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Optimization of Hydrogen Production Planning Through Electrolysis

TESI DI LAUREA MAGISTRALE IN
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Abstract

The research at hand has been conducted to analyze the optimization of Hydrogen onsite production through electrolysis for a Hydrogen refueling station (HRS), which has a specific hourly Hydrogen demand that needs to be met. This HRS utilizes a specific configuration (including an electrolyzer, a compressor, a storage system, and a distribution network). The objective of the thesis is to determine an optimal configuration in terms of electrolyzer and storage installed capacities and hourly setpoints, and to further investigate the price and the CO₂ content of each kilogram of Hydrogen in each of the five case studies.

We proposed a mixed integer programming for the treated optimization problems, which we solve with CPLEX. Several models have been developed. These models use either the Cost Minimization (energy/electricity costs and CAPEX and OPEX costs) approach or the CO₂ Minimization Approach. The used data as inputs for these models are real time data of hourly electricity prices, hourly renewable energy sources (RES) production profile, and hourly CO₂ content of 1 MWh (grid related emissions) for France and Germany in 2019.

The results have shown that allocating Frequency Containment Reserve (FCR) does not affect the price of Hydrogen. Furthermore, the Carbon Dioxide content of each Kg of Hydrogen will not be affected considerably and as a result, due to the risk of aging that it will bring for the configuration, integration of FCR does not make any sense.

Also, technological advancements analysis regarding electrolyzers and its following reductions in CAPEX in the next upcoming years were evaluated. The investigation showed that these matters are not going to make massive changes in configuration in terms of electrolyzer and storage capacity used, while the reductions in the price of Hydrogen in the market is considered to be noteworthy.

Moreover, integrating RES as one of the sources to provide electricity for the system in addition to the electricity coming from the grid and making it a priority source for the electrolyzer was the last examined topic. Results showed that RES integration will exceptionally change the CO₂ content of each kilogram of Hydrogen by reducing the consumption of fossil fuels for electricity production. However, the price of each Kg of Hydrogen will be affected in a reverse manner due to the high prices of each MWh of electricity coming from RES. Thus, reductions in RES price can heavily contribute

to making the RES Hydrogen competitive in the market since it makes of a huge part of the RES Hydrogen price.

Key-words: Hydrogen production, Electrolysis, Renewable electricity, Optimization, CPLEX

Abstract in italiano

La ricerca in corso è stata condotta per analizzare l'ottimizzazione della produzione di idrogeno in loco attraverso l'elettrolisi per una stazione di rifornimento di idrogeno (HRS), che ha una specifica domanda oraria di idrogeno che deve essere soddisfatta. Questo HRS utilizza una configurazione specifica (comprendente un elettrolizzatore, un compressore, un sistema di accumulo e una rete di distribuzione). L'obiettivo della tesi è quello di determinare una configurazione ottimale in termini di capacità installate di elettrolizzatori e accumulo e di setpoint orari, e di approfondire ulteriormente il prezzo e il contenuto di CO₂ di ogni chilogrammo di idrogeno in ciascuno dei cinque casi studio.

Abbiamo proposto una programmazione mista intera per i problemi di ottimizzazione trattati, che risolviamo con CPLEX. Sono stati sviluppati diversi modelli. Questi modelli utilizzano l'approccio di minimizzazione dei costi (costi di energia/elettricità e costi CAPEX e OPEX) o l'approccio di minimizzazione di CO₂. I dati utilizzati come input per questi modelli sono dati in tempo reale dei prezzi orari dell'elettricità, del profilo di produzione oraria delle fonti di energia rinnovabile (RES) e del contenuto orario di CO₂ di 1 MWh (emissioni relative alla rete) per Francia e Germania nel 2019. orario di CO₂ di 1 MWh (emissioni relative alla rete) per Francia e Germania nel 2019.

I risultati hanno dimostrato che l'allocazione della riserva di contenimento della frequenza (FCR) non influisce sul prezzo dell'idrogeno. Inoltre, il contenuto di Anidride Carbonica di ogni Kg di Idrogeno non ne risentirà notevolmente e di conseguenza, a causa del rischio di invecchiamento che comporterà per la configurazione, l'integrazione di FCR non ha alcun senso.

Inoltre, è stata valutata l'analisi dei progressi tecnologici riguardanti gli elettrolizzatori e le sue successive riduzioni di CAPEX nei prossimi anni a venire. L'indagine ha mostrato che questi aspetti non apporteranno enormi cambiamenti nella configurazione in termini di elettrolizzatore e capacità di stoccaggio utilizzata, mentre le riduzioni del prezzo dell'idrogeno sul mercato sono considerate degne di nota.

Inoltre, l'ultimo argomento esaminato è stato l'integrazione delle RES come una delle fonti per fornire elettricità al sistema in aggiunta all'elettricità proveniente dalla rete e renderla una fonte prioritaria per l'elettrolizzatore. I risultati hanno mostrato che l'integrazione delle RES modificherà eccezionalmente il contenuto di CO₂ di ogni chilogrammo di idrogeno riducendo il consumo di combustibili fossili per la produzione di elettricità. Tuttavia, il prezzo di ogni Kg di Idrogeno sarà influenzato in

maniera inversa a causa dei prezzi elevati di ogni MWh di energia elettrica proveniente da RES. Pertanto, le riduzioni del prezzo delle RES possono contribuire pesantemente a rendere l'idrogeno da RES competitivo sul mercato poiché costituisce una parte enorme del prezzo dell'idrogeno da RES.

Parole chiave: Produzione di Idrogeno, Elettrolisi, Elettricità rinnovabile, Ottimizzazione, CPLEX.

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Introduction

The Hydrogen industry and market are considered to be well established now. Hydrogen, due to its chemical and physical characteristics, has been used extensively in different sectors of industry and economy and the demand has grown in the past century, a representation of which can be seen in Fig. 1 and Fig. 2. Considering the emission generation correlated with Hydrogen's diverse production routes, its great penetration in each sector cannot be ignored at all and needs to be evaluated (Liu, 2021) (Kramer, 2006).

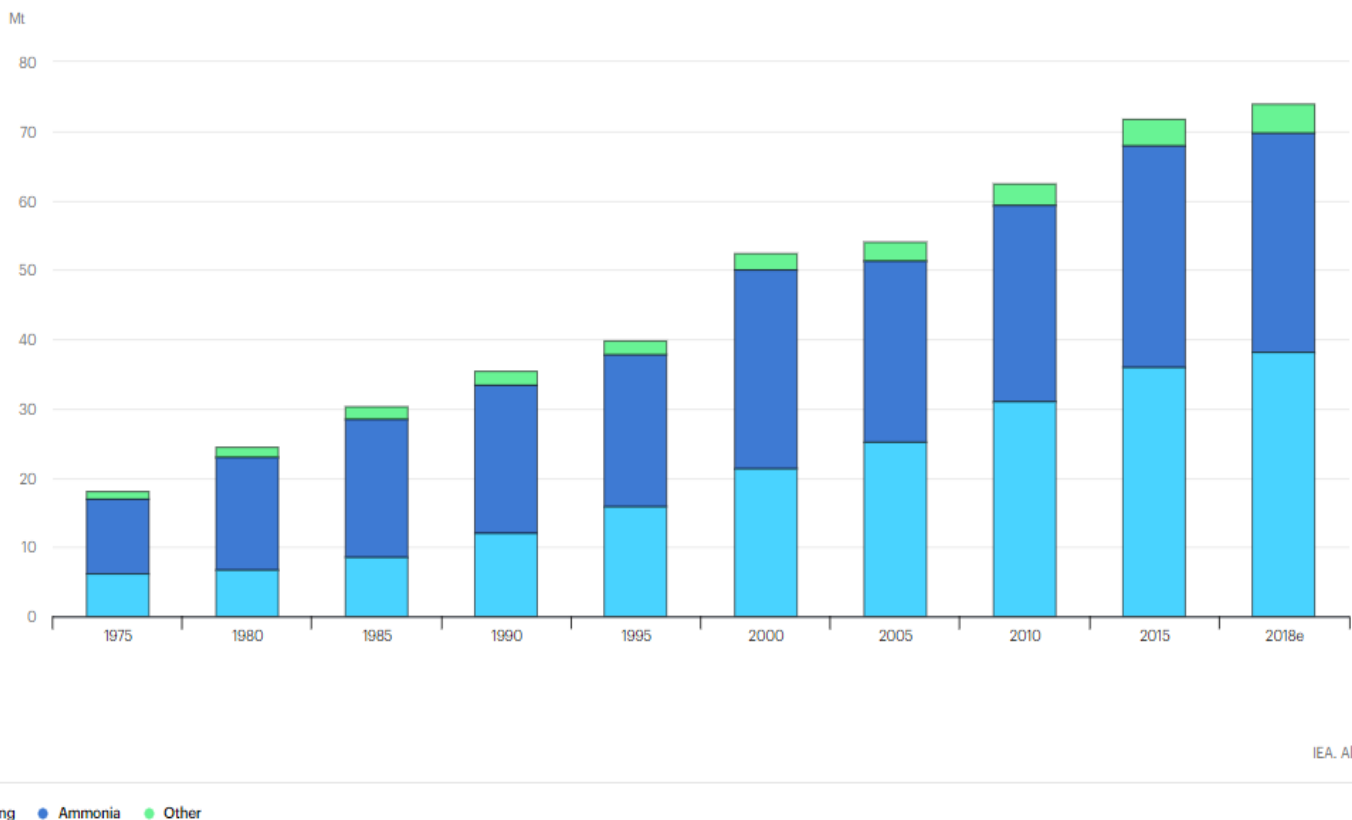


Figure 1 Demand for pure Hydrogen worldwide between 1975-2018 (source: (IEA, 2019))

Also, the potential of further utilization of Hydrogen in the transport and energy sector, is another reason for Hydrogen being of high importance all over the world. Therefore, a lot of attention has been dedicated to Hydrogen Market nowadays. Moreover, due to all the laws and regulation defined for reaching the decarbonization goals for countries all over the world, Hydrogen gains much more attention due to its

characteristics, features like its high energy value and the ability to decrease fossil fuel utilization. Consequently, several steps come to mind while dealing with Hydrogen penetration study. Investigating all of the Hydrogen production routes and their related emission production factor, evaluating Hydrogen demand points especially in EU, and forecasting the pattern for future consumption come in the first step. Then, examining the regulation defined by the governments to promote Hydrogen use, and studying the infrastructure which helps this Hydrogen penetration happen come in the second step (Atilhan, 2021) (Kramer, 2006) (Hosseini, 2016) (The Council Of The European Union, 2020) (Fuel Cells and Hydrogen Joint Undertaking, 2019). This analysis has been done in the first chapter of this thesis.

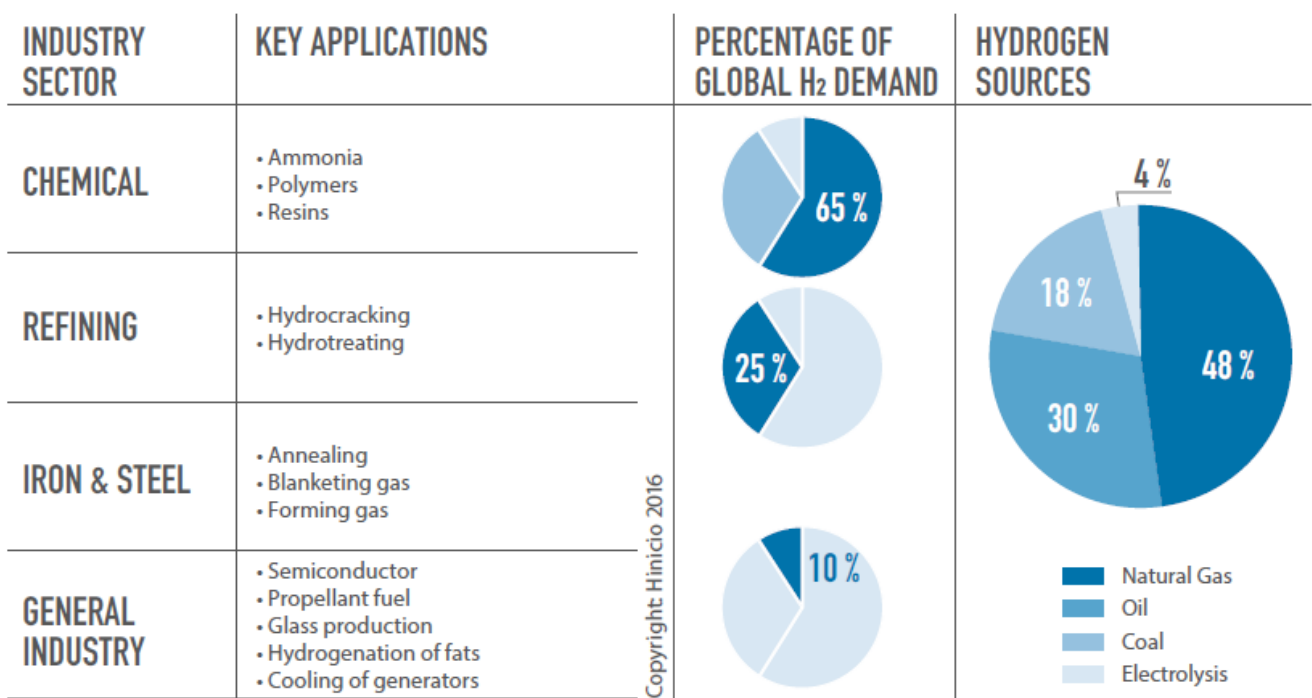


Figure 2 Hydrogen market elements in details (source: (IRENA, 2018))

Analysis (Fuel Cells and Hydrogen Joint Undertaking, 2019) has shown that Hydrogen penetration into all industry sectors is the only solution that can allow Europe to reach all the energy and environmental targets set for 2030 and 2050. This Hydrogen utilization also aids in further penetration of renewable energies in the energy market by assisting in setting up a buffer, in terms of time, sector, and place between production and consumption. This crucial buffer leads to an increase in the possibility of short and long-term energy storage, which then results in stability and high efficiency of the power system. Experts (Fuel Cells and Hydrogen Joint Undertaking, 2019) claim that Hydrogen is by far the best solution being utilized to mitigate the imbalances that happens to the grid because of the unequal supply and demand in

several nodes of consumption and in some time periods of the year. Moreover, the advancements in the utilized technologies which lead to cost reductions in hydrogen-related configurations are helping the process of Hydrogen being much more penetrable than before as well as being competitive compared to electricity coming from renewables. Furthermore, at-scale decarbonization, especially gas grid decarbonization, can only take place by the help of Hydrogen since other options, like biogas or electrification with heat pumps, are not available at the desired needed scale or are costly to be implemented into old infrastructure. The current gas grid in Europe has the task of providing for 15% of Europe's power generation and more than 40% of household heating (The Council Of The European Union, 2020). Some sectors, like transportation, are hard to get decarbonized, unless Hydrogen and hydrogen-based fuels play the main role. In the transport sector, which accounts for almost one-third of total CO₂ emissions emitted in Europe, the most promising fuel, called as fuel of the future, is Hydrogen. This gains high importance now since batteries do not show a promising future yet due to a lower range of movement for the vehicle (because of a lower energy density), a not efficient recharging process, and high costs. The aviation industry, as well, considers Hydrogen as the only available at-scale fuel, suitable for the purpose of decarbonization. Sectors of industry involving feedstock, are in the same situation as transportation in terms of needing to be involved with Hydrogen and hydrogen-based fuels. Using Hydrogen as feedstock, either directly or indirectly for industrial purposes, alongside with the possibility of using it together with CO₂ lead the way to replace hydrocarbons and use CO₂ instead of emitting it (Fuel Cells and Hydrogen Joint Undertaking, 2019) (The Council Of The European Union, 2020) (IRENA, 2018) (Kakoulaki, 2021) (Kramer, 2006) (Atilhan, 2021) (Sharma, 2015) (Hosseini, 2016) (Dincer, 2012).

Because of the reasons mentioned above, in the second chapter of this research, providing the hourly demand of a HRS has been studied as an example of Hydrogen penetration in transportation. The specific configuration (an electrolyzer, a compressor, a storage system, and a distribution network) and their related characteristics are all discussed in detail in this chapter. The mathematical models utilize different sets of input data in terms of the price of 1MWh of electricity, demand profiles, and hourly CO₂ content of 1 MWh (grid related emissions). The methodology used is designed in a way to identify optimal configurations, assess the price of Hydrogen in each case, and find the CO₂ content of each kilogram of Hydrogen produced while looking into the hourly operating setpoints and economics of the configuration. Reviewing the price and the CO₂ content of each Kg of Hydrogen can give insight for considering strategies like Hydrogen penetration as fuel in the sectors or coupling RES electricity and grid electricity together for Hydrogen production.

The goal of this research is to investigate using onsite Hydrogen production through a renewable process (electrolysis) which get its electricity from either fossil fuels or

renewable resources with the two approaches of finding the most environmentally friendly and economical solution. We used data based on the actual electricity price and Hydrogen demand data coming from two different countries of Germany and France.

The mathematical models are developed to answer the aforementioned research goals. Several experiments are done in order to examine whether Hydrogen injection into the mobility industry as a fuel makes sense in terms of the price of each kilogram of output Hydrogen and its relative CO₂ content or not. The numerical results can further shed light on the strategy for further penetration of renewable resources for electricity production and Hydrogen use. Discussing the results of these experiments have been done in chapter three of this thesis.

Finally, in the last chapter of this thesis, chapter five, the conclusions are reviewed to sum up the most important notions understood from the experiments.

