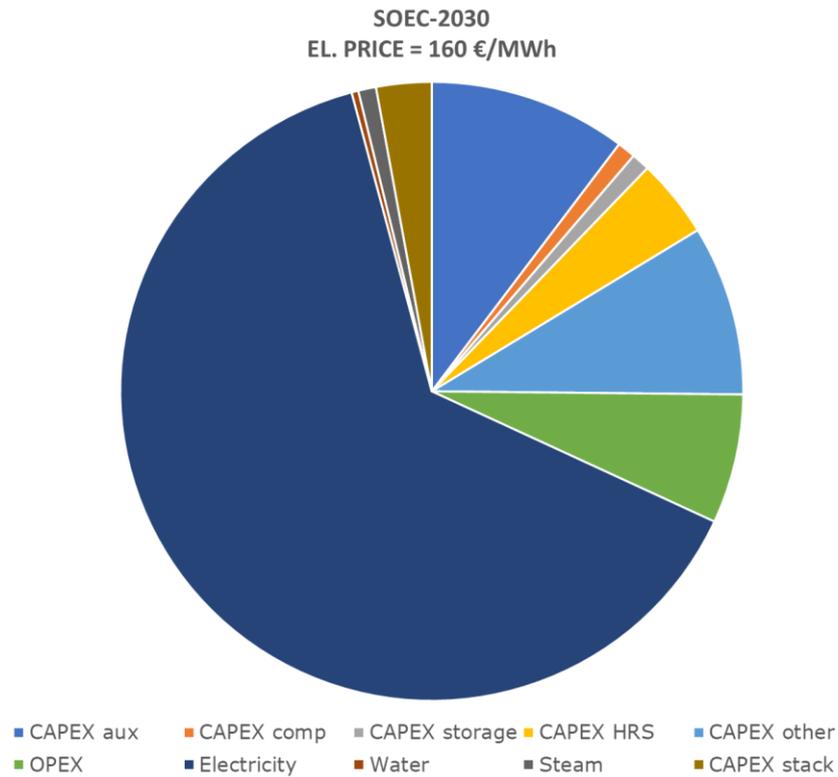


Figure 23. SOEC-2030: Contributions to the cost of hydrogen with $C_{el} = 160$ €/MWh

Furthermore, to make the impact of the cost of electricity on technologies even more evident, they are plotted simultaneously on the same graph, for the two temporal scenarios. They are reported making use of three different electricity price C_{el} equal to 160, 80 and 40 €/MWh. This is important to assess at which C_{el} the three technologies becomes competitive to replace fossil diesel fuel, and if it can occur in both the temporal scenarios, or only in the future one, in the case it is not yet feasible in the current state of the art.