1 Literature Review

1.1 Hydrogen Properties

Hydrogen is the first element on the periodic table. It was discovered in 1766 by Henry Cavendish and it is shown with symbol H. Hydrogen, the most common element around us, has the atomic number of one. This element is in the shape of gas at room temperature, and it is known to be colorless as well as odorless. Hydrogen can easily get ignited and it is known to be one of the most flammable elements ever. It can also be considered as an energy carrier that relatively to mass, has the higher and lower heating value of almost three times of famous fuels, like Methane or Natural Gas. This shows that relatively to mass, Hydrogen is very valuable due to being able to provide almost three times the amount of energy provided by a complete combustion.

1.2 Production Routes

Nowadays, no one can ignore the enormous penetration of Hydrogen in all aspects of industry globally, as well as the potential of the further penetration of Hydrogen in the transportation and the energy sectors. This is due to the fact that H_2 is the reactant for many industrial processes because of its physical and chemical properties and when using it as an energy source, huge amounts of energy are accessible.

Since Hydrogen is widely used everywhere, it is principal to analyze how Hydrogen's production methods are affecting the environment. This is where low-carbon Hydrogen production routes, like electrolysis, come into the frame. By integrating these concepts in H_2 production, decarbonization can effectively takes place. Accordingly, climate change mitigation as well as a decline in the amount of greenhouse emissions can happen. As a result, all Hydrogen production routes and technologies are gaining much more attention in the recent decades.

Generally, the production routes of Hydrogen can be divided into two main groups: fossil fuel based (normally Natural Gas, Coal, and Oil) and renewable source based (Biomass and Water). Although the production of Hydrogen through renewable resources has

gained so much attention and investments in the past years, obtaining Hydrogen through fossil fuels is still the method that is mainly used (Liu, 2021).

There are several methods used in industry, and also in small scale, to get to Hydrogen. In case of using fossil fuels, steam reforming, partial oxidation and also gasification are carried out. In case of having renewable resources, water electrolysis and biomass gasification could be used. Fig. 3 shows a comparison between the popularity of these routes worldwide.

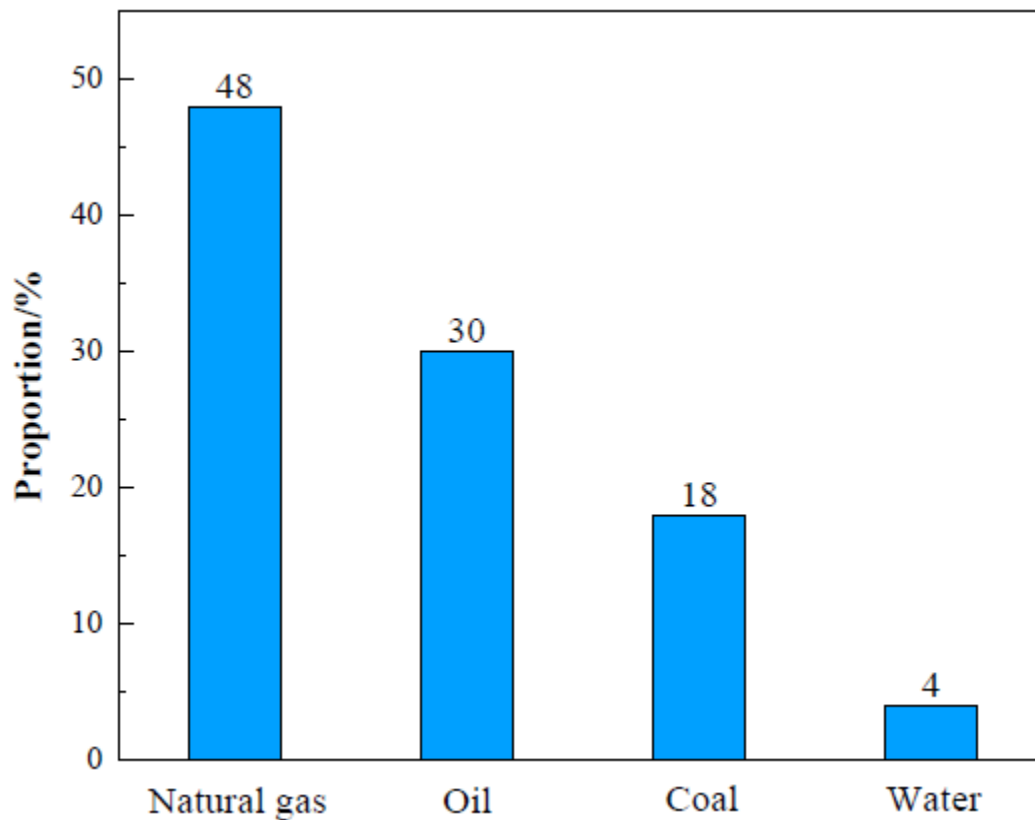


Figure 3 Comparison between different H₂ production routes (source: (Liu, 2021))

1.2.1 Fossil Hydrogen Production

1.2.1.1 Steam Methane Reforming (SMR)

This production route nowadays is a commercialized and mature method which dates to almost 100 years ago and accounts for almost 50% of the worldwide Hydrogen production. SMR uses Natural Gas to generate Hydrogen through four main processes which are steam reforming, carbon dioxide reforming, auto-thermal reforming, and partial oxidation reforming.

The first method, steam reforming, having the efficiency of 65%-70%, is the most common and one of the least expensive methods, which happens through four main steps. First, the impurity from Natural Gas needs to be removed in order to heat up the mixed gas of steam and Natural Gas. This way, CO and H₂ are obtained. Then, the conversion of CO and water to H₂ and CO₂ through the catalytic water-gas shift reaction takes place. After this, the obtained H₂ needs to be purified for further use (Liu, 2021) (Sharma, 2015). The stoichiometric reactions can be found in Table 1 below. Formally, these two reactions, mentioned above, together result into the 3rd reaction, known as GRR or Global Reforming Reaction (Garbarino, 2020):

Reaction	Acronym	ΔH_{298}^o (kJ mol ⁻¹)
$\text{CH}_4 + \text{H}_2\text{O} \rightleftharpoons \text{CO} + 3 \text{H}_2$	SMR	206.63
$\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2$	WGS	-41.16
$\text{CH}_4 + 2 \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + 4 \text{H}_2$	GRR	165.47

Table 1 SMR, WGS, and GRR reactions (source: (Garbarino, 2020))

The other methods of carbon dioxide reforming, auto-thermal reforming, and partial oxidation reforming have a lot in common with the first method, however, they all have some advantages and disadvantages compared to the main steam reforming production route which are mentioned in Table 2.

Moreover, the amount of Carbon Dioxide produced throughout any industrial reaction is of high importance since it will directly affect the environment and the strategies and investments which are going to target climate change and emission control. In average, for each Kg of hydrogen produced through SMR, 9 kg of CO₂ is emitted, which is not negligible at all (U.S. Department of Energy, 2021).

Methods	Advantages	Disadvantages
Steam reforming	<ul style="list-style-type: none"> ◆ No oxygen consumption, ◆ Lower temperature ◆ High ratio of H₂/CO ◆ High efficiency ◆ More mature technology and extensive application 	<ul style="list-style-type: none"> ◆ Additional heating required ◆ High CO₂ emissions ◆ Complex system ◆ High re-requirements for NG quality
Partial oxidation reforming	<ul style="list-style-type: none"> ◆ No catalyst required ◆ High conversion efficiency ◆ Simple system ◆ Small scale production ◆ Low desulfurization demand 	<ul style="list-style-type: none"> ◆ Oxygen required ◆ Low ratio of H₂/CO ◆ Higher temperature ◆ High pressure of dust treatment
Auto-thermal reforming	<ul style="list-style-type: none"> ◆ Lower temperature than partial oxidation reforming ◆ High conversion efficiency ◆ Lower oxygen consumption than partial oxidation reforming 	<ul style="list-style-type: none"> ◆ Oxygen required ◆ Less industrial production
Carbon dioxide reforming	<ul style="list-style-type: none"> ◆ CO₂ as raw material ◆ Low reforming temperature 	<ul style="list-style-type: none"> ◆ Additional heating required ◆ Low ratio of H₂/CO ◆ Under investigation

Table 2 Summary of SMR (source: (Liu, 2021))

1.2.1.2 Coal Gasification

Another commercialized and mature method used for the production of Hydrogen is Coal gasification which uses the abundant sources of coal. The type of the Coal Gasification method depends on how the contact between the coal and the gasifier has been set.

Generally, there are three types of coal gasification which are entrained flow gasification, fixed bed gasification, and fluidized bed gasification of which the first one is the most

common one (Sharma, 2015). The overall stoichiometric reactions can be found in Table 3 (Huang, 2014):

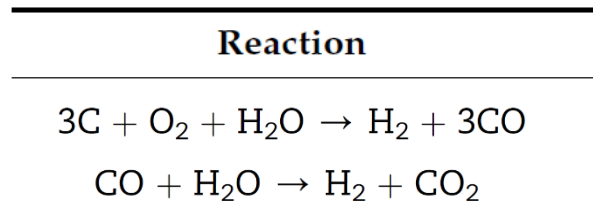


Table 3 Coal gasification reactions (source: (Huang, 2014))

This production route in terms of the maturity of technology and the economic performance is superior to the other methods and can be considered as the cheapest especially if direct access to coal is possible. However, the efficiency is lower compared to previous discussed methods (the efficiency is around 55%) and the needed CAPEX is higher (Liu, 2021) (Sharma, 2015).

Just like the previous case, it is crucial to take into consideration the amount of Carbon Dioxide produced throughout this reaction. In average, for each Kg of hydrogen produced through Coal Gasification, 22.25 kg of CO₂ is emitted (Burmistrz, 2016).

1.2.2 Renewable Hydrogen Production

1.2.2.1 Biomass Gasification

Biomass, materials like wood and forestry and agricultural residues, is considered to be a valuable input since it can be used as input for several procedures which then release Hydrogen.

The most common way to obtain Hydrogen from Biomass is Gasification (a thermochemical method) in which Biomass must go through a partial oxidation process at high temperature (usually more than 723°C). This process converts the input material with the help of gasifying agents, like air, steam, and oxygen into a syngas which is a mixture of CO, CO₂, CH₄, and also H₂. This method now is known as one of the most advanced biomass-based methods of clean Hydrogen production with no emissions yet with a high efficiency which is also an economic option as well. At present, the amount of Hydrogen present in the syngas is between 40% to 60%, however, the stability of the catalysts in the reaction, as well as their recyclability are still under investigation and have become limitations for expanding this method of production to a large-scale one (Sharma, 2015) (Liu, 2021).

1.2.2.2 Electrolysis of water

Using electricity to split water into Hydrogen and Oxygen is now considered to be a mature and commercialized method for Hydrogen production. This method is now used to obtain around 5% (Liu, 2021) of the total global Hydrogen used. Nowadays, the integration of renewable energies to provide the needed electricity with almost no environmental emissions and very low (even zero) cost of fuel have been the focus of many industrial production sites and studies at the same time.

Regarding the technology used for electrolysis, two commercially mature type of electrolyzers are available in the market: the Proton Exchange Membrane electrolyzer (PEMEL) (which is used in the case of this thesis) and Alkaline electrolyzer (AEL). (Liu, 2021) (Sharma, 2015) (Nikolaidis, 2017). The way that these two types of electrolysis systems work are different, summary of which is presented in the Table 4 below:

Electrolysis can give pure Hydrogen (around 99.99%) as its output. However, there are still some disadvantages which needs to be taken care of. The barriers regarding providing the input energy and the relatively high CAPEX associated with the equipment needed for electrolysis have made the electrolytic production of Hydrogen being small in scale and have slowed down the pace of this method being spread out (Liu, 2021) (Sharma, 2015).

Apart from all these production methods, there is also another method for producing Hydrogen based on nuclear energy. Since it is a niche technology with very low TRL (Technology Readiness Level) at the moment, the thesis won't detail it further. Following references might be useful for interested readers (Liu, 2021) (Sharma, 2015).

1.3 Types of Hydrogen

The worldwide demand for Hydrogen is growing. However, not all countries have access to the same technology for Hydrogen production, storage, and transportation, resources, and geopolitical outlook to use it. Consequently, there are limitations and opportunities bound to each method which have been developed to get to Hydrogen for the past century. These matters also affect the final price for the user due to the barriers each section has.

All the procedures for Hydrogen generation have been codified based on colors in order to reach a better understanding of each one of them. The colors, describing the main production routes, are as follows: grey (or brown/black), blue hydrogen, green hydrogen, yellow (or purple) hydrogen.

Also, the type of Hydrogen produced is sometimes called out by names like Clean Hydrogen, Renewable Hydrogen, and Low-carbon Hydrogen as well (Noussan, 2020).

In Fig. 4, a summary of all types of Hydrogen can be seen in the picture and the detailed explanation follows:

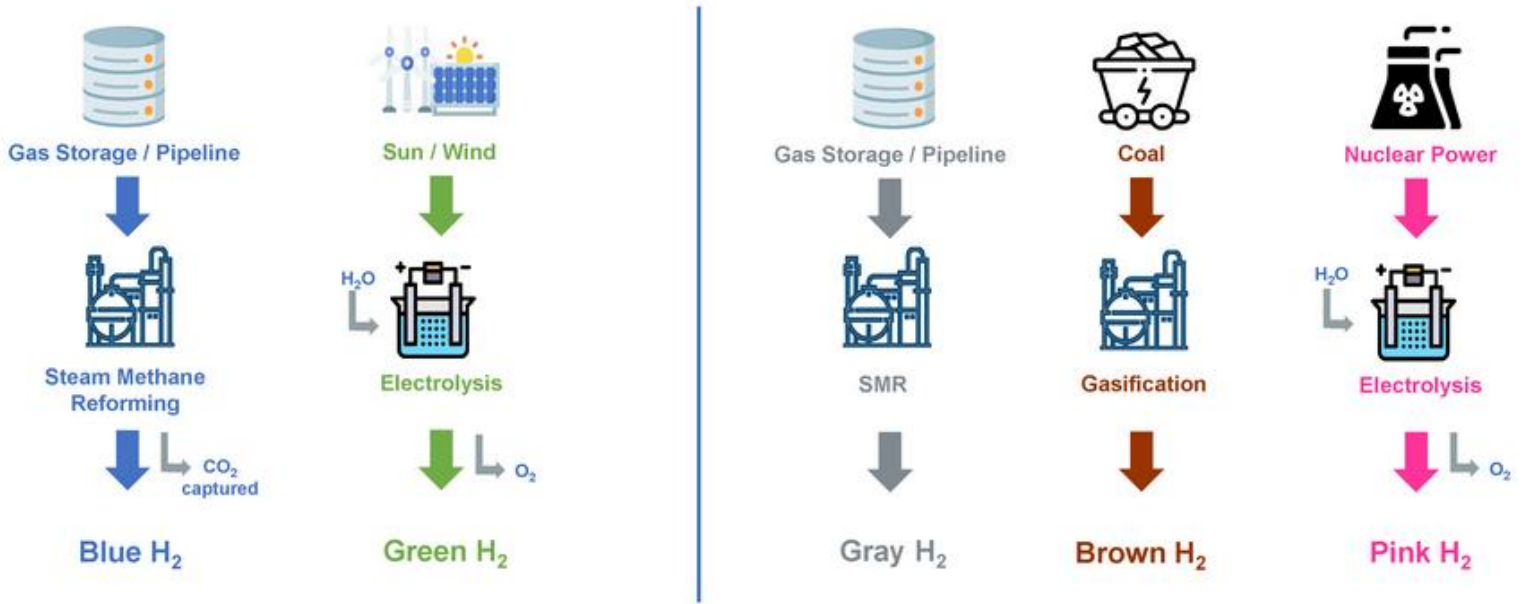


Figure 4 A summary of Hydrogen colors and their production route (source: (Droege, 2021))

1.3.1 Green Hydrogen

Green Hydrogen is the outcome of using electricity from renewable resources coupled electrolysis, which is water getting split water by electricity (Fig. 5). Several technologies are being used for electrolysis which are explained in detail in section 1.4 of this thesis. However, generally, electricity coming from zero-emission solar panels or wind turbines, or hydropower is sent through the device, releasing Oxygen and Green Hydrogen as its only two products. The Oxygen is normally vented into the air, and it doesn't have any effect on the environment. Generating this type of Hydrogen, since it is coming from renewable clean energy sources, is known to be zero emission and almost eliminates the CO₂ (in general carbon emissions) (Noussan, 2020) (Liu, 2021) (Kakoulaki, 2021) (Abad, 2020) (Hosseini, 2016) (Dincer, 2012) (Nikolaidis, 2017).

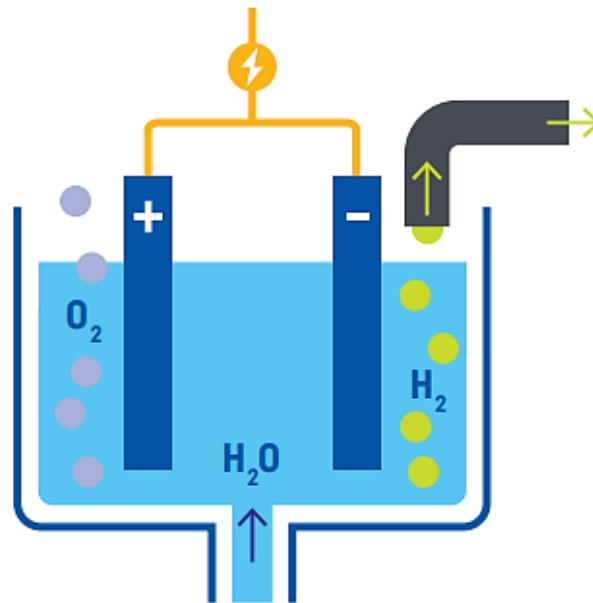


Figure 5 The schematic procedure for Green Hydrogen production (source: (ATCO Corporate, 2021))

The ratio of Hydrogen energy content and electrolysis total power consumption, called electrolysis average efficiency, is in the range 65%–70% with the output pressure of the electrolyzer in the range of 10–30 bar.