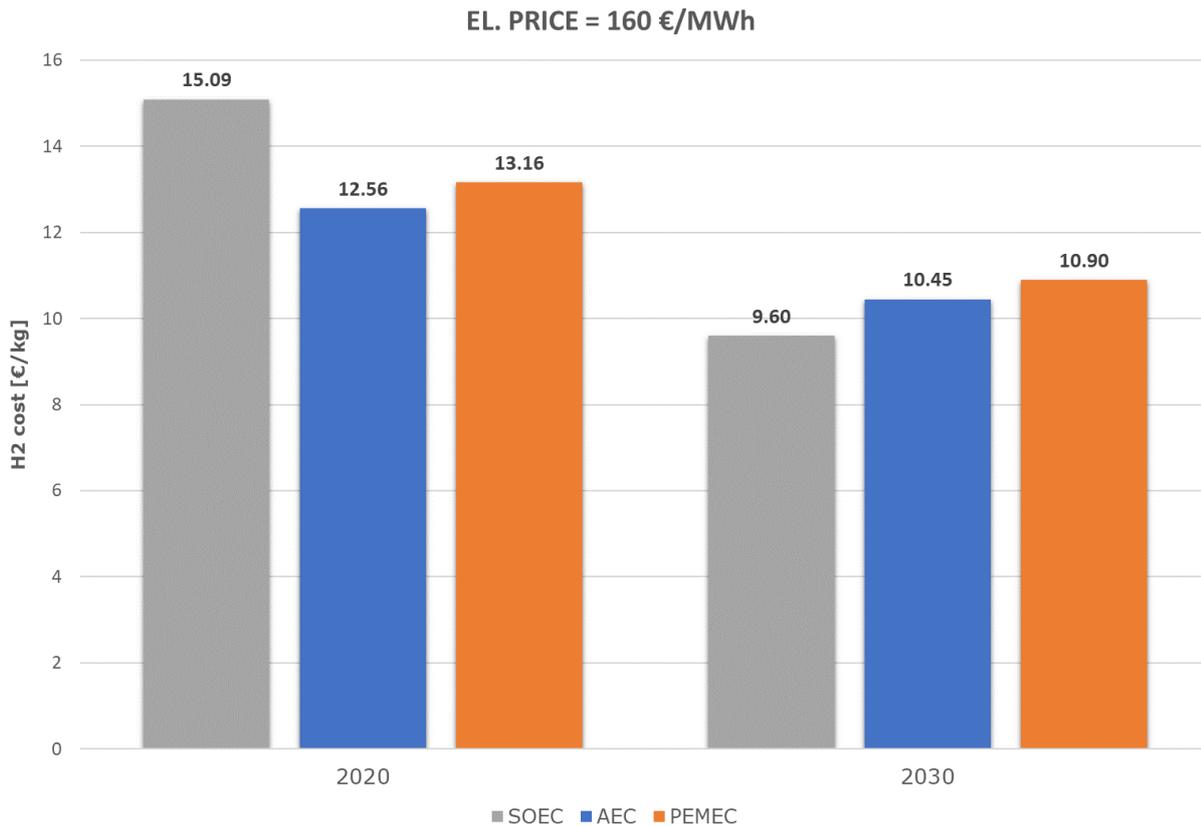


Figure 24. Comparison of 2020 and 2030 scenarios with $C_{el} = 160 \text{ €/MWh}$

Form Figure 24, 25 and 26 becomes evident the fact that at high level of C_{el} the low temperature water technologies are subjected to a steep rise of the LCOH, almost reaching the value of the SOEC, for the 2020 case. Instead, observing the 2030 context, the high temperature machine results to be the most competitive solution, showing a LCOH of 9.60 €/kg compared with the 10.45 €/kg and 10.90 €/kg price of the alkaline and proton exchange membrane, respectively.

On the contrary, when the price of electricity C_{el} goes down the AEC and PEMEC become more competitive, being less impacting the lower efficiency and making the reduced investment costs prevail. This is always true for the 2020, where in particular, the alkaline machine is constantly the cheaper solution, though slightly compared to PEM trend.

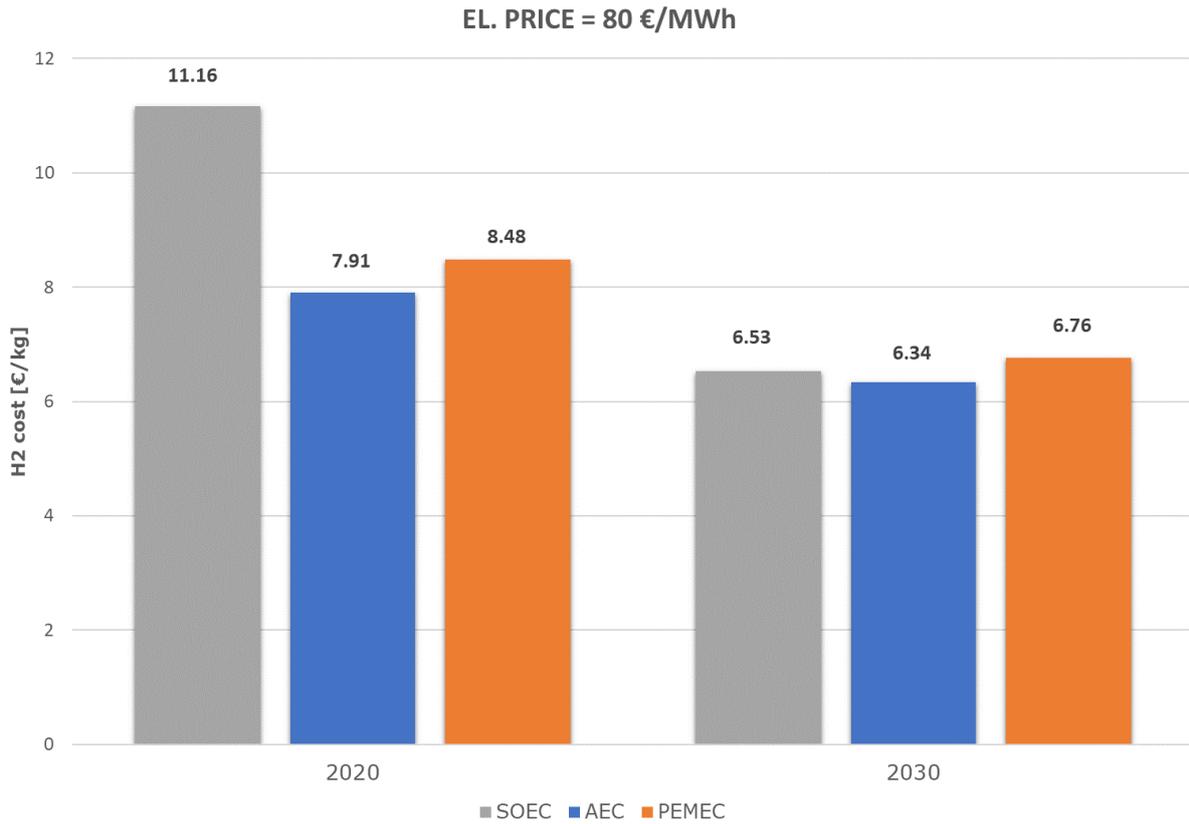


Figure 25. Comparison of 2020 and 2030 scenarios with $C_{el} = 80 \text{ €/MWh}$

On the other hand, for the 2030 scenario, the SOEC technology seems to reach the cost parity, even for lower electricity price C_{el} , as in the case of 80 €/MWh in Figure 25, showing LCOH of 6.53 €/kg with respect to 6.34 €/kg and 6.76 €/kg of the AEC and PEMEC, respectively. However considering an extreme scenario of very low C_{el} , as in the example of Figure 26, compared to the 160 €/MWh baseline case study adopted, it is worth to point out that the alkaline electrolyser shows again the lowest LCOH, followed by PEMEC. Nevertheless the price of hydrogen seems to settle at almost the same value for all the three water electrolysis technologies, resulting in a very promising alternative solution to diesel fuel.