Moreover, the amount of fresh water and the electricity consumed by the electrolyzer depend on the type as well as size of the electrolyzer and its working conditions (most important its output pressure). The amount of water consumed by the device is in the

range of 20-50 liters per each kilogram of Hydrogen output. This is a serious matter to bear in mind especially in regions in which water scarcity is a critical problem.

In such regions, the shortage of water coupled with the equipment cost have made Green Hydrogen production the most expensive Hydrogen production method available (Noussan, 2020) (Nikolaidis, 2017).

Green Hydrogen can also come from bioenergy pathways. Biomass, like agricultural residues, wood, and forestry, have been used extensively, especially in the recent years, as a clean renewable source of energy which can produce a huge amount of Hydrogen through biological and thermochemical procedures, namely solid biomass gasification and pyrolysis and biomethane reforming, which were explained previously in different production routes of Hydrogen section. However, for now, biomass alteration, although being clean, is not used extensively to produce Hydrogen at large scale, yielding to a competitive price in the market due to the CAPEX and OPEX of the facilities needed for the process (Liu, 2021) (Kakoulaki, 2021) (Kramer, 2006) (Dincer, 2012) (Navarro, 2009).

Within European union, Germany together with Netherlands are the leaders in establishing projects of Green Hydrogen projects (Hydrogen Europe Intelligence Department, 2020). Other countries like Norway (hybrid PV+ Wind generators), Greece (hydro generators), and Spain (P2P system integration for cooling facilities) are also noteworthy examples of the production of Green Hydrogen (Noussan, 2020).

In this thesis, Green Hydrogen production (Hydrogen being produced through electrolysis with use of renewable electricity coming from the sun and wind), is investigated. To have a better understanding of other types of Hydrogen, readers are referred to Noussan, M. et al (2020).

1.4 Electrolysis in the Considered Case Study

As explained in the previous part, the electrolysis is one of the main Hydrogen production routes. Since the case study examined in this thesis involves electrolysis, this method is going to be discussed here thoroughly.

Water electrolysis happens by the help of electrolyzer, for which different technologies are available. Alkaline electrolyzers (AEL), being the state of the art, and Proton Exchange Membrane (PEM) are the two main technologies which are commercialized and extensively used.

AEL, since 1920s, has been widely used for industrial applications. Its capital cost is relatively low compared to other technologies and it is known to be available extensively while being durable. AEC operates at a relatively low pressure and with a low current density. It also shows a bit of inflexibility when confronted with frequent load changes (as rare as they can happen since it is usually operated at steady state unless for maintenance) and start-ups. In consequence, the overall efficiency of AEC has some limitations and cannot exceed a certain range.

In 1960s, PEM was introduced to the market as a more modern technology trying to diminish the defects of AEL technology. As a result, it operates with a higher flexibility while dealing with variance in load and power while providing a faster startup, a quicker response to load changes, and also a better and more efficient energy consumption. The efficiency is also higher in this case. Although the benefits mentioned here are crucial for in the comparison between PEM and AEL, there are a number of disadvantages that are cardinal as well. Using expensive materials in the complex structure of this electrolyzer, a shorter lifetime, and requiring a pure source of water have made the use of this type of electrolyzer limited to small-scale applications.

There is another technology introduced as well, being called Solid Oxide electrolyzers (SOEC). However, this technology is still in the R&D phase, and has a higher CAPEX. Operating temperatures are relatively higher in this technology, so the main limitation is the material degradation in presence of high temperatures, although there is a higher electrical efficiency.

The future progress in improving the electrolysis and electrolyzer technology is possible in all three types of technologies explained above. All these improvements will cause declines in the CAPEX costs and in the final Hydrogen price. For AEL, future improvements are focused on dealing with a better coupling with intermittent and unprogrammable RES. In the case of PEM, reaching a less complex structure and manufacturing line in addition to using less noble and expensive materials are the solutions for the future. Lastly, for SOEC, stabilizing the electrolysis process to get to the commercial use by trying to figure out how to operate at lower temperatures (from 650°C - 1000°C to 500°C - 750°C) and developing new suitable materials are the goals. In all cases, economies of scale are the next step in the path to reaching a competitive price for Hydrogen produced through electrolysis (Schmidt, 2017) (Noussan, 2020).

The schemes of all these three technologies are shown below in Fig. 6:

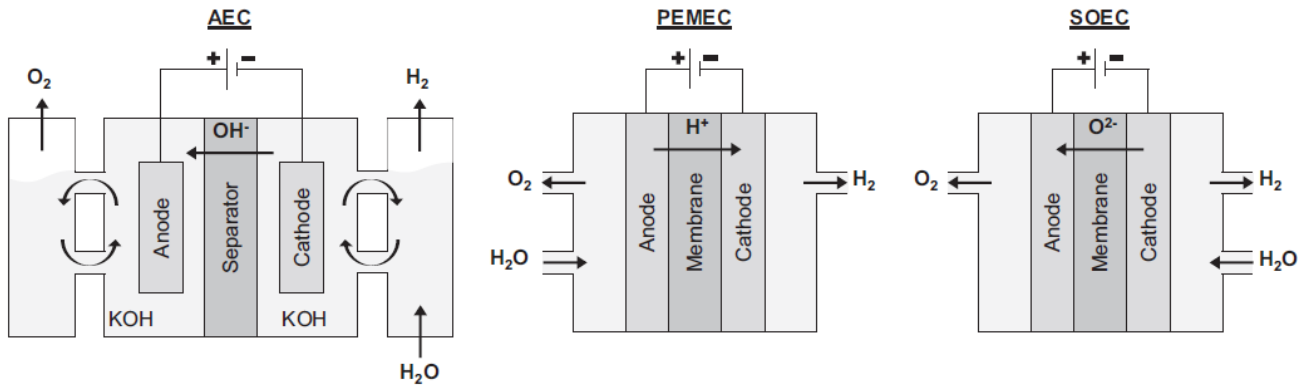


Figure 6 Schemes of the three electrolyzer types (source: (Schmidt, 2017))

1.5 Hydrogen Market

1.5.1 Hydrogen Uses in Industry

The share of industrial uses of Hydrogen is now dominating all other uses; oil refining, ammonia production, methanol production, and steel production are the sectors with the highest shares of H₂ consumption. The large-scale Hydrogen production to meet the needs of industrial sectors, nowadays, mostly takes place using three main fossil fuels: natural gas, oil, and coal and hence, a lot of pollution is emitted into the air (IRENA, 2018). Green Hydrogen can be the ideal solution for providing the H₂ that these sectors need since it is not polluting the environment. Because of this matter, some claims that Green Hydrogen use is going to be twenty-two times bigger by 2030, although considerable barriers are still in place regarding providing enough electricity from RES (Noussan, 2020) (Matthew Farmer, 2021) (Kakoulaki, 2021).

As it is clear, the largest demand share belongs to the chemicals sector (Ammonia production and refining) while other shares of the global Hydrogen demand are much smaller. For production, more than 95 % of current global production is coming from fossil-fuels (Steam-methane reforming (SMR) being the most common method of production while coal gasification and oil are in the next places). It is also useful to bear in mind that globally, only about 4 % of Hydrogen production comes via electrolysis, mostly using chlor-alkali processes (IRENA, 2018).

1.5.1.1 Hydrogen in Oil Refining

Up to 25% of the Hydrogen in the world is consumed by oil refining, which is converting crude oil into different final products. In oil refineries, Hydrogen, which can be feedstock, energy source, as well as reagent, is mainly used in the two processes of hydrocracking (converting heavy oil residuals into oil products with a higher value) and hydrotreatment (removing impurities especially Sulphur). Hydrogen also plays a role in the process of upgrading oil sands (removing Sulphur) as well as biofuel hydrotreatment (the process of removing oxygen and improving the quality of the fuel) in refineries too. Moreover, some Hydrogen, which cannot get economically recovered after using them in these processes, is used as fuel and consequently, it is burned. The final products after desulphurization can be fuels for transportation or the feedstock used in the petrochemical sector.

The Hydrogen used in the oil Refining has two main sources: almost 60% of the Hydrogen comes from fossil fuels (specifically Natural Gas) and the rest (40%) is provided through the by-product Hydrogen coming from chemical plants or in general, any other facility that produces Hydrogen, but not as the main product. Thus, oil refining Hydrogen use (the share that comes directly from the fossil fuels) is responsible for the emission of almost 20% of the total refinery emissions. This amount of emission contains around 230 Mton of CO₂ per year. In the recent years, the air pollutant standards have been getting tougher, especially regarding Sulphur, and there have been many policies and laws introduced to the market regarding the allowed amount of industrial pollution. This matter and the future regulation will lead to an increase in the amount of H₂ needed for this sector to substitute the conventional energy sources and that is why it is believed that the Hydrogen market is going to have a boost (by at least 7% by 2030) as a cleaner alternative. Of course, the abundance of crude oil can have an impact on the increase in Hydrogen use since it is a must for the whole process. The future predictions and plans show that there are not going to be many new refineries built and that is why it is needed for the old ones to be retrofitted by using a proper Carbon Capture and Storage System for reducing emissions (IEA, 2019).

1.5.1.2 Hydrogen in Ammonia and Methanol production

The chemical sector is the next main consumer of Hydrogen. This sector mainly produces Ammonia (more than 31 Mt H₂/year of hydrogen needed for Ammonia production) and Methanol (more than 12 Mt H₂/year for Methanol production), which are the next two main players of the Hydrogen market. The chemical sector is also one of the biggest producers of by-product Hydrogen. This Hydrogen can be utilized both by the same sector or it can be transferred to another sector or other purposes.

Ammonia coming from the chemical sector is mainly (around 80% of it) used for manufacturing fertilizers (Ammonium Nitrate and Urea). The rest (around 20%) is used for other industrial purposes, such as manufacturing synthetic fibers or explosives) which are also really important, and their demand is never diminishing. Methanol, on the other hand, is used for manufacturing of industrial materials such as methyl methacrylate, various solvents, as well as formaldehyde. It is also an important part of the procedure that converts Natural Gas and Coal to Gasoline (a process which is called Methanol-to-Gasoline).

Just like the case of refineries, this sector mostly consumes the Hydrogen which comes from the fossil fuels (due to them being cheap and accessible). Natural Gas reforming or Coal Gasification are the main processes used in this sector, of which, the former is more efficient and that is why it accounts for almost 65% of Hydrogen production for the chemical sector. The regional Natural Gas prices also influence this matter. It has been estimated that the demand for Methanol and ammonia is going to increase in the sector by 2030 and due to high number of associated emissions (greenhouse gases) with fossil fuels used in the process, switching to low-carbon (low-emission) methods to acquire Hydrogen in parallel with working on increasing the efficiency of the chemical process is the possible solution to mitigate the harmful environmental impacts.

1.5.1.3 Hydrogen in Steelmaking

Steelmaking industry uses Hydrogen as the reducing agent (either sole reducing agent or auxiliary reducing agent). To be more precise, Hydrogen is used instead of coke in the furnace and consequently, reduces the amount of coke used and a decline in the correlated emissions is seen due to the fact that Hydrogen will form water while reacting with iron ore (and not Carbon Dioxide like coke). Thus, steelmaking sector accounts for the fourth-largest demand of Hydrogen worldwide now (around 4 Mt H₂/year). The estimations have shown that the demand for Steel is going to rise around 6% by 2030. This matter confirms the fact that the demand for Hydrogen will rise notably in the upcoming decades too.

Large quantities of Hydrogen (around 14 Mt H₂/year, not in a pure form, but as a mixture like coke oven gas) is also a particular by-product of this sector, just like the chemical sector, and just as the previous case, this Hydrogen can be used internally within the same sector (around 9 Mt H₂/year), or it can be transferred to other sectors.

The Hydrogen which is utilized in the Steelmaking sector is mostly coming from fossil fuels (just like the two previously explained sectors). The emissions coming from the steelmaking sector is also an issue since around 1.4 tons of direct Carbon Dioxide

emission is produced as a result of producing 1 tons of crude Steel (around 4% of Europe CO₂ emissions). This calls for efforts to first, implement the low-carbon Hydrogen in the cycle (to substitute the currently coming directly from Natural Gas and Coal Hydrogen) as well as integrating the CCUS systems to recover the produced Carbon Dioxide as much as possible. The second option is still not developed completely, like the Chemical sector case, and it is on the way of being commercialized. The last step is to try to substitute Hydrogen instead of Carbon Monoxide as the main reducing agent in the DRI process. The latter is the last phase of the plan due to the fact that the large-scale plant capable of doing so is going to be ready approximately in 2030 (IEA, 2019).

1.5.2 Hydrogen Uses in Mobility

In most of the countries all over the world, a massive amount of energy is being used up by the transportation means. Until the recent decades, conventional fuels (mostly fossil fuels) were extensively being used which then had resulted in huge amounts of harmful gases as well as greenhouse gases (like SO₂, NO₂, NO, CO, and CO₂) being emitted in the air. These gases also have caused an increase in the average temperature of earth and global warming related issues. All these environmental problems as well as fossil fuels' stock being finite, have made societies think of an alternative fuel for passenger vehicles, buses, and trucks. This is when Hydrogen was suggested.

It is safe to say that basically, every means of transport can be powered by Hydrogen. In the case of mobility and the use of Hydrogen, two cases can be evaluated. First is to use H₂ as the direct fuel of the transportation vehicle (known as Hydrogen-based fuels, including Ammonia, Methanol, synthetic Methane, and synthetic liquid fuels), and second, is to use Hydrogen, indirectly, through fuel cells (Hydrogen fuel cell electric vehicles or FCEVs) as the power train of the vehicle. Hydrogen can be used in cars, Buses, trucks, other goods vehicles, as well as in Maritime, Railway, and Aviation sectors. (IEA, 2019) (Greene, 2020).

1.5.3 Hydrogen Uses for Heating and Power Production

This sector, providing heat and power for the buildings, is the origin of 28% of the global emissions and requires almost 34% of the global energy demand, the energy which is used for cooking as well as space heating and hot water production. Around 85% of this energy comes from fossil fuels (IEA, 2019). Mitigating this amount of emission by substituting the low-carbon fuel alternatives, reducing the energy demand by improving the energy efficiency of buildings, while reducing the use of conventional fuels in order to switch to cleaner and greener fuels has been one of the main objectives in countries' strategies for the global energy transition program although there are a limited number of solutions for

it. One of these limited solutions, which has shown to be of the most cost-efficient ones, is to involve Hydrogen by utilizing Hydrogen boilers for heating and fuel cell CHPs (combined heat and power). This integration of Hydrogen in Building sector has not really advanced yet and needs much more investment and focus (Hydrogen Council, 2020) (IEA, 2019).

Also, nowadays, Hydrogen has not been fully integrated in the Electricity and Power sector as well, for instance around 0.2% of the total electricity production comes from Hydrogen now. In addition, pure Hydrogen is not used as the direct fuel for power generation. However, as one of the most influential steps, Hydrogen can be used, more widespread, for balancing the supply and demand electricity. Remote areas of the world, like islands, still have some challenges for meeting the electricity demand of their people and there is also no objection that economic stability and electricity are closely related. In these areas, renewable energy resources in great scales can be utilized to be the greener alternatives for electricity production for these areas even considering their unprogrammability. This is when Hydrogen can enter the game and benefits the grid by offering the possibility of using the green energies and also being stored for later use. In addition, Hydrogen as well as Hydrogen-based fuels like Ammonia (which can be co-fired in Coal-fired power plants for decreasing Coal consumption, used in gas turbines or CCGTs) and synthetic Natural Gas are other good solution which can contribute to declining the number of emissions that the power sector is producing by providing low-carbon alternatives (Matthew Farmer, 2021) (Noussan, 2020) (IEA, 2019).

1.5.4 Policies and Regulations in Europe

Just like any other sector, the regulations and policies affect the energy and Hydrogen sector enormously. In recent decades, the focus of governments has been specifically redirected to promoting carbon-free energy carriers, like Hydrogen (Hydrogen Europe Intelligence, 2020).

First, the 'Energy Union', formed in 2015 with the five main pillars of energy efficiency, energy security, decarbonization, the internal energy market, and research & innovation, has had the purpose of defining EU's legislations to reach such agenda proposed as its pillar. Then, in 2019, 'Clean Energy Package', was introduced. The European Chamber, at its gathering on 12 December 2019, embraced the target of accomplishing a climate-neutral EU by 2050, an agreement which is known as 'Green Deal' as well (Hydrogen Europe Intelligence, 2020). This arrangement targets to present Europe as the leader of the energy transition in the world, aiming for a carbon-free mainland by 2050, through handling biodiversity misfortune as well as changing inefficient utilization of assets by moving to a more roundabout economy (Hydrogen Europe Intelligence, 2020) (Fuel Cells

and Hydrogen Joint Undertaking, 2019). Generally, it is said that the EU's plan for fighting the climate change is very ambitious, yet possible. The first main set of initiatives are mentioned as follows:

1. Embody climate-neutrality into the laws of EU (known as European Climate Law)
2. Promotion of climate actions for the citizens to get them involved as much as possible (known as European Climate Pact)
3. Reduce the amount of greenhouse gas emitted into the atmosphere by more than 50% by 2030 (known as 2030 Climate Target Plan)
4. Reach a climate-resilient society (fully implemented the policies and laws of climate change) by 2050 (known as New EU Strategy on Climate Adaptation)

Other policies and legislations designed are stated below:

- Further promotion of reduction in the amount of greenhouse gas emissions produced by introducing EU Emissions Trading System (EU ETS) for industry, the power sector, and transportation within the EU itself
- Reduction of greenhouse gas emissions in the transport sector, for instance through introduction of well-set standards for CO₂ emitted by vehicles
- Reduction of greenhouse gas emissions in buildings and the agriculture sector by setting national targets
- Promotion of ad-hoc low-carbon technologies
- Protect the ozone layer
- Reach an improved energy efficiency and higher penetration of renewable energies
- Make the transition from fossil fuel to cleaner energy as easy as possible
- More investment in cutting-edge research and technologies as well as related climate actions (European Commission for Green Deal, 2021)

It is worth to mention that this whole revolution has started by Paris agreement in order to try to limit the damages that humans have done to the environment through industrialization and the global warming that has happened afterwards due to the enormous amount of CO₂ which is emitted into the atmosphere. An example of such damage can be seen in Fig. 7 that depicts the CO₂ emissions from different sectors from 2010 to 2050. The countries involved in this agreement have consented to submit broadly decided commitments to quickly lessen their CO₂ produced in their energy sector to regulate the worldwide temperature increment to well underneath 2°C above preindustrial levels while seeking methods to even restrict this temperature more, and to 1.5°C. This agreement directly affects the whole process of energy production and use, namely generation, storage, distribution, and consumption, while promoting energy

efficiency and decarbonization in the industry, power, buildings, and transport sectors too (European Alternative Fuels Observatory, 2021) (IEA, 2019) (The Council Of The European Union, 2020) (IRENA, 2018).

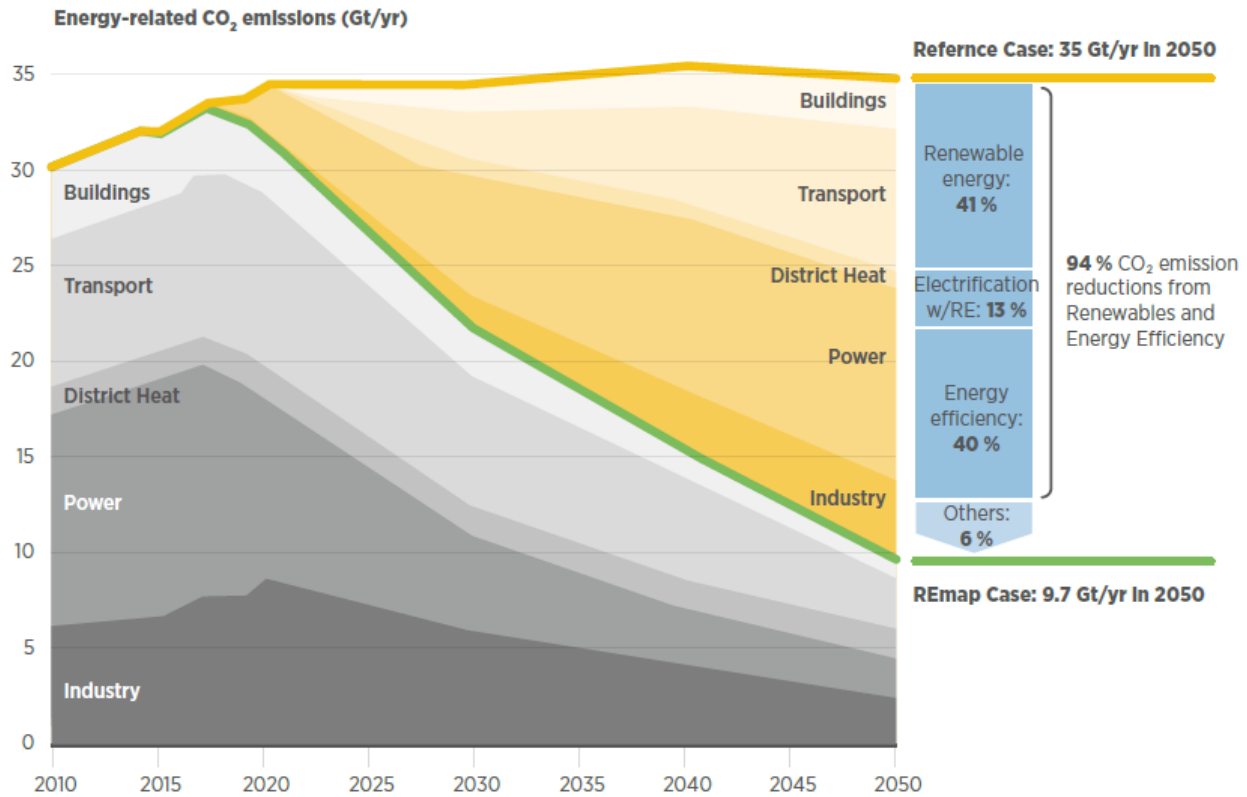


Figure 7 CO₂ emissions from different sectors from 2010 to 2050 (source: (IRENA, 2018))

While coming up with ideas and notions to further implement the Paris agreement, one thing seemed so vital in every proposed model being evaluated. The necessary factor was the integration of Hydrogen production, storage, and distribution at large scale in every winner scheme, although one third of all the emissions related to energy sector cannot be eliminated due to not having a viable economical option to handle (IRENA, 2018) (The Council Of The European Union, 2020) (Hydrogen Europe Intelligence Department, 2020) (Kakoulaki, 2021) (Kurtz, 2019) (Abad, 2020) (Dincer, 2012). As shown in Fig. 8, Hydrogen will be more than enough for all sectors.

Consequently, the European Commission has been focused more than ever in supporting Member states in upscaling of supply of Hydrogen, by defining a thorough legal frameworks and principles to ensure competition in a liquid market by attracting necessary investments and introducing an efficient carbon pricing mechanism. Other outcomes of these directives will be affordable prices while securing the supply at all

points to reach economy of scale for this expanding market of switching to decarbonized energy carriers (The Council Of The European Union, 2020) (Kakoulaki, 2021) (Kurtz, 2019) (Abad, 2020) (Hosseini, 2016).

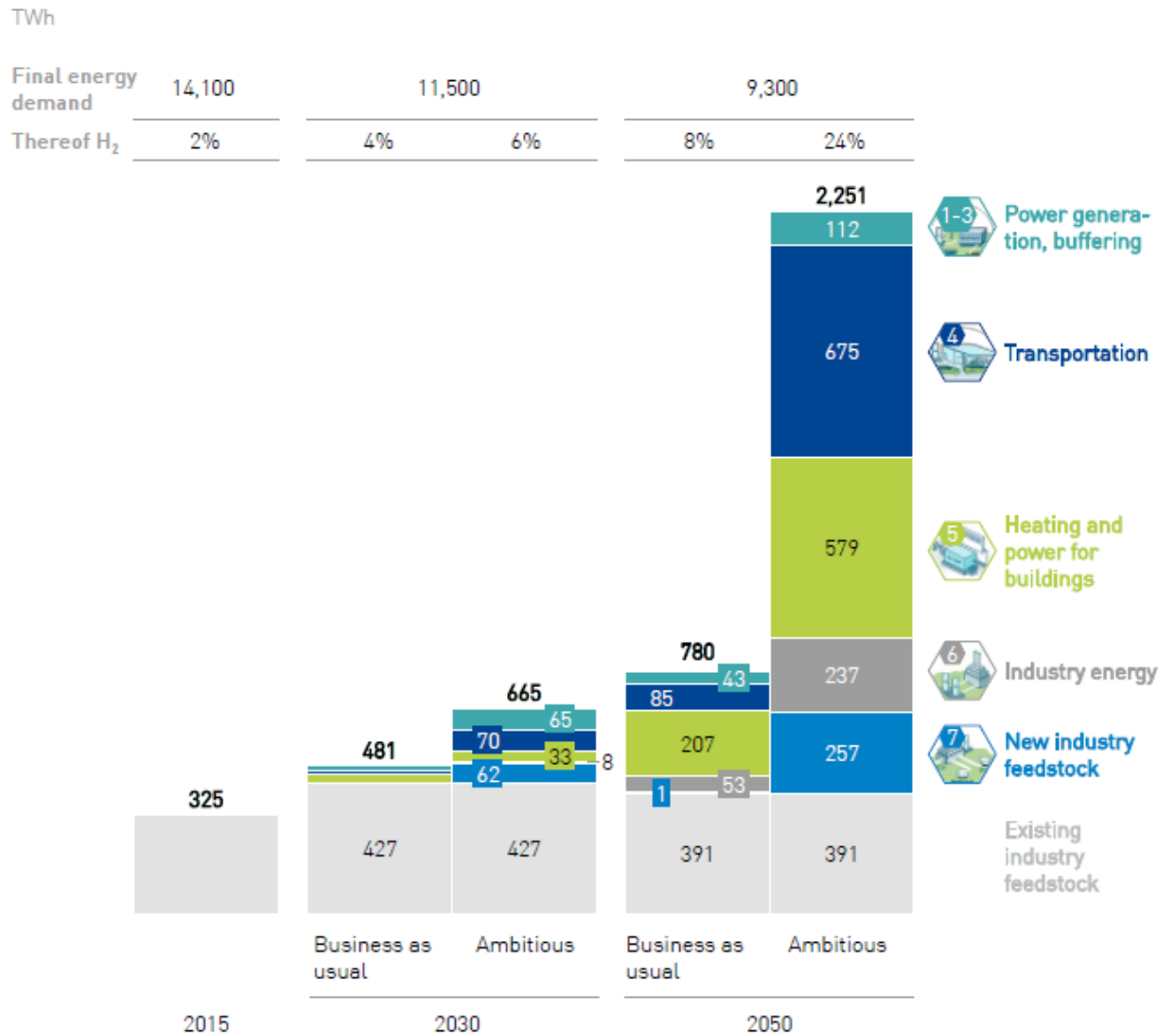


Figure 8 Hydrogen providing total energy demand (source: (Fuel Cells and Hydrogen Joint Undertaking, 2019))

1.5.5 Hydrogen Infrastructure for Transportation

An infrastructure which operates to provide the Hydrogen from a storage system to vehicle, to be used either as a direct fuel in internal combustion engines (ICE) or as an Indirect fuel for the vehicle as the Hydrogen needed for fuel cells (FC), is called a Hydrogen refueling stations (or in short HRS). A refueling bus station is an example of the Hydrogen infrastructure for delivering Hydrogen to a specific group of users. Nowadays in the transportation sector, dispensing Hydrogen for Hydrogen-used vehicles for direct combustion in ICEs for the case of buses, the case of study in hand in this thesis, the Hydrogen being distributed is mostly in gaseous form. The scheme of a typical Hydrogen refueling station is shown below in Fig. 9. The main parts of each HRS as a production site, a compression and a storage system which then is followed by a dispensing device or method (Reuter, 2017) (Kurtz, 2019) (European Alternative Fuels Observatory, 2021).

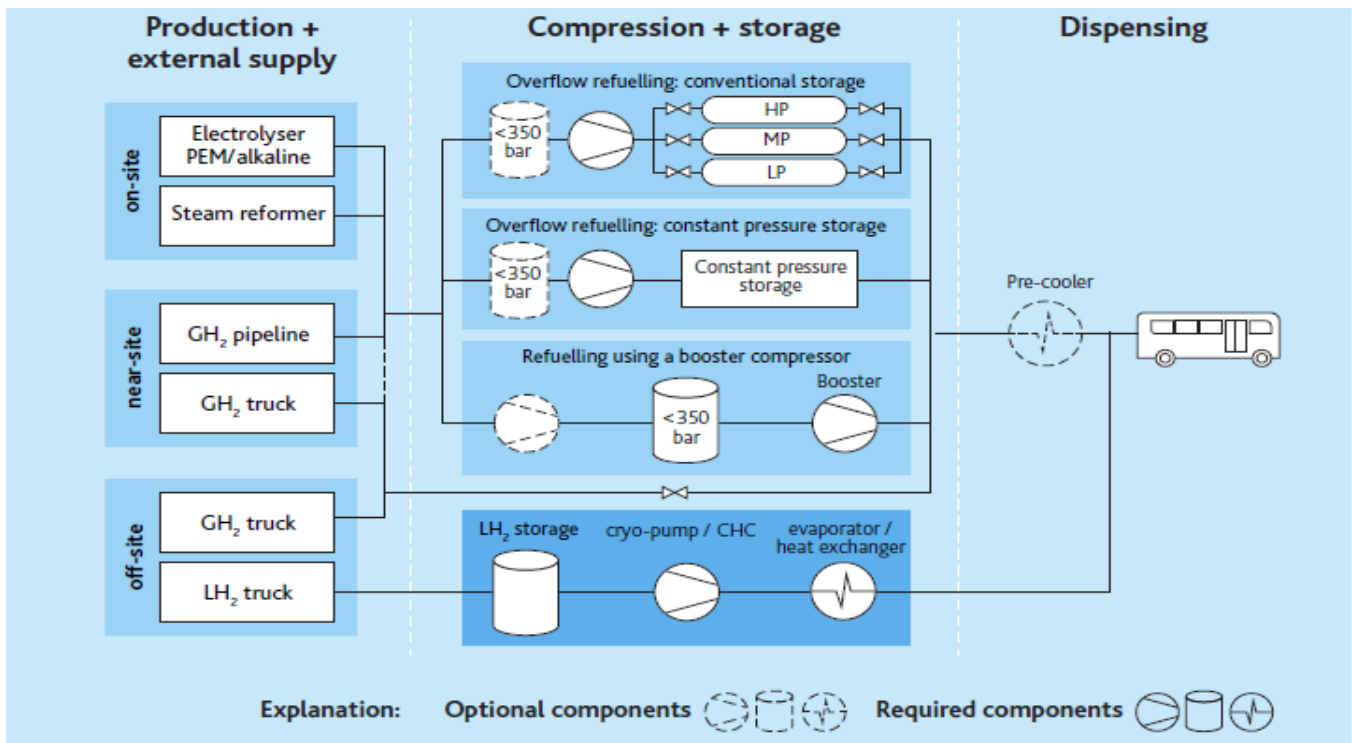


Figure 9 Scheme of a Hydrogen refueling station (source: (Reuter, 2017))

2 Optimization Methodology

2.1 Scope of the Research

This research focuses on optimizing the production procedure of the needed Hydrogen for a refueling bus station utilizing a specific configuration. This configuration works in a way that there are four parts, including an electrolyzer, a compressor, a storage system, and a distribution network, that by consuming electricity produce Hydrogen from water to fulfill a known demand of one refueling station. This analysis in hand intends to investigate working conditions and economics of this onsite production through electrolysis depending on different optimization objective functions (minimizing the cost, minimizing CO₂ footprint) and under different CAPEX assumption. This is established using different sets of input data in terms of price of 1MWh of electricity, demand profiles, and hourly CO₂ content of 1 MWh (grid related emissions). The details regarding this data and their sources are presented in section 2.4.

The goal is then to assess the price of Hydrogen in each case and identify optimal configurations. Additionally, the analysis regarding the CO₂ content of each kilogram of Hydrogen can help in evaluating whether using Hydrogen instead of other conventional fuels can be backed up by ultimate reduced environmental impacts.

2.2 Optimization Tools

In order to model the desired configurations of the Hydrogen production plant, mixed integer programming using CPLEX was chosen. In this analysis, CPLEX (version 20.10) was used as the solver which has the ability to solve all types of linear programming and quadratic problems as well as integer and mixed-integer ones. This solver has been used through AMPL, which is known to be one of the best computer languages used for large-scale optimization due to its flexibility to carry out repeated runs in a relatively short period of time as well as its easy-to-use notation and syntax, diverse solvers, and interactive environment. Using AMPL, algebraic modeling with the help of state-of-the-art interpreters convert the problem into a readable format for the CPLEX for the solver

to deal with the problem directly or turn it into interrelated subproblems and handle them (AMPL Inc., 2021).

Additionally, the system used for carrying out the optimization of the models had the characteristics stated below:

- Processor: Intel(R) Core (TM) i5-3337U CPU @ 1.80GHz (4 CPUs), ~1.8GHz
- Memory: 8192MB RAM
- Available OS Memory: 8082MB RAM

2.3 General Overview

This study is categorized in five major sections. In section one, the model investigates the conditions under which the sum of electricity costs throughout the year is minimized based on different demand profiles which are needed to be provided and considering difference maximum allowances for FCR (Frequency Containment Reserve) allocation. The second model focuses on the minimization of the Carbon Dioxide produced per MWh of electricity used in 1 year and the third model takes into consideration the CAPEX and OPEX numbers as well as the sum of electricity costs for the whole configuration with the goal of finding the best and wisest installed capacity for both the main two components of the system (Electrolyzer and Storage).

The basis of all these models is the same, however, there are several modifications for the objective function which needs to be optimized and the constraints and input data differ based on the desired scheme. Moreover, this study considers the actual electricity data from two countries. The input data (the prices of electricity which is withdrawn from the grid as well as the prices for FCR and the amount of CO₂ produced per MWh of electricity) are provided from Germany and France. Also, the output of the models, with any type of input, has been a .csv file with the main numbers regarding the cost of the whole configuration in KEuros, the cost of each Kilogram of Hydrogen in Euros, and the CO₂ content of each Kg of Hydrogen and also, a .xlsx file containing the hourly set points for electrolyzer in KW and storage in Kg.