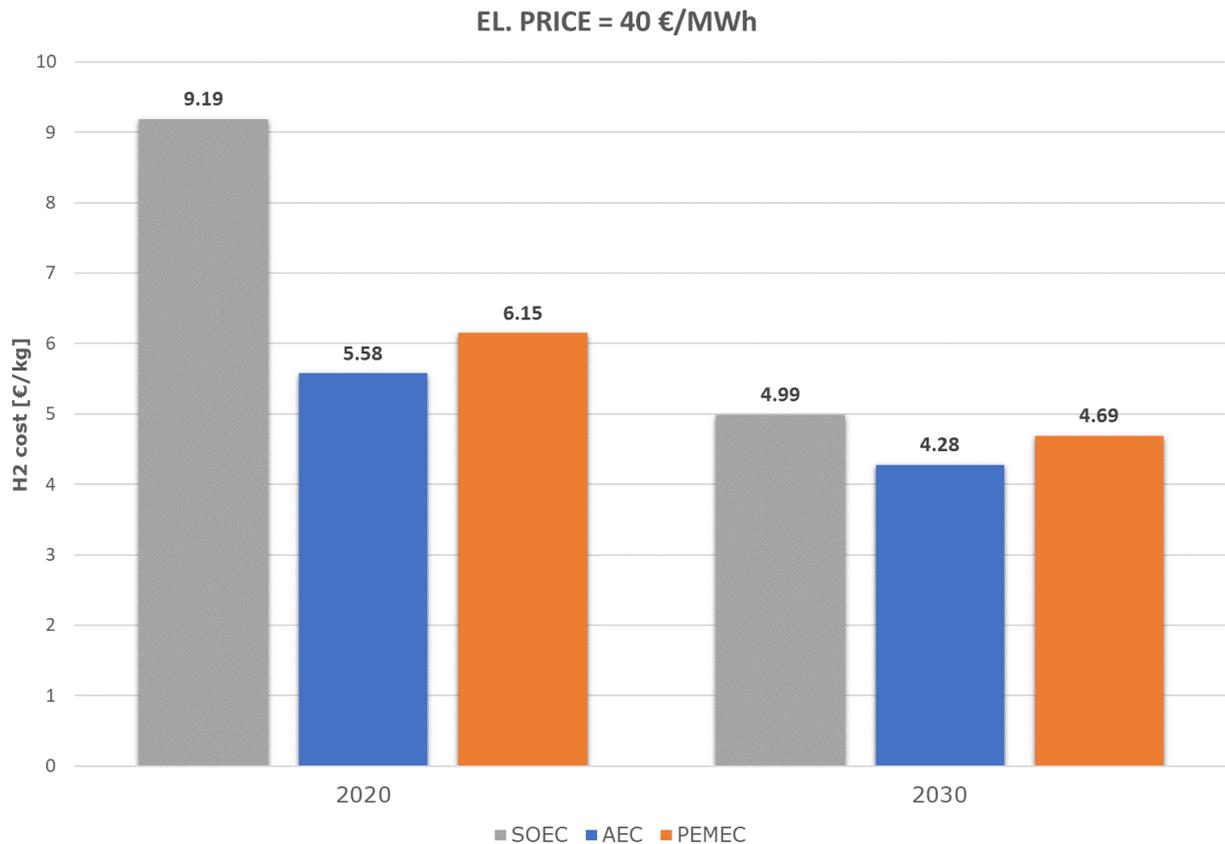


Figure 26. Comparison of 2020 and 2030 scenarios with $C_{el} = 40 \text{ €/MWh}$

In addition, in Figure 27 is proposed a graph relating to the year 2030 showing the cost of hydrogen, as a function of the capacity factor (CF), with the cost of electricity set at 160 €/MWh. The decrease in the capacity factor leads to a reduction in the frequency with which the stack replacement occurs. However, the hydrogen demand to be met remains the same, but this time with a shorter period of plant operation. Therefore to be satisfied, an increase in the size of the electrolyser system with a consequent increase of the investment costs is required. As shown in Figure 27, the overall trend is an increase in LCOH, as the capacity factor decreases.

Furthermore, the extent of the variation in the cost of hydrogen becomes marked only for CF values below 30%, for SOEC technology characterized by higher CAPEX, and below 25%, for alkaline and proton exchange membrane solution. In particular, observing the graph, a very steep increment of LCOH can be highlighted between 20% and 10% of CF, concerning SOEC context. As a matter of fact this reduction of the CF leads to double the electrolyser capacity making the investment costs clearly prevail, being necessary to increase the size of the global plant in such a way as to supply the same hydrogen demand.

For CF higher than these values, the impact on the profitability of the plant is limited due to a trade-off between:

- the working hours of the electrolyser system, namely the production of more or less hydrogen, the more or less the CF rises, impacting on the size of the machine to be adopted;
- the CAPEX_{stack} replacement, which is reduced as the number of operating hours of the plant decreases.

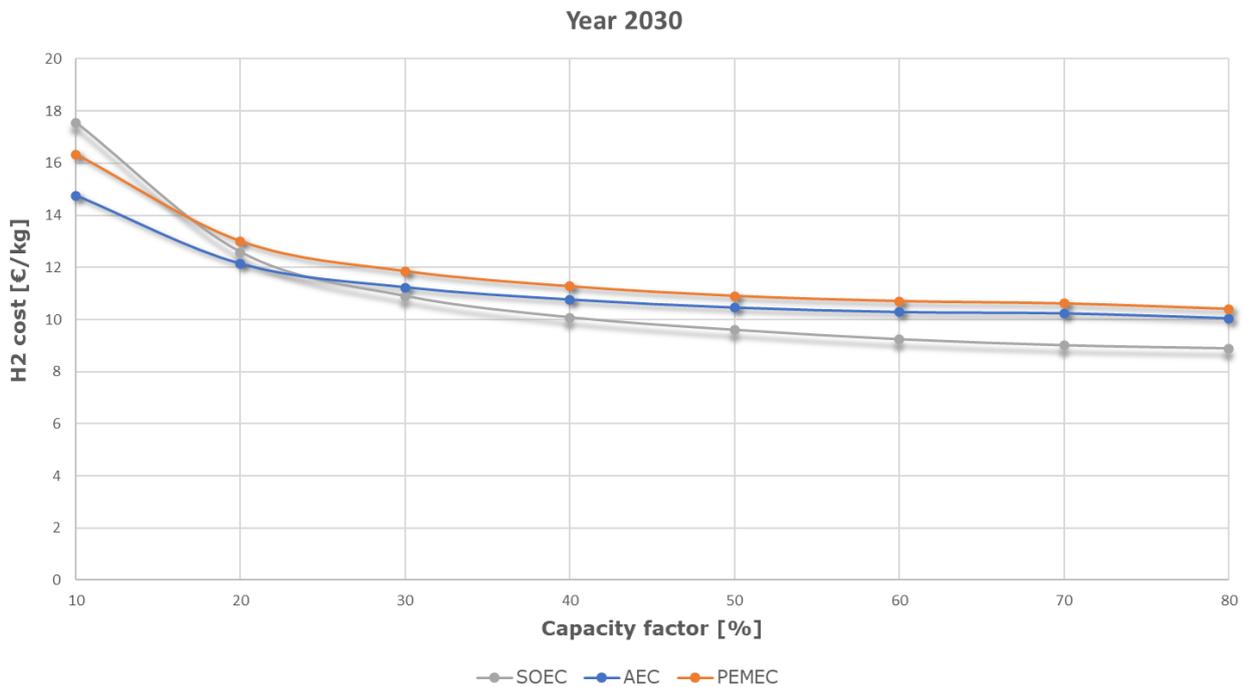


Figure 27. Year 2030: H₂ cost as a function of the price of the capacity factor with $C_{el} = 160 \text{ €/MWh}$

Finally, it has been chosen to verify the LCOH trend, increasing the number of the FCEBs to be supplied, for all three investigated technologies, with reference to the 2030 scenario.

Previous results have been obtained considering multiple modules of a certain defined size: 1000 kW for AEC and PEMEC, and 500 kW for SOEC. This has been done to make the analysis really implementable with the commercial units currently available. In the following Table 12, however, it is possible to see the real electrolyser global capacity required for the two years investigated.

Table 13. Global system capacity required

Global system capacity [MW]	2020	2030
AEC	6.33 [MW]	5.00 [MW]
PEMEC	6.94 [MW]	5.10 [MW]
SOEC	5.24 [MW]	3.70 [MW]

The highest value of global system capacity is for PEMEC technology, and it corresponds to a size of 6.94 MW, for the 2020 scenario. On the contrary, the lowest one is the MW required to satisfy the hydrogen demand by means of the solid oxide electrolyser cell, for a value equal to 3.70 MW, and for the case of the 2030 context. In this way, thanks to the Table 13, it is shown a prospective of the global system capacity required to satisfy the demand of a fleet of 47 FCEBs, adopted for the region of Cologne and Wuppertal.

The increase of the hydrogen demand, that occurs with a larger fleet of FCEBs, leads to rise the electrolyser capacity, in order to generate a sufficient amount of H_2 , necessary to cover the request.

Therefore, in this type of analysis, a unique size of the system has been evaluated to firstly verify that a reasonable size of the plant could be obtained as the fleet increased. In particular, the previously cost function, also reported in the Appendix, has been used to obtain the new specific investment cost ($CAPEX_{system}$ [€/kW]) and then the CAPEX for the stack replacement is assessed as a percentage of the previous value.