2.4 Case Study Details

The following points are mutual between all models in terms of the input:

- + The data regarding hourly electricity prices and hourly FCR remuneration prices are actual data from France and Germany. Also, this input data varies by year as

well. The data for both years of 2019 and 2020 has been used. Separate optimization runs have been carried out for each country in each year separately with its own specific data. Since for some analysis, France was used as the core, below, in addition to the depiction of spot prices of France and Germany throughout 2019, spot prices of France have separately been compared to the 2019 average of spot prices in France and the average of 200 cheapest prices of the year 2019 as well. A noteworthy piece of information here is that before the integration of the market, Germany and France had different markets for electricity and consequently, the hourly spot price was different in each country. However, after the integration of the markets, now, they have almost the same price for most hours of the year, and this is completely evident in the graphs below (Fig. 10 to Fig. 12). These data mentioned above are gathered from ENTSO-E, which is the short form for the European Network of Transmission System Operators for Electricity. This association has the goal to bring together the 42 TSOs who come

from 35 countries for further securing Europe's electricity network (ENTSO-E, 2021).

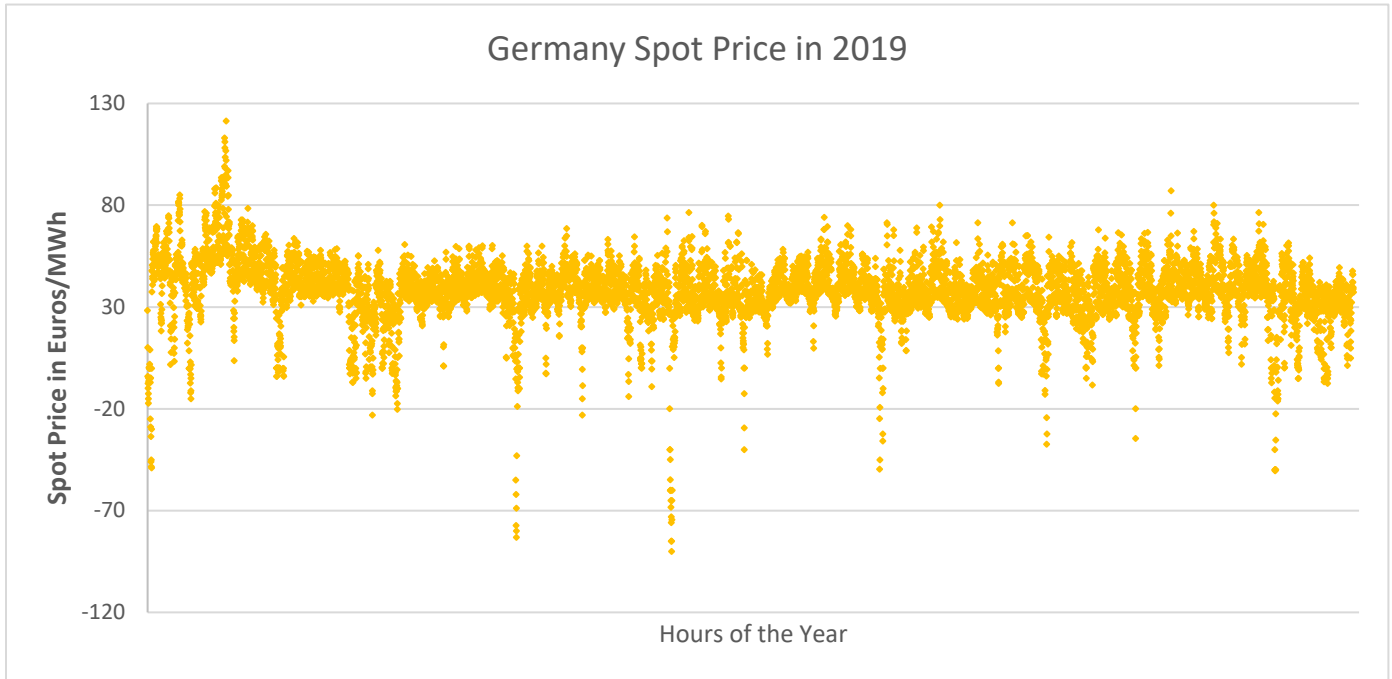


Figure 11 Germany Spot price in 2019 in Euro/MWh throughout the year

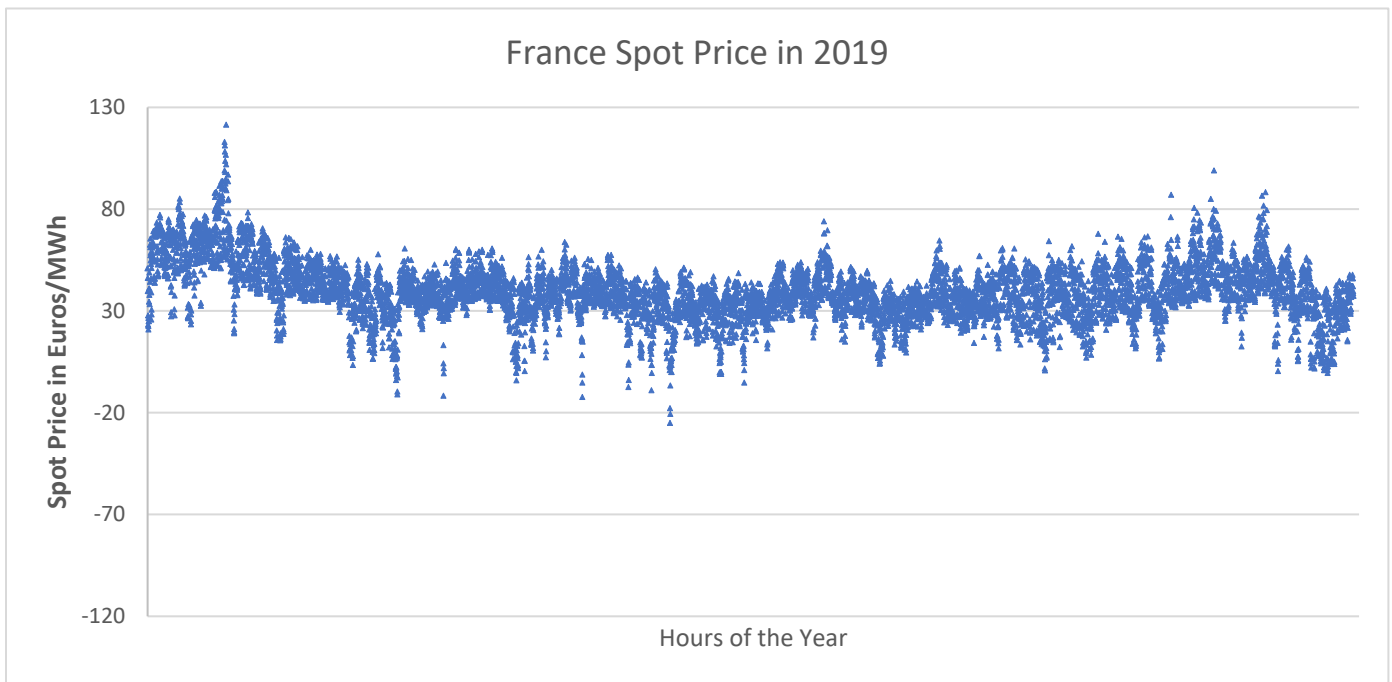


Figure 10 France Spot price in 2019 in Euro/MWh throughout the year

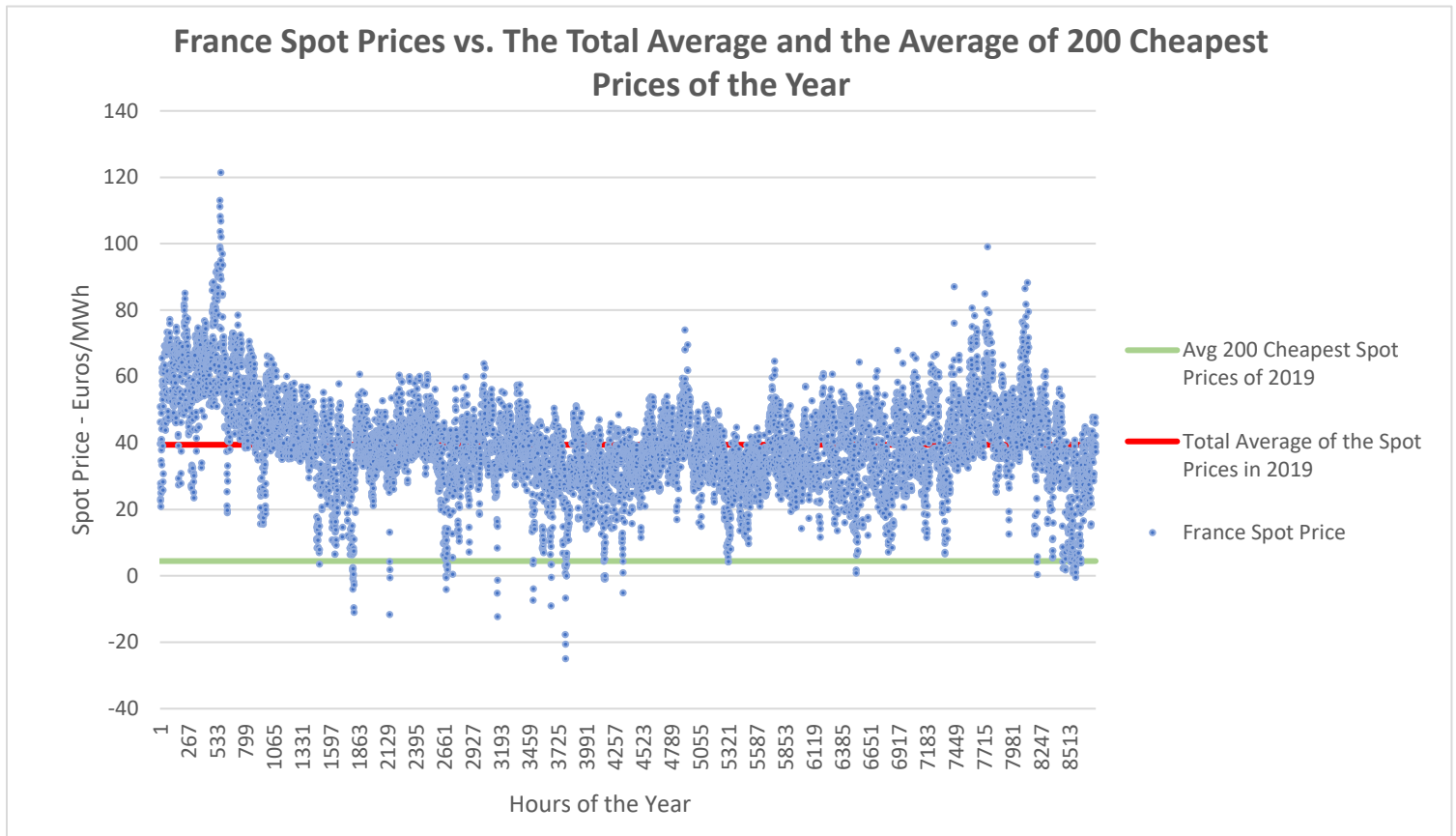


Figure 12 France Spot Prices vs. The Total Average and the Average of 200 Cheapest Prices of the Year

- + The hourly demand profile is related to the Hydrogen demand of a bus refueling station. The demand profile is the same for each week of the year: the same hourly demand profile has been repeated for all the weeks. However, the demand profile given to this model, is not unique. For understanding the power of different demand profiles and how this input can affect the results of the optimization, a sensitivity analysis has been implemented by changing the demand profile for the whole year by changing the desired amount of Hydrogen in weekdays and weekends. There are four different hourly demand profiles available: 1a, 2a, 1b, and 2b.

- + Between these four demand profiles, in profile 1a and 1b the total weekly Hydrogen demand is 2130 Kg whereas in demand profiles 2a and 2b this value is 2640 Kg. This is why some analysis has been done between 1a and 1b and then 2a and 2b separately. Additionally, because of this difference in the total weekly Hydrogen demand in these demand profiles, the initial condition for the storage is different between 1a/1b and 2a/2b. For the case of 1a/1b, this amount has been set to 30% of the storage volume while for 2a/2b this amount is set to 37.5%. The demand profiles used in the optimization models can be found in Fig.13 and Fig.14:

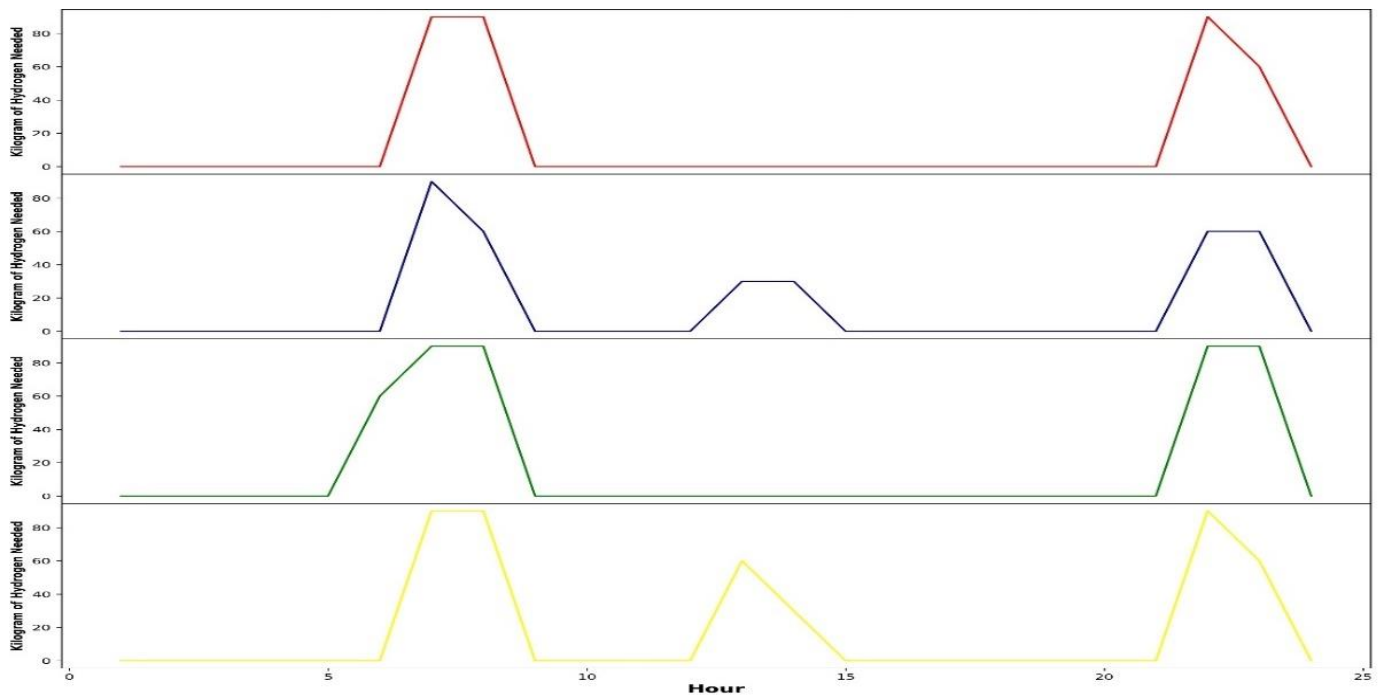


Figure 13 Hourly demand profiles (in the order of: 1a-1b-2a-2b) for weekdays (Mon-Fri)

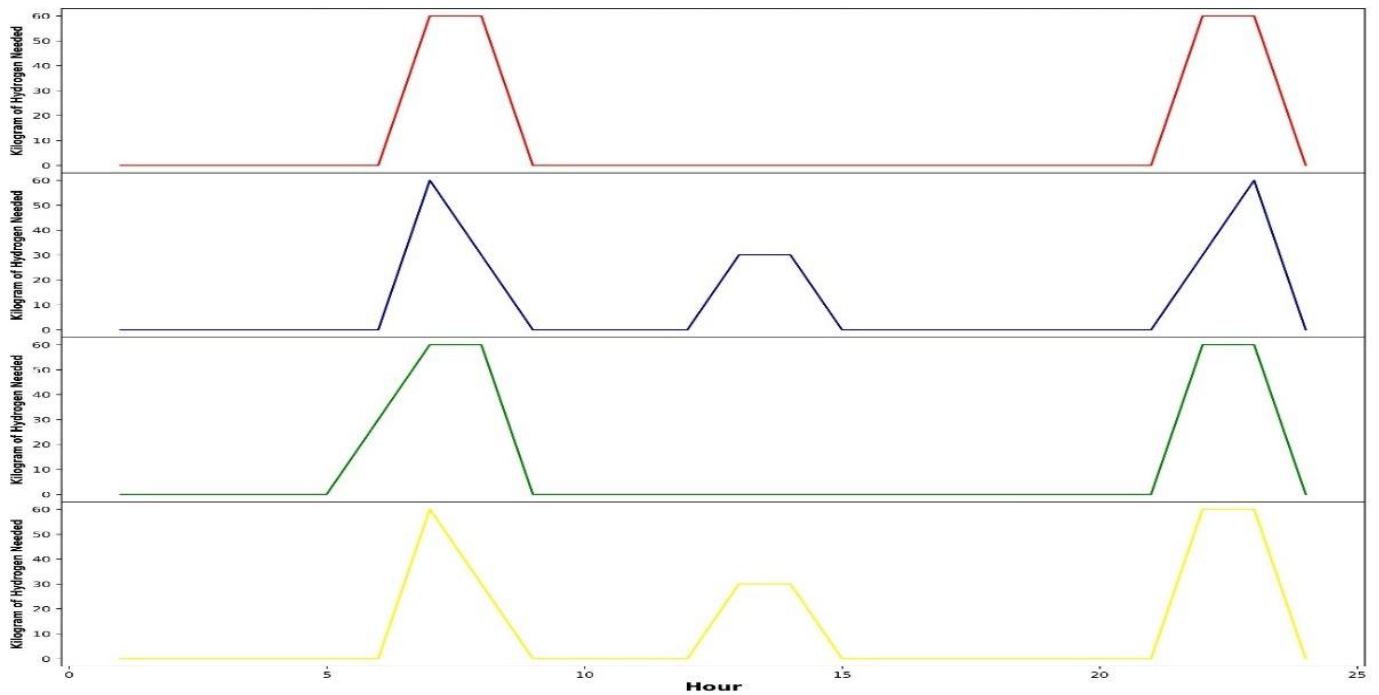


Figure 14 Hourly demand profiles (in the order of: 1a-1b-2a-2b) for Weekends (Sat-Sun)

- + The data regarding hourly average CO₂ content per 1 MWh are actual data from France and Germany (shown in Fig. 15 and Fig.16) and both sets of data are for 2019. Separate optimization runs have been carried out for each country separately with its own specific data.
- + These data for the hourly average CO₂ content per 1 MWh for France has been gathered from RTE resources. This entity is the administrator of the French Electricity Transmission Network. (RTE, 2021) For Germany, the data from Agora Energiewende has been used. This entity is operating as a branch of the non-profit Smart Energy for Europe Platform (SEFEP) (Agora Energiewende, 2021).