The results can be examined, looking the Table 14, 15 and 16, for SOEC, AEC and PEMEC, respectively. The analysis is carried out taking into account the promising future scenario of the 2030 years, and fixing the electricity price to 160 €/MWh to be consistent with the other values previously acquired.

Table 14. LCOH vs. N° FCEB, SOEC 2030

SOEC 2030 (EL. PRICE = 160 €/MWh)				
N° FCEBs	CAPEX_{system} [€/kW]	CAPEX_{stack repl.} [€/kW]	Total capacity [MW]	LCOH [€]
47	1800	270	3.70	9.60
100	955	143	7.88	8.45
200	814	122	15.76	8.15
300	742	111	23.63	8.01
400	694	104	31.51	7.91
500	659	99	39.39	7.85
600	632	95	47.27	7.80
700	610	92	55.15	7.76

As it is possible to see, SOEC shows the lower LCOH, rising the number of FCEBs, reaching also the lower value of CAPEX for the stack replacement. The maximum total capacity is achieved for a number of FCEBs equal to 700 and it corresponds to a value of 55.15 MW. For this size the LCOH is equal to 7.76 €/MWh.

Table 15. LCOH vs. N° FCEB, AEC 2030

AEC 2030 (EL. PRICE = 160 €/MWh)				
N° FCEBs	CAPEX_{system} [€/kW]	CAPEX_{stack repl.} [€/kW]	Total capacity [MW]	LCOH [€]
47	713	249	5.00	10.45
100	477	167	10.65	10.05
200	424	148	21.29	9.84
300	396	138	31.94	9.76
400	377	132	42.58	9.69
500	363	127	53.23	9.64
600	352	123	63.88	9.61
700	343	120	74.52	9.58

Regarding the alkaline electrolyser cell, the total capacity increases, for a fleet of 700 FCEBs, reaching values of about 75 MW. It shows the lowest value of specific investment cost for the system equal to 343 €/kW, and the final LCOH is 9.58 €/MWh.

Table 16. LCOH vs. N° FCEB, PEMEC 2030

PEMEC 2030 (EL. PRICE = 160 €/MWh)				
N° FCEBs	CAPEX _{system} [€/kW]	CAPEX _{stack repl.} [€/kW]	Total capacity [MW]	LCOH [€]
47	1000	400	5.10	10.90
100	667	267	10.86	10.33
200	593	237	21.72	10.10
300	553	221	32.58	9.98
400	527	211	43.44	9.90
500	507	203	54.29	9.85
600	492	197	65.15	9.81
700	479	192	76.01	9.77

Instead, for what concern the proton exchange membrane electrolyser, a very similar trend compared to the alkaline one can be observed. The maximum total capacity is achieved for a value of about 76 MW leading to a LCOH of 9.77 €/MWh.

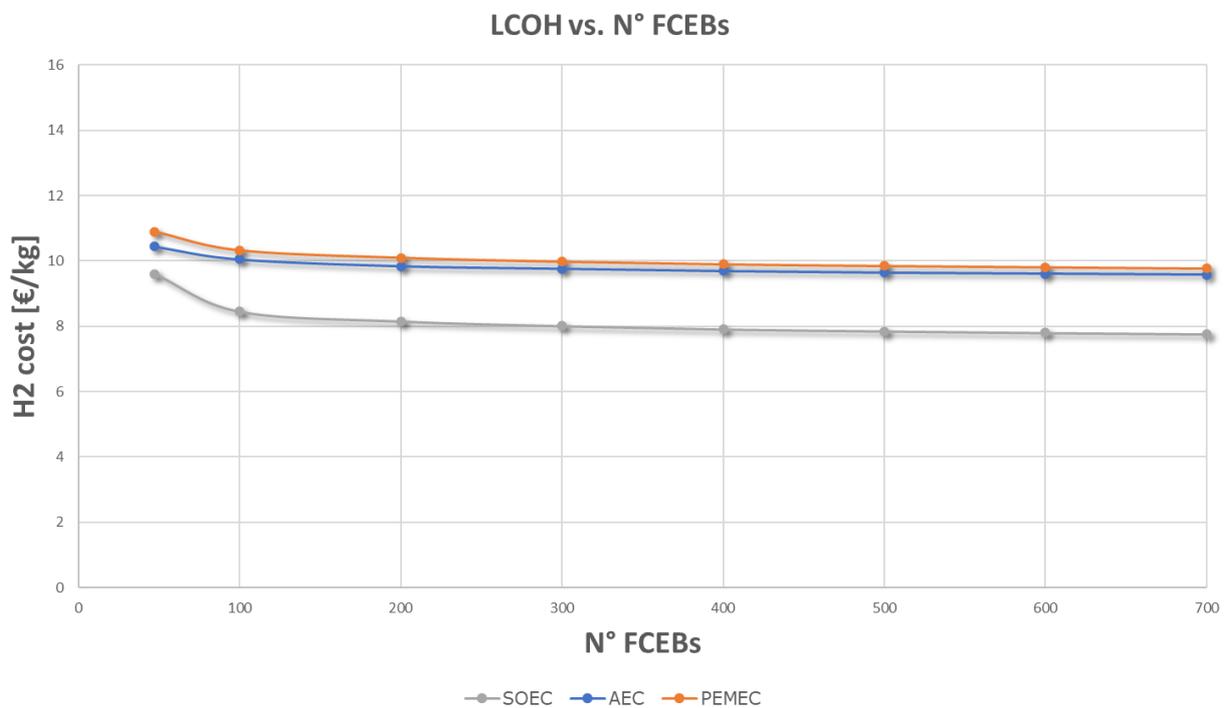


Figure 28. Year 2030: Cost of H₂ as a function of the number of FCEBs with C_{el} = 160 €/MWh

In the Figure 28, it is possible to see , in a single graph, the previously data reported in Table 14, 15 and 16. In particular the representation of the trend of the LCOH as a function of the number of fuel cell electric buses can be analysed.

The maximum number of 700 units of fuel cell electric buses is selected because, observing the Figure 28, a negligible variation can be noticed already starting from values of about 200 FCEBs, for the SOEC machine, and even before for AEC and PEMEC. For the latter, in fact, small changes no longer occur for values above 100 units. Instead, for lower numbers of fuel cell electric buses, especially for SOEC, a reduction of the levelized cost of hydrogen can be pointed out. This is explained by the scale effect on the investment cost of the electrolyser due to the cost function exploited to assess it, and also reported in Appendix.

7. Final considerations

The previous results allow to get an overview on the price of hydrogen produced by means of a water electrolysis machine, to be sold at the dispenser of the hydrogen refuelling station in order to power the FCEBs. For what concerns the evaluation of the competitiveness of the gas produced, it is fundamental to understand and verify if, nowadays or in a future scenario, it can completely replace the traditional diesel fossil fuel.

As it is possible to see from the graph below of Figure 29, considering the last three years, namely 2019, 2020 and 2021, the price of diesel has been characterized by a not stable trend, undergoing numerous strong fluctuations [73].

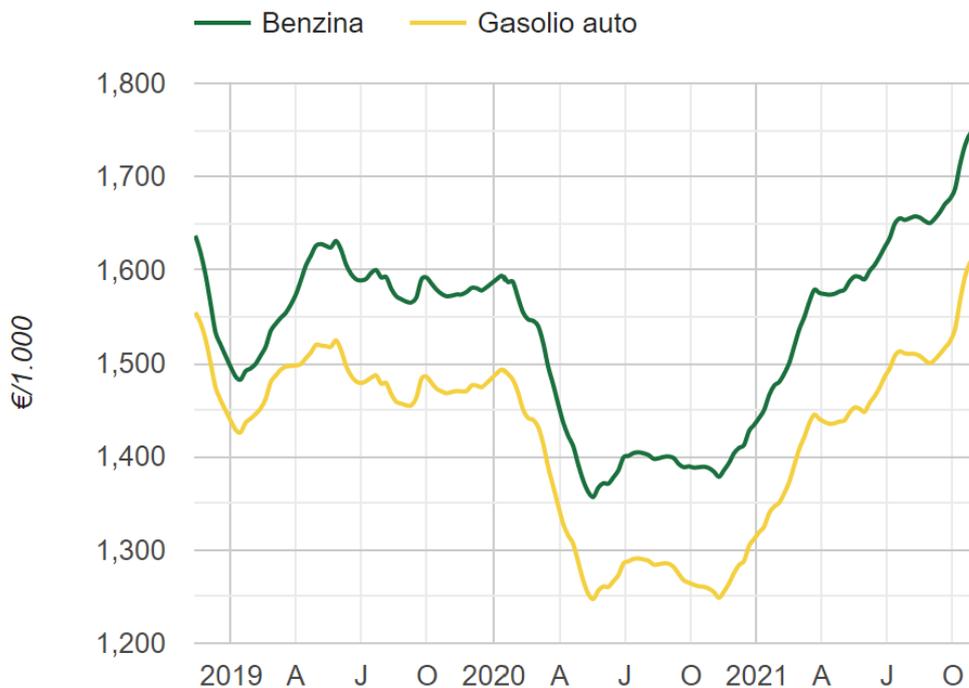


Figure 29. Trend of the average weekly price up to the survey of 08/11/2021 [73]

Therefore, observing the Figure 29, a price of diesel of about 1.61 €/L for the current scenario can be selected, and up to 1.92 €/L for the 2030 scenario, as a possible forecast highlighted by the “Piano Nazionale di Sviluppo – Mobilità Idrogeno, Italia” [54].

As anticipated in previous sections regarding the bus diesel fuel consumption, a value of 38.04 L/100km and 34.40 L/100km can be assumed for the 2020 and 2030, respectively [54].

Starting from that and making use of the previously reported prices, the value in € per 100km of distance covered by the buses can be derived:

- around €61.24, for the 2020 context;
- around €66.05, for the 2030 temporal scenario.

In case of public transport, with the adoption of hydrogen buses, like FCEBs, values slightly lower than 10 kg of hydrogen to cover 100 km are required [54]:

- 8.88 kg/100 km adopted for the year 2020;
- 7.30 kg/100 km selected for the year 2030.