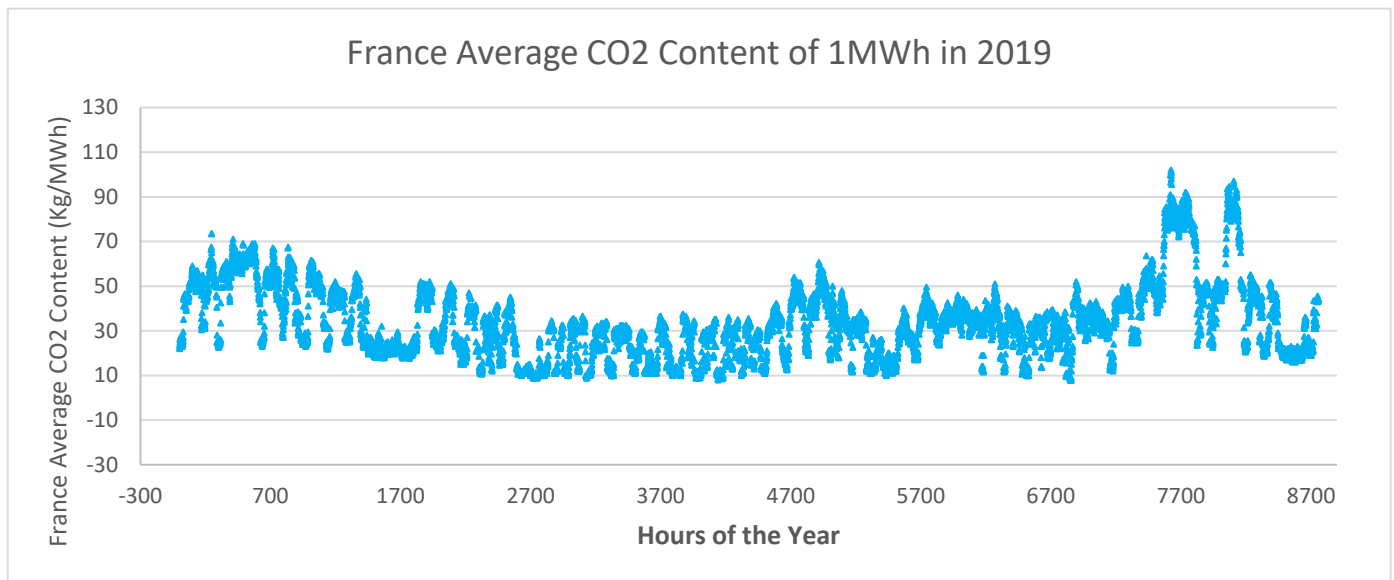


Figure 15 France Average CO2 Content (Kg/MWh)

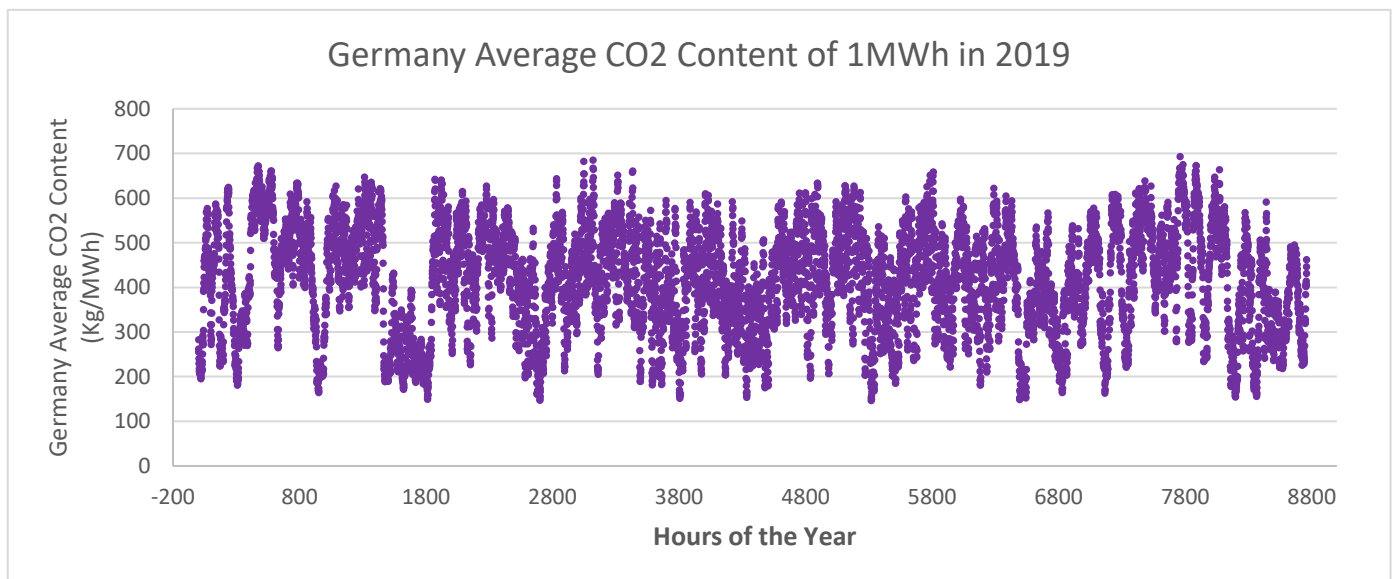


Figure 16 Germany Average CO2 Content (Kg/MWh)

- + The hourly electricity production profile of the wind turbine (the source of RES electricity in this thesis that we going to use its electricity in Models 4 and 5), is shown below in Fig. 17:

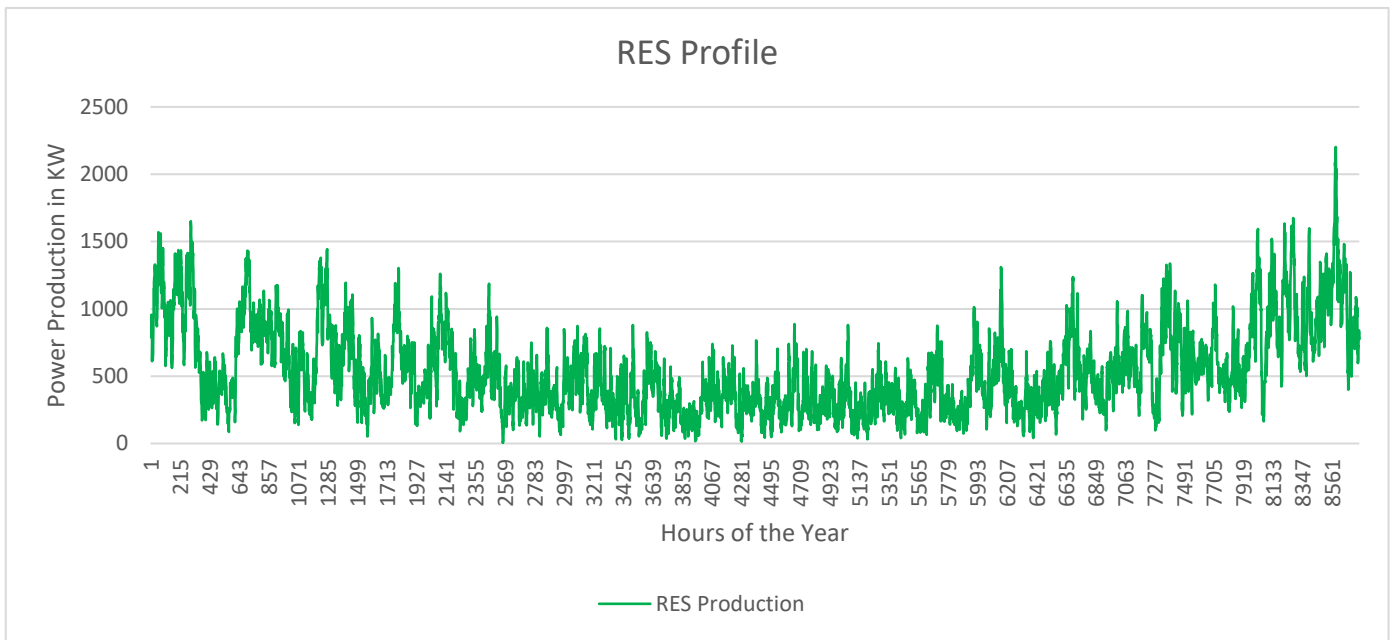


Figure 17 RES power production profile in KW

2.4.1 Model 1: Normal Cost Function Minimization

The main problem in hand, which is mutual between all models, is that there is a known hourly demand for Hydrogen, throughout a year, which needs to be fulfilled. This is going to happen with the help of an electrolyzer, which withdraws electricity from the grid to produce Hydrogen through electrolysis. The Oxygen which comes from this device is released into the air and the Hydrogen, which is the target element goes through compression, storage, and then it is distributed to the Hydrogen station as anticipated from before.

The electrolyzer works at 30 bars, and it gets its power from the electricity withdrawn from the grid. The possible working range for this equipment is between 15% load to full load. In this model, electrolyzer works at the rated power of 1 MW. Consequently, the working range will be between 150 kW and 1000 kW. This electrolyzer also has the specific consumption of 55 KWh/Kg of H₂.

The Hydrogen coming from this electrolyzer is then compressed to be ready to be stored at the final pressure of 500 bars. This compressor has a specific consumption for each kilogram of H₂ which is 5 KWh. The use the of compressor is determined by the rate at which the electrolyzer is being utilized. The compressor is coupled with the electrolyzer in terms of rate of working because the use of this component is to make the Hydrogen coming from the electrolyzer ready for storage.

The compressed H_2 is then gathered to be stored in a storage which has its own limitations; it has a specific dead volume which cannot be used and can be treated as the minimum amount of H_2 which needs to be present in the storage. In the last stage, the Hydrogen from the storage is distributed through the system to meet the known demand and the desired stations. It is possible to say that the process of providing the demand is focused on the storage, to turn on the electrolyzer as less as possible due to the changing hourly electricity prices and use the already existing Hydrogen in the storage. This means using less electricity at the hours with higher electricity prices and consequently, forcing less cost on the system. There is no other cost associated with turning the electrolyzer on. The overall scheme of the plant is shown in below in Fig. 18:

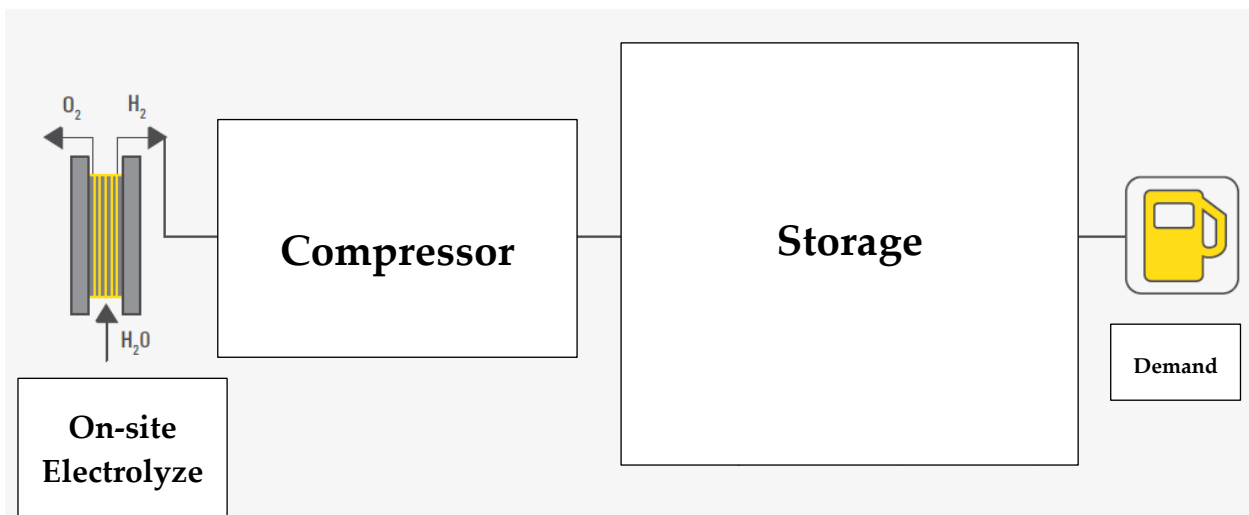


Figure 18 Scheme of the plant being analyzed

Additionally, this Hydrogen production configuration is supposed to provide Frequency Containment Reserve (FCR).

FCR is the solution for the problem of frequency change in the grid. Frequency of the grid, which needs to be maintained at 50 or 60 Hz (depending on the country), depends on the speed of the synchronous generators which produce electricity. When this level of generation (supply) and demand are not balanced, the deviations from the frequency setpoint happens. Although these allowed deviations are really small, they need to be handled in a matter of seconds. The Transmission System Operators (TSO) in each country, use balancing services for this reason. The type of balancing service which is used for this frequency imbalance is called Frequency Containment Reserves which is implemented automatically in case of any deviation within seconds to make the level of demand and supply equal again. In consequence, FCR is the first response of the system, and this is exactly what is considered to happen in this model for the

configuration at hand as well. (Austria's independent transmission system operator (TSO), APG, 2021) (Next Virtual Power Plant Operator & Power Trader, 2021)

Having FCR implemented in the model means that at each hour, the whole configuration has the possibility to offer to the grid a part or all of the electricity it had previously bid to buy from the grid. This can happen in two manners: the possibility of ramping up or ramping down (at the same time). Ramping up and down means utilizing more electricity or less electricity from the grid, respectively, to change the available electricity in the network for other users. This amount of ramp up or down (in MWh) can be sold to the Transmission System Operators (TSO) with a specific hourly price which is known as well, like the hourly electricity price. This matter, as a result, counts as a remuneration for the configuration and not a cost, like the hourly electricity usage. It should be taken into consideration that this ramping up or down can happen, of course, with respect to the electrolyzer's minimum and maximum level of technical feasibility which is 15% to 100% of its power. One last issue regarding FCR is that at each hour, the amount proposed for ramping up or down should be symmetrical. So, FCR allocation can only happen if the electrolyzer has the ability to ramp up and down at the same time within its feasible power region. The FCR explanation can also be found in Fig. 19.

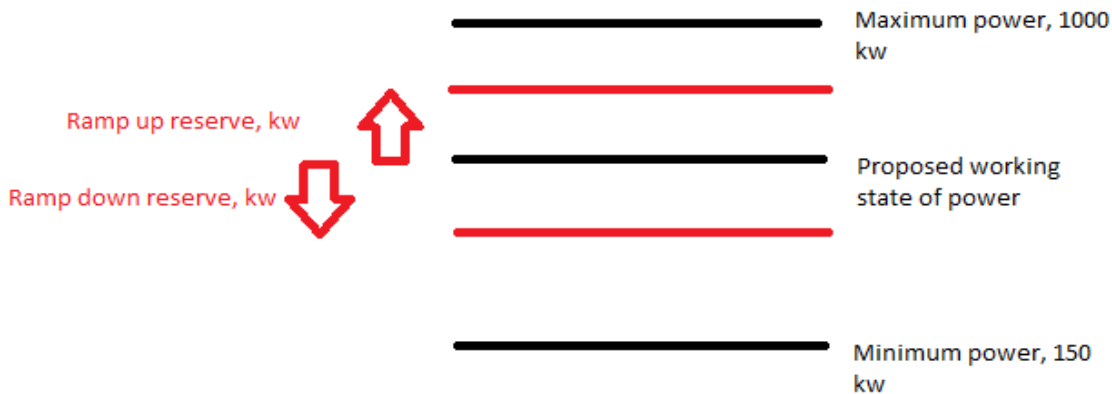


Figure 19 FCR explanation

Model 1 has the aim to find out the hourly rate (in KW) at which the electrolyzer is working based on the hourly electricity prices while determining the optimized amount of FCR allocated in each hour.

2.4.1.1 Model's Specific Characteristics

There are some features only related to the input data of this model:

- + For the case of France, to also evaluate how much the maximum allowed FCR allocation affects the state at which electrolyzer is working at in an hourly manner and more generally how this additional term can affect the problem at hand, this maximum allowance has been set to 0 %, 10 %, and 25 % of the rated electrolyzer power (which here is 1 MW) for each demand profile as well. For the case of Germany, the optimization has been carried out only using the 1a demand profile with 0 % maximum FCR allocation because the input data of spot prices and FCR remuneration prices throughout the year are almost the same for both countries and the evaluation of one can show the overall results.

2.4.2 Model 2: CO₂ Minimization

The main problem in this part is just as what it was presented in Model 1: there is a known hourly demand for Hydrogen, throughout a year, which needs to be fulfilled. This is going to happen with the same configuration discussed in the previous section, with the help of an electrolyzer, compressor, storage, and distribution network. The major difference is the objective of the optimization. In Model 2 we aim at finding out the hourly rate (in KW) at which the electrolyzer is working at. But the goal of the optimization is to minimize the amount of CO₂ associated with the production of each kilogram of H₂ in a year. In fact, this CO₂ is the result of electricity production which is later used by the configuration for Hydrogen production. Consequently, in this model, the average CO₂ content for 1 Mwh is given to the model for each hour of the year too. The outcome of the optimization, in the markets, can later be used by the regulatory entities to define penalties for CO₂ produced by the plants. The numbers vary between hours of a day and also between countries (Germany and France) due to the electricity being produced under different circumstances and using different types of powerplants.

All other assumptions regarding the working range and requirements of all the equipment, meaning the electrolyzer (the minimum possible load, the specific consumption, and the pressure), the compressor (the inlet and outlet pressure as well as the specific consumption), storage (the dead volume, the specific consumption, and the pressure), and the distribution system (its specific consumption) are all the same as before.

Regarding providing Frequency Containment Reserve (FCR), the findings of Model 1 can assist in finding the strategy. Since Model 1 showed that there is no added value for having FCR allocated in general because it will not lead to economic gain whereas the risk of aging for the equipment will be higher, In Model 2, the maximum amount of allocated FCR will be set to 0%.

Just as Model 1, the process of providing the demand is mainly focused on the storage, because turning on the electrolyzer and withdrawing electricity continuously from the grid leads to an increase in the amount of CO₂ content of the Hydrogen produced. This can be explained by pointing out that using less electricity at the hours with higher CO₂ content puts less CO₂ content on the system.

In the real market and real-world cases, the carbon intensity of the electricity grid used for Hydrogen production is the element that determines the carbon intensity of each kilogram of Hydrogen produced. In the case of European countries, reporting average CO₂ content, the CO₂ footprint changes from 0 kg CO₂/kg H₂ in Iceland (due to having an electricity grid which is completely decarbonized, a case which can be considered as renewable Hydrogen) to 46.1 kg CO₂/kg H₂ in Estonia. Furthermore, if the Hydrogen production configuration is connected to a grid and it is using a part of the electricity which if not utilized, is going to be curtailed, the CO₂ footprint of each kilogram of Hydrogen would be zero.

There are several industrial and governmental thresholds for the CO₂ footprint of each kilogram of Hydrogen produced in Europe. The key ones are listed below in Table: (Hydrogen Europe Intelligence Department, 2020)

Name of the Regulation/Benchmark	Related Range (Kg CO₂ / Kg H₂)
RED II threshold for RFNBO	3.384
CertifHy threshold for low carbon hydrogen	4.4
EU Taxonomy threshold for sustainable hydrogen manufacturing	5.8
EU ETS Benchmark	8.85

Table 4 Main thresholds for CO₂ content of 1 Kg of H₂ in Europe (source: (Hydrogen Europe Intelligence Department, 2020))

Moreover, in Fig. 20 the average CO₂ content of each kilogram of Hydrogen produced with the electricity coming from the grid has been compared to the benchmarks stated in the table above for several European countries:

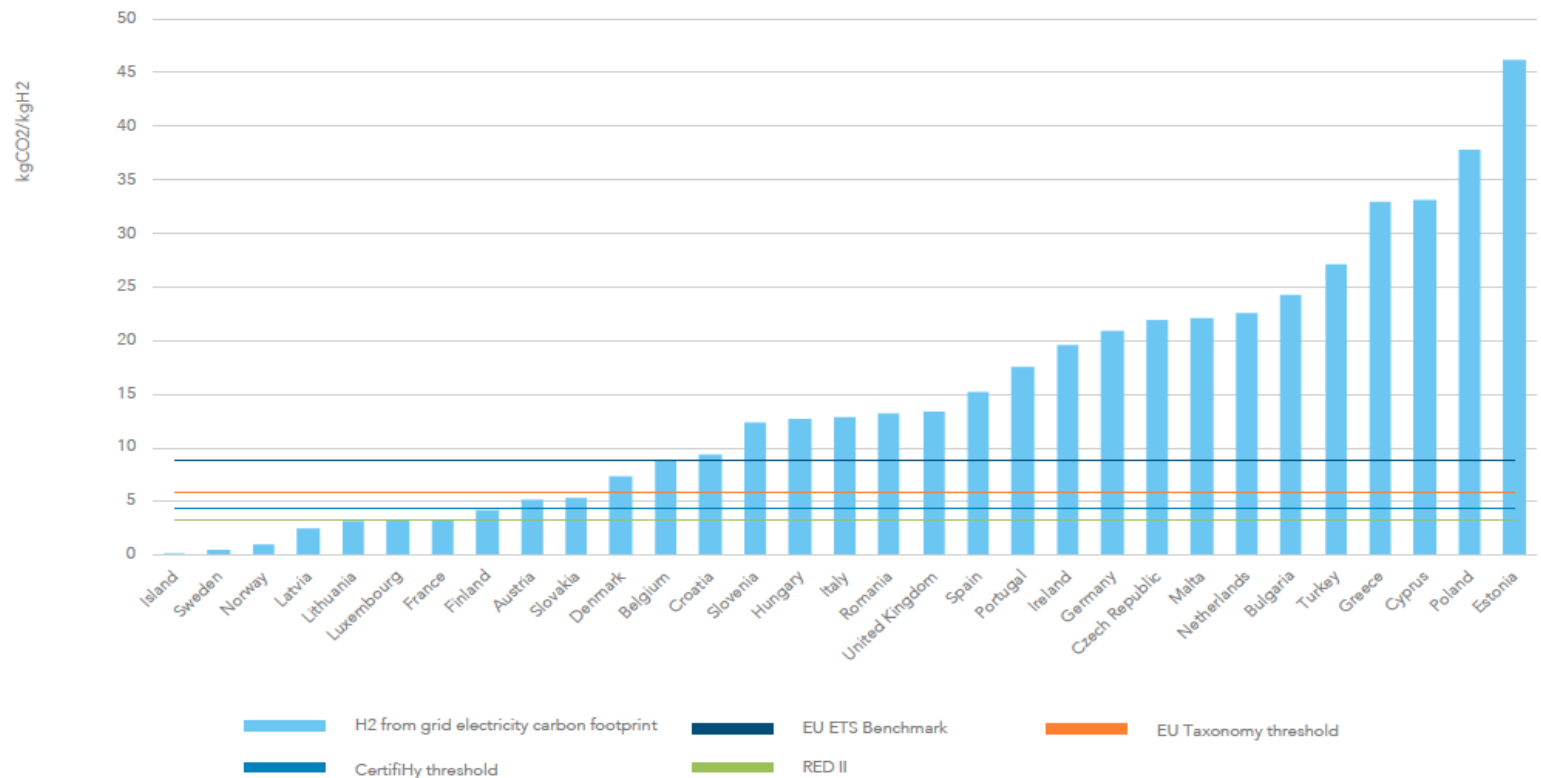


Figure 20 Average CO2 content of 1 kilogram of H2 in EU countries compared to several benchmarks (source: (Hydrogen Europe Intelligence Department, 2020))

2.4.2.1 Model's Specific Characteristics

There are some features only related to the input data of this model:

- + Only demand profile 1a has been used with the total weekly Hydrogen demand of 2130 Kg.
- + For both France and Germany, although as explained above the amount of FCR allocated in each hour would be 0 due to it not having any benefit for the optimization case in hand, the maximum FCR allocated amount has been set to 0 as input for the models to have the possibility of comparing electrolyzer's setpoints in Germany and France with each other as well as comparing electrolyzer's setpoints in CO₂ minimization case and cost minimization case.

2.4.3 Model 3: Optimization of the Installed Capacities of Electrolyzer and Storage

The main problem in this part is just as what it was presented in Model 1: there is a known hourly demand for Hydrogen, throughout a year, which needs to be fulfilled.

This is going to happen with the same configuration discussed in the previous section (electrolyzer, compressor, storage, and distribution network). However, the installed capacities and storage are yet to be found through optimization of the total costs of the system. The total cost of the system in this model consists of two major parts: the cost of energy throughout the year and the CAPEX and OPEX of the configuration. The former, cost of energy, is exactly what we have separately in Model 1 to minimize and the later, hardware costs, is the added term which partly depends on the capacities installed of storage and electrolyzer and partly on the constant cost of the distribution network. This model, just like the two previous models, also aims to find out the hourly rate (in KW) at which the electrolyzer is working at. The point of this model and this optimization session is to find the final price of each kilogram of Hydrogen in a desired year, considering the total OPEX and CAPEX of the production route. The outcome of the optimization can be used to further examine the impact of technological advancements in the price of Hydrogen as the new findings in electrolyzer production technologies will lead to reductions in the CAPEX costs of electrolyzer and stack replacement.

All other assumptions regarding the working range and requirements of all the equipment, meaning the electrolyzer (the minimum possible load, the specific consumption, and the pressure), the compressor (the inlet and outlet pressure as well as the specific consumption), storage (the dead volume, the specific consumption, and the pressure), and the distribution system (its specific consumption) are all the same as before.

Regarding providing Frequency Containment Reserve (FCR), as it was shown in the first model, for a given demand profile, there is not going to be grand reductions in the total price of one kilogram of Hydrogen while increasing the maximum allowed percentage of FCR. So, FCR allocation has been omitted from this model (its maximum allowed percentage for allocation has set to 0).

2.4.3.1 Model's Specific Characteristics

There are some features only related to the input data of this model:

- + The hourly demand profile is 1a.
- + The input data are all for France and for 2019. The optimization has only been carried out for France because the cost of the Hardware, CAPEX, is basically the same in both Germany and France. Huge differences are only seen in cases which have specific configurations which are not discussed here.
- + This model also evaluates the effect of technology advancements in electrolyzer production line. This has been done by implementing a parameter in the model which determines the amount of CAPEX reduction in that run of the optimization model. This parameter can take the values of 100% (full CAPEX

costs), 80%, 60%, and finally 40%. This parameter affects the CAPEX cost of electrolyzer as well as the stack replacement due to it being dependent on electrolyzer's costs.

2.4.4 Model 4: Normal Cost Function Minimization + RES

This model is exactly the same as Model 1 with only one main difference. The electricity needed for the electrolyzer can be supplied through both the electricity grid and a wind turbine, which its production profile throughout the year is known. The price of electricity coming from this wind turbine is set to be 0 for all hours throughout the year. This is due to the fact that electricity coming from renewable energy resources has the priority of dispatch for feeding the electrolyzer in the configuration and to implement this concept in the model, the price of the electricity produced by this wind turbine can be set to zero.

The rest of the configuration and the circumstances under which the equipment is operating, are exactly the same as Model 1. In terms of FCR allowance, to have a clear understanding of how the model and the configuration behaves compared to the case which RES does not exist, maximum FCR allowance percentage has been set to 0 (in other terms, no FCR is allocated).

The model here in this approach again has the aim to find out the amount of grid-electricity and RES-electricity which the electrolyzer is consuming to provide the specific demand.

2.4.4.1 Model's Specific Characteristics

There are some features only related to the input data of this model:

- + All the input data are the same as Model 1.
- + One extra set of data added here, compared to Model 1, is a sample hourly electricity production profile of a wind turbine throughout the year (Agora Energiewende, 2021).

2.4.5 Model 5: Optimization of the Installed Capacities of Electrolyzer and Storage using Grid + RES Electricity

This model is exactly the same as Model 3 with only one main difference. The electricity needed for the electrolyzer can be supplied through both the electricity grid and a wind turbine, which its production profile throughout the year is known. It is possible to say that this model is a combination of Model 3 and 4. The price of electricity coming from this wind turbine is set to be 0 for all hours throughout the year. Although as explained in the previous section regarding Model 4, the prices are

set to be zero only to force a prioritized dispatch, after performing the optimization, it is mandatory to add the average price of electricity coming from RES to the final price of each kilogram of Hydrogen.

The rest of the configuration and the circumstances under which the equipment is operating, are exactly the same as Model 3, in which the goal was to find the installed capacities as well. Additionally, just as before, no FCR is allocated.

This model has the aim of finding the optimum installed capacities of electrolyzer and storage while minimizing the total cost of the system which includes the energy cost (electricity which comes from grid and RES) as well as the CAPEX and OPEX costs.

2.4.5.1 Model's Specific Characteristics

There are some features only related to the input data of this model:

- + All the input data are the same as Model 3.
- + The hourly electricity production profile of the wind turbine has been used here too.
- + To point out the time frame, all the input data are for France and only the data for 2019 has been used in this model. The optimization has only been carried out for France since as mentioned in the previous sections, the cost of the Hardware is basically the same in both Germany and France. Huge differences are only seen in cases which have specific configurations which are not discussed here.
- + The effect of technological advancements in electrolyzer production prices has been examined in this model just like Model 3 by implementing a CAPEX impact parameter in the model, determining the amount of reduction of electrolyzer and stack CAPEX. This parameter takes the values of 100% (full CAPEX costs), 80%, 60%, and finally 40% in different runs of the optimization program.

The information presented in the previous section can be summarized in the Table 5 below.

Name of the Model	Objective Function	Inputs					Outputs
		Demand Profile	Electricity Provided by	FCR Allocated	Timeseries Data	Country	Numbers
Model One	Energy Cost Minimization	1a/1b/2a/2b	Grid	0%-10%-25% for each demand profile	Hourly Price of Electricity from Grid	France - Germany	CO2 Footprint + Price
Model Two	CO2 Minimization	1a	Grid	0%	Hourly CO2 Content of Each MWh of Electricity	France	CO2 Footprint + Price
Model Three	Total Cost Minimization (Energy + CAPEX + OPEX)	1a	Grid	0%	Hourly Price of Electricity from Grid	France	CO2 Footprint + Price
Model Four	Energy Cost Minimization	1a	Grid + RES	0%	Hourly Price of Electricity from Grid + Hourly RES Electricity Production	France	CO2 Footprint + Price
Model Five	Total Cost Minimization (Energy + CAPEX + OPEX)	1a	Grid + RES	0%	Hourly Price of Electricity from Grid + Hourly RES Electricity Production	France	CO2 Footprint + Price

Table 5 Overall summary of all the cases analyzed in this Thesis

2.5 Mathematical Formulation

2.5.1 Model 1

In this section, the mathematical model used for optimization of Model 1 is described. To do so, first, the parameters and variables are explained in order for the objective function and constraints to be understandable.

Here, due to having hourly data for the Hydrogen demand and also the prices, we have two parameters of *start*, which is 0, and *end*, which is 8760 (in other words the hours of one year), and they are used as numerators for hourly data. As we have four main parts in our configuration, *eq* here works as a numerator for these parts and by using this numerator in $cons_{eq}$ we talk about the specific consumption in KWh per Kg of Hydrogen being handled of each of the equipment. To complete this explanation, it is needed to bear in mind that in *eq*, $\{ 'e', 'c', 's', 'd' \}$, each of the elements stand for the electrolyzer, the compressor, the storage, and the distribution network, respectively. Additionally, we have e_{kw} and e_{min} that are related to electrolyzer's feature, its Hydrogen production capacity (in KW) and the technical minimum rate (as a percentage of its Hydrogen production capacity) at which it can operate. Then, the characteristics of the storage need to be defined, s_{low_p} as its minimum amount of Hydrogen that should remain in the storage at any given point in time as a percentage of its Hydrogen storage capacity and s_{kg} as its Hydrogen storage capacity in Kg. The parameter of pcr_p is defined as the maximum allowable amount of primary containment reserve (PCR or FCR) as a percentage of the electrolyzer's capacity. Then we have the hourly defined parameters, sp_{mwh_h} , pcr_{mwh_h} , h_{kg_h} , and $CO2_{mwh_h}$. For each hour, these parameters show the hourly spot price (price of electricity at the spot market), hourly remuneration of PCR, hourly Hydrogen demand of the refueling bus station, and the average hourly Carbon Dioxide content of the used electricity, respectively.

Parameter Definition

$start = 0$: the start of a year at point 0

$end = 8760$: the end of a year, when going from 0 to 1, hour 1 is done

$hour = \{start, \dots, end\}$: a set defined for going through the year hour by hour

$eq = \{ 'e', 'c', 's', 'd' \}$: numerator for our equipment which are electrolyzer, the compressor, the storage, and the distribution network

e_{kw} : Hydrogen production capacity of the electrolyzer in KW

e_{min} : minimum possible working rate of the electrolyzer as a percentage of its Hydrogen production capacity

s_{low_p} : minimum possible level of the storage as a percentage of its Hydrogen storage capacity

s_{kg} : storage Hydrogen storage capacity in Kg, the mass of the storage has been defined as the Kg of Hydrogen that it can contain at the pressure coming out of the compressor

pcr_p : maximum allowed amount of the PCR as a percentage of the electrolyzer's capacity

sp_mwh_h : electricity price for hour h , known as spot price for hour h , in MWh, given for 8760 hours of the year

pcr_mwh_h : PCR remuneration price for hour h in MWh, given for 8760 hours of the year

h_kg_h : Hydrogen demand for hour h in Kg, given for 8760 hours of the year

$CO2_mwh_h$: average CO_2 content of the electricity consumed for hour h in Kg per MWh, given for 8760 hours of the year

$cons_{eq}$: specific electricity consumption of each of equipment eq in KWh per Kg of Hydrogen produced

For completely defining our problem, we need to have four variables:

1. x_{e_h} : This is a binary variable that takes 1 when the electrolyzer is on at hour h and 0 if otherwise.
2. x_{p_h} which shows the rate at which the electrolyzer is working at hour h , which can take any amount between 0 and 1 (in other words, from 0% until 100%).
3. y_h is the variable related to the level of the storage, the amount of gas inside the storage in Kg at hour h .
4. z_h is defined as a variable that shows the PCR allocated at hour h , as a percentage of the electrolyzer's capacity.