Hence, as shown in Figure 30 and 31, this means that in order to be competitive or completely replace diesel fuel, the resulting price to the end user must show a value of about 6.90€ and 7.44€ per kilogram of hydrogen produced for 2020 and 2030, respectively.

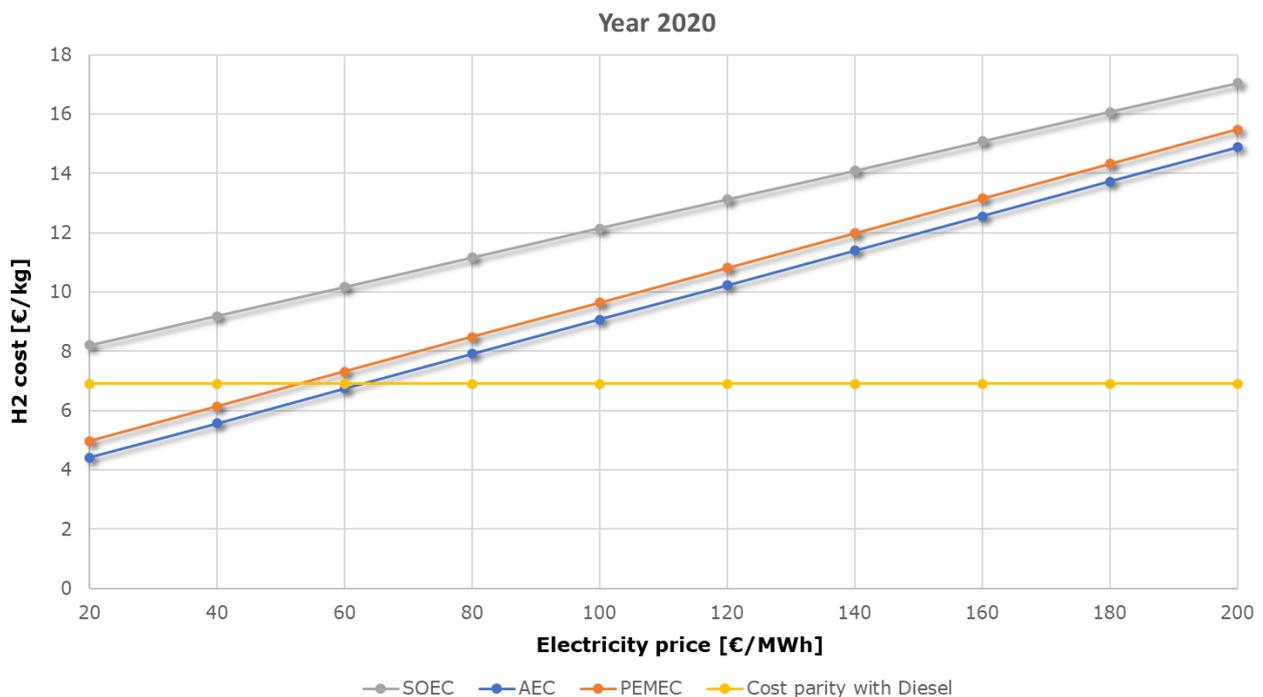


Figure 30. Year 2020 - H₂ cost as a function of the price of electricity with the threshold of competitiveness with diesel



Figure 31. Year 2030 - H₂ cost as a function of the price of electricity with the threshold of competitiveness with diesel

This is the starting point to evaluate the feasibility of using hydrogen as a fuel, relying on the techno-economic analysis developed in this thesis for mobility purpose. Indeed, as it is highlighted in Figure 30, SOEC does not seem to be a feasible solution in the current state of the technology, for no value of electricity price. Instead, regarding the low temperature machines, they result to be an alternative to diesel when low C_{el} occurs (such as 55-60 €/MWh). This condition can be obtained, for instance, when there are many RES available and a lot of excess energy to be exploited.

A completely different trend occurs in 2030 and shown in Figure 31, where approximately for electricity price lower than 100 €/MWh, all three technologies become competitive and moreover, as the C_{el} increases, SOEC technology becomes the best solution to be adopted. Even if it seems to be only at the beginning, the road has already been traced and the commitments stipulated, in particular, by the European Union, are strongly determined to install an enormous quantity of electrolysers capacity, in a very short time. To do this SOEC appears to be a promising solution in the coming decades, above all because, as shown in the Figure 28, it will be the best choice, if the goal is to enlarge the amount of hydrogen produced, spending less energy.

Furthermore, another final consideration that can be extracted from the Figure 28, is that, it is not convenient to build plant with a too high total capacity to satisfy the increased hydrogen demand. This is related to the fact that for values higher than 100-150 FCEBs, the scale effect associated to the increase of the size plant, becomes negligible and consequently, the reduction of LCOH is no more significative. In fact, a balance between the increase of hydrogen demand and the enormous growth in capital cost for the electrolyser capacity is established, leading to a flattening of the hydrogen cost trend. This can even be more underlined by the reduction of specific investment costs, that becomes more and more limited as the number of buses increasing, as shown in the Table 13, 14 and 15.

It is worth to point out that is evident how the integration of this hydrogen production plant system with renewable energy sources becomes fundamental in order to make use of the surplus of electricity to produce a green and sustainable gas to be used for mobility purpose.

Finally, it must be emphasized that the values obtained from the proposed techno-economic analysis are the results of an elaboration carried out in a precautionary manner and therefore reliable from the point of view of hydrogen production technologies for the 2020 scenario. The same approach has been pursued for low temperature technologies, in case of the 2030 context. For the latter scenario, however, a much more evident reduction in investment costs, due to a higher learning rate and economy of scale, has been supposed for SOEC, with respect to PEM and AEC. This assumption is confirmed and validated in all the scientific papers consulted.

Nevertheless, for the high temperature machine, $CAPEX_{stack}$, $CAPEX_{aux}$ and degradation rates cover a very wide range of values, due to the immaturity of the technology. Thus, a choice in their selection has been carried out, but always taking into account to get an economic evaluation that reliably represented the state of the art of the technologies, and then an effectively achievable future scenario.

Appendix

As regards the compressor component, the formula reported in the reference [41] has been used:

$$CAPEX_{compression} = A \cdot \left(\frac{Q}{Q_{ref}}\right)^a + B \cdot \left(\frac{Q}{Q_{ref}}\right)^b \cdot \left(\frac{p_{out}}{p_{in}}\right)^c \cdot \left(\frac{p_{out}}{p_{ref}}\right)^d \quad (1)$$

Where:

- p_{in} corresponds to the compressor inlet pressure, that means, the electrolyser outlet;
- p_{out} represents the compressor outlet pressure;
- p_{ref} is a parameter which corresponds to the reference pressure of 30 bar;
- Q_{ref} represents the reference flow rate equal to 50 kg/h.

Furthermore, for what concerns the coefficients related to the CAPEX compression formula, the values are reported in the following Table 17:

Table 17. Coefficients related to the CAPEX formula of the compression system

Coefficient	Value
A	100000 €
B	300000 €
a	0.66
b	0.66
c	0.25
d	0.25

Instead, in order to evaluate the electricity required to drive the compressor, the technical work has to be assessed exploiting the following relationship:

$$l_c = \left(\frac{k}{k-1} \right) \cdot R^* \cdot T \cdot \left(\beta^{\frac{k-1}{k}} - 1 \right) \quad (2)$$

Where:

- k corresponds to 1.408;
- R^* with a value of 4157 J/(kg K);
- T assumed equal to 293 K;
- β as the parameter that represents the ratio between the outlet and inlet pressure.

For what concern the evaluation of the CAPEX related to the Hydrogen Refuelling Station (HRS), the following formula has been chosen [41]:

$$CAPEX_{station} = A \cdot \left(\frac{Q}{Q_{ref}} \right)^{0.66} \quad (3)$$

With:

- Q_{ref} is the reference capacity of the station equal to 200 kg /day ;
- Q corresponds to the kg/day of the system capacity investigated;
- A is taken equal to 750 k€;
- 0.66 is the adopted scaling factor.

Instead, for the assessment of the civil work costs, the formula reported below has been used [41]:

$$CAPEX_{civil\ work} = (A + B) \cdot (S_{adjust} \cdot A_{equip}) \quad (4)$$

considering the coefficient values to be adopted, reported in the following Table 18:

Table 18. Coefficients of the $CAPEX_{civil\ works}$ expression

Coefficient	Definition	Value
A	Base cost	950 €/m ²
B	Additional cost	150 €/m ²
S_{adjust}	Surface adjustment	150%

The A_{equip} parameter, representing the total surface area occupied by the various components, such as the electrolyser, the auxiliary components, compressor and storage, has been estimated taking into account the following values:

Table 19. Surface area of the different components adopted

Coefficient	Value
AEC	0.095 m ² /kW
PEMEC	0.048 m ² /kW
SOEC	0.10 m ² /kW
Compressor	11 m ²
Storage	0.09 m ² /kW

Finally, taking into account additional CAPEX items, such as:

- Engineering;
- control and management system;
- interconnection;
- commissioning and start-up;

an expression that is a function of the total size of the electrolyser system, has been exploited [41]:

$$Other\ costs = 10\% \cdot \left(\frac{2.5MW}{P_{project}} \right) + 35\% \quad (5)$$

where $P_{project}$ is the size of the investigate plant.

Finally, for completeness, it is proposed, in this appendix of the dissertation, the formulation for the assessment of the cost function, written in terms of power, with the costs expressed as specific investment costs. In fact, it is also used in Section 6, to evaluate the LCOH trend as a function of the number of FCEBs:

$$\frac{C_a}{C_b} = \left(\frac{S_a}{S_b} \right)^{n1} \quad (6)$$

$$\frac{c_a \cdot S_a}{c_b \cdot S_b} = \left(\frac{S_a}{S_b} \right)^{n1} \quad (7)$$

$$\frac{c_a}{c_b} = \left(\frac{S_a}{S_b} \right)^{n1} \cdot \frac{S_b}{S_a} \quad (8)$$

Therefore, considering:

$$n_2 = n_1 - 1 \quad (9)$$

the following expression can be obtained:

$$\frac{c_a}{c_b} = \left(\frac{S_a}{S_b} \right)^{n_2} \quad (10)$$

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