The objective function is defined in Equation 1. The target is to minimize the costs of consumed electricity while taking into account the only remuneration obtained by selling PCR to the grid. To further clarify the objective function, the first term only points out the cost of the electricity consumed by the electrolyzer at hour h . The second term refers to the cost of the electricity consumed by the compressor at hour h . However, the amount of electricity utilized here depends on the amount of Hydrogen produced by the electrolyzer at that hour and that is why first, this amount in Kg is calculated, and then, amount of electricity which the compressor requires for handling the produced Hydrogen is being computed. The third term refers to the cost of electricity needed for the distribution of demanded Hydrogen at hour h , which does not have anything to do with the Hydrogen produced at that hour. The demand needs to be provided by either the Hydrogen, which is just produced, or the amount of

Hydrogen which is already stored in the storage from previous hours. So, the total demand of hour h is being handled by the distribution network. The last term points out to the remuneration of PCR at hour h , the amount of which is determined through a variable as a percentage of the electrolyzer's Hydrogen production capacity.

As for the constraints, the initial conditions of the storage (constraint 2), the electrolyzer's state in terms of being on and off and also its rate (constraints 3 and 4), and the PCR rate (constraint 5) need to be defined. Then, it should be dictated to the model that the storage can contain only a specific amount of gas (constraints 6 and 7). Then, there is constraint 8, which is a very important constraint since it connects the state of storage at hour h with its previous hour of $h-1$, to find out the storage level at hour h by considering the amount of Hydrogen that has left the storage at hour $h-1$ and the amount of Hydrogen produced at hour h . After dealing with the storage, it is time for regulating the PCR, which can take only specific amount, shown in constraints 9 and 10. In the two constraints of 11 and 12, the connection between electrolyzer's rate and the amount of PCR have been discussed by pointing out that the final rate at which the electrolyzer is working at, should not pass the minimum or maximum allowed levels (PCR can be positive or negative in the sense that electricity can be sold to the electrolyzer again or bought from it). In the last four constraints of 13 to 16, the domain of each of the variables has been defined.

Objective Function Definition

$$\text{Min} \sum_{h \in \text{hour}} (sp_mwh_h \times (e_kw \times x_p_h) + sp_mwh_h \times (e_kw \times x_p_h \div cons_e \times cons_c) + sp_mwh_h \times (h_kg_h \times cons_d) - pcr_mwh_h \times z_h \times e_kw)$$

Equation 1

Subject to

$$y_0 = 2 \times s_{low_p} \times s_{kg} \quad \text{Equation 2}$$

$$x_{e_0} = 0 \quad \text{Equation 3}$$

$$x_{p_0} = 0 \quad \text{Equation 4}$$

$$z_0 = 0 \quad \text{Equation 5}$$

$$y_h \geq s_{low_p} \times s_{kg} \quad h \in \{ 1, \dots, end \} \quad \text{Equation 6}$$

$$y_h \leq s_{kg} \quad h \in \{ 1, \dots, end \} \quad \text{Equation 7}$$

$$y_h = y_{h-1} - h_{kg}g_{h-1} + (e_{kw} \times x_{p_{h-1}} \div cons_e) \quad h \in \{ 1, \dots, end \} \quad \text{Equation 8}$$

$$z_h \leq pcr_p \quad h \in \{ 1, \dots, end \} \quad \text{Equation 9}$$

$$z_h \geq 0 \quad h \in \{ 1, \dots, end \} \quad \text{Equation 10}$$

$$x_{p_h} + z_h \leq 1 \times x_{e_h} \quad h \in \{ 1, \dots, end \} \quad \text{Equation 11}$$

$$x_{p_h} - z_h \geq e_{min} \times x_{e_h} \quad h \in \{ 1, \dots, end \} \quad \text{Equation 12}$$

$$x_{e_h} \in \{ 0, 1 \} \quad h \in \{ 1, \dots, end \} \quad \text{Equation 13}$$

$$0 \leq x_{p_h} \leq 1 \quad h \in \{ 1, \dots, end \} \quad \text{Equation 14}$$

$$0 \leq y_h \quad h \in \{ 1, \dots, end \} \quad \text{Equation 15}$$

$$0 \leq z_h \leq 1 \quad h \in \{ 1, \dots, end \} \quad \text{Equation 16}$$

2.5.2 Model 2

Here, due to having hourly data for the Hydrogen demand and also the prices, we have two parameters of *start*, which is 0, and *end*, which is 8760 (in other words the hours of one year), and they are used as numerators for hourly data. As we have four main parts in our configuration, *eq* here works as a numerator for these parts and by using this numerator in $cons_{eq}$ we talk about the specific consumption in KWh per Kg of Hydrogen being handled of each of the equipment. To complete this explanation, it is needed to bear in mind that in *eq*, $\{ 'e', 'c', 's', 'd' \}$, each of the elements stand for the electrolyzer, the compressor, the storage, and the distribution network, respectively. Additionally, we have *e_kw* and *e_min* that are related to electrolyzer's feature, its Hydrogen production capacity (in KW) and the technical minimum rate (as a percentage of its Hydrogen production capacity) at which it can operate. Then, the characteristics of the storage need to be defined, *s_low_p* as its minimum amount of Hydrogen that should remain in the storage at any given point in time as a percentage of its Hydrogen storage capacity and *s_kg* as its Hydrogen storage capacity in Kg. The parameter of *pcr_p* is defined as the maximum allowable amount of primary containment reserve (PCR or FCR) as a percentage of the electrolyzer's capacity. Then we have the hourly defined parameters, sp_mwh_h , pcr_mwh_h , h_kg_h , and $CO2_mwh_h$. For each hour, these parameters show the hourly spot price (price of electricity at the spot market), hourly renumeration of PCR, hourly Hydrogen demand of the refueling bus station, and the average hourly Carbon Dioxide content of the used electricity, respectively.

Parameter Definition

start = 0 : the start of a year at point 0

end = 8760 : the end of a year, when going from 0 to 1, hour 1 is done

hour = $\{ start, \dots, end \}$: a set defined for going through the year hour by hour

eq = $\{ 'e', 'c', 's', 'd' \}$: numerator for our equipment which are electrolyzer, the compressor, the storage, and the distribution network

e_kw : Hydrogen production capacity of the electrolyzer in KW

e_min : minimum possible working rate of the electrolyzer as a percentage of its Hydrogen production capacity

s_low_p : minimum possible level of the storage as a percentage of its Hydrogen storage capacity

s_kg : storage Hydrogen storage capacity in Kg, the mass of the storage has been defined as the Kg of Hydrogen that it can contain at the pressure coming out of the compressor

pcr_p : maximum allowed amount of the PCR as a percentage of the electrolyzer's capacity

sp_mwh_h : electricity price for hour h , known as spot price for hour h , in MWh, given for 8760 hours of the year

pcr_mwh_h : PCR remuneration price for hour h in MWh, given for 8760 hours of the year

h_kg_h : Hydrogen demand for hour h in Kg, given for 8760 hours of the year

$CO2_mwh_h$: average CO_2 content of the electricity consumed for hour h in Kg per MWh, given for 8760 hours of the year

$cons_{eq}$: specific electricity consumption of each of equipment eq in KWh per Kg of Hydrogen produced

For completely defining our problem, we need to have four variables:

1. x_{e_h} : This is a binary variable that takes 1 when the electrolyzer is on at hour h and 0 if otherwise.
2. x_{p_h} which shows the rate at which the electrolyzer is working at hour h , which can take any amount between 0 and 1 (in other words, from 0% until 100%).
3. y_h is the variable related to the level of the storage, the amount of gas inside the storage in Kg at hour h .
4. z_h is defined as a variable that shows the PCR allocated at hour h , as a percentage of the electrolyzer's capacity.

The objective function is defined in Equation 17. The target is to minimize the average Carbon Dioxide content of each kilogram of Hydrogen produced, which is directly correlated with the amount of electricity consumed at each part of the configuration. To further clarify the objective function, the first term only points out the Carbon Dioxide content for the electricity consumed by the electrolyzer at hour h . The second term refers to the Carbon Dioxide content of the electricity consumed by the compressor at hour h . However, the amount of electricity utilized here depends on the amount of Hydrogen produced by the electrolyzer at that hour and that is why first, this amount in Kg is calculated, and then, amount of electricity which the compressor requires for handling the produced Hydrogen is being computed. The third term refers to the Carbon Dioxide content of the electricity needed for the distribution of demanded Hydrogen at hour h , which does not have anything to do with the Hydrogen produced at that hour. The demand needs to be provided by either the Hydrogen, which is just produced, or the amount of Hydrogen which is already stored in the storage from previous hours. So, the total demand of hour h is being handled by the distribution network.

As for the constraints, the initial conditions of the storage (constraint 18), the electrolyzer's state in terms of being on and off and also its rate (constraints 19 and 20), and the PCR rate (constraint 21) need to be defined. Then, it should be dictated to the model that the storage can contain only a specific amount of gas (constraints 22 and 23). Then, there is constraint 24, which is a very important constraint since it connects the state of storage at hour h with its previous hour of $h-1$, to find out the storage level at hour h by considering the amount of Hydrogen that has left the storage at hour $h-1$ and the amount of Hydrogen produced at hour h . After dealing with the storage, it is time for regulating the PCR, which can take only specific amount, shown in constraints 25 and 26. In the two constraints of 27 and 28, the connection between electrolyzer's rate and the amount of PCR have been discussed by pointing out that the final rate at which the electrolyzer is working at, should not pass the minimum or maximum allowed levels (PCR can be positive or negative in the sense that electricity can be sold to the electrolyzer again or bought from it). In the last four constraints of 29 to 32, the domain of each of the variables has been defined.

Objective Function Definition

$$\text{Min } \sum_{h \in \text{hour}} (CO2_mwh_h \times (e_kw \times x_p_h) + CO2_mwh_h \times (e_kw \times x_p_h \div cons_e \times cons_c) + CO2_mwh_h \times (cons_d \times h_kg_h))$$

Equation 17

Subject to

$$y_0 = 1.5 \times s_low_p \times s_kg \quad \text{Equation 18}$$

$$x_e_0 = 0 \quad \text{Equation 19}$$

$$x_p_0 = 0 \quad \text{Equation 20}$$

$$z_0 = 0 \quad \text{Equation 21}$$

$$y_h \geq s_low_p \times s_kg \quad h \in \{ 1, \dots, end \} \quad \text{Equation 22}$$

$$y_h \leq s_kg \quad h \in \{ 1, \dots, end \} \quad \text{Equation 23}$$

$$y_h = y_{h-1} - h_kg_{h-1} + (e_kw \times x_p_{h-1} \div cons_e) \quad h \in \{ 1, \dots, end \} \quad \text{Equation 24}$$

$$z_h \leq pcr_p \quad h \in \{ 1, \dots, end \} \quad \text{Equation 25}$$

$$z_h \geq 0 \quad h \in \{ 1, \dots, end \} \quad \text{Equation 26}$$

$$x_p_h + z_h \leq 1 \times x_e_h \quad h \in \{ 1, \dots, end \} \quad \text{Equation 27}$$

$$x_p_h - z_h \geq e_min \times x_e_h \quad h \in \{ 1, \dots, end \} \quad \text{Equation 28}$$

$$x_e_h \in \{ 0, 1 \} \quad h \in \{ 1, \dots, end \} \quad \text{Equation 29}$$

$$0 \leq x_p_h \leq 1 \quad h \in \{ 1, \dots, end \} \quad \text{Equation 30}$$

$$0 \leq y_h \quad h \in \{ 1, \dots, end \} \quad \text{Equation 31}$$

$$0 \leq z_h \leq 1 \quad h \in \{ 1, \dots, end \} \quad \text{Equation 32}$$

2.5.3 Model 3

In Model 3 several changes have been implemented which are going to be discussed as follows.

Here, due to having hourly data for the Hydrogen demand and also the prices, we have two parameters of *start*, which is 0, and *end*, which is 8760 (in other words the hours of one year), and they are used as numerators for hourly data. Another numerator, *cap*, has also been defined here which is going to be used only when the one-time costs of CAPEX and OPEX need to be considered later in the objective function. As we have four main parts in our configuration, *eq* here works as a numerator for these parts and by using this numerator in $cons_{eq}$ we talk about the specific consumption in KWh per Kg of Hydrogen being handled of each of the equipment. To complete this explanation, it is needed to bear in mind that in *eq*, {'e', 'c', 's', 'd'}, each of the elements stand for the electrolyzer, the compressor, the storage, and the distribution network, respectively. Additionally, we have *e_min* and *s_min* that are the technical minimum rates (as a percentage) of the Hydrogen production capacity of the electrolyzer and the Hydrogen storage capacity of the storage, respectively. In contrary to Model 1 and Model 2, the Hydrogen production capacity of the electrolyzer and the Hydrogen storage capacity of the storage are not known and figuring out the optimal capacities is one of the main goals of this model. Furthermore, PCR has been deleted in this model and it will not be implemented in Model 3 because of the findings of the previous Two Models. These findings will be discussed in the results chapter. Then we have the hourly defined parameters, sp_{mwh}_h , h_{kg}_h , and $CO2_{mwh}_h$. For each hour, these parameters show the hourly spot price (price of electricity at the spot market), and hourly Hydrogen demand of the refueling bus station, and the average hourly Carbon Dioxide content of the used electricity, respectively. More parameters are defined in this model as well due to the one-time costs mentioned a few lines earlier. Model 3 considers all the CAPEX and OPEX related to the equipment and the WACC. So, $e_{C_{cap}}$, $st_{C_{cap}}$, $c_{C_{cap},s}$, $c_{C_{cap}}$, and $s_{C_{cap}}$ point out the CAPEX of the electrolyzer, the stack replacement, the storage, the compressor, and the storage while $e_{O_{cap}}$, $c_{O_{cap}}$, and $d_{O_{cap}}$ are the parameters inserted in the model for the OPEX of the electrolyzer, the compressor, and the distribution system. These parameters are all in euros. Also, to fully analyze the economics of the configuration and have a real-life case, $wacc$, $lwacc$, $shwacc$, and C_{dec} are also introduced into the model as well which are economic parameters.

Parameter Definition

$start = 0$: the start of a year at point 0

$end = 8760$: the end of a year, when going from 0 to 1, hour 1 is done

$hour = \{start, \dots, end\}$: a set defined for going through the year hour by hour

$eq = \{ 'e', 'c', 's', 'd' \}$: numerator for our equipment which are electrolyzer, the compressor, the storage, and the distribution network

$c = 1$: used for the another numerator for the one-time costs

$cap = \{1, \dots, cap\}$: numerator to be used only when the one-time costs of CAPEX and OPEX need to be considered.

e_{min} : minimum possible working rate of the electrolyzer as a percentage of its Hydrogen production capacity

s_{min} : minimum possible level of the storage as a percentage of its Hydrogen storage capacity

sp_{mwh}_h : electricity price for hour h , known as spot price for hour h , in MWh, given for 8760 hours of the year

pcr_{mwh}_h : PCR remuneration price for hour h in MWh, given for 8760 hours of the year

h_{kg}_h : Hydrogen demand for hour h in Kg, given for 8760 hours of the year

$CO2_{mwh}_h$: average CO₂ content of the electricity consumed for hour h in Kg per MWh, given for 8760 hours of the year

$cons_{eq}$: specific electricity consumption of each of equipment eq in KWh per Kg of Hydrogen produced

$e_{C_{cap}}$: the electrolyzer's CAPEX in euros

$st_{C_{cap}}$: the stack replacement's CAPEX in euros

$c_{C_{cap}}$: the compressor's CAPEX in euros

$s_{C_{cap}}$: the storage's CAPEX in euros

$d_{C_{cap}}$: the distribution network's CAPEX in euros

$e_{O_{cap}}$: the electrolyzer's OPEX as a percentage of its CAPEX

$c_{O_{cap}}$: the compressor's OPEX as a percentage of its CAPEX

$d_{O_{cap}}$: the distribution network's OPEX as a percentage of its CAPEX

$Lwacc$: amortization factor resulted from the weighted average cost of capital for the equipment with the longer lifetime of 20 years (unitless) which is 0.101852

$Shwacc$: amortization factor resulted from the weighted average cost of capital for the equipment with the longer lifetime of 10 years (unitless) which is 0.149029

C_{dec} : CAPEX decrease, presented as a percentage, an economic parameter that shows how much the CAPEX will increase throughout the years as a result of technological advancement, it can take the amounts of 1, 0.8, 0.6, and 0.4 .

$tot_h = \sum_{h \in hour} h_kg_h$: total demanded calculated for further computations in the objective function

$$h \in \{ start, \dots, end \}$$

Here, compared to Model 1, there are some changes in the variables defined:

1. x which is the Hydrogen production capacity of the electrolyzer in KW, and its optimal value needs to be found.
2. x_{e_h} : This is a binary variable that takes 1 when the electrolyzer is on at hour h and 0 if otherwise.
3. x_{p_h} which shows the rate at which the electrolyzer is working at hour h in KW, which can take any amount above 0.
4. y which is the Hydrogen storage capacity of the storage (mass of Hydrogen getting stored) in Kg and its optimal value needs to be found.
5. y_{p_h} is the variable related to the level of the Hydrogen stored in the storage in Kg, or in other words, the mass of the of gas inside the storage in Kg at hour h .

The objective function is defined in Equation 33. The target is to minimize the costs of electricity consumed at each part of the configuration while taking into account the economic considerations, including the CAPEX and OPEX of each of the equipment in their respective lifetime and the WACC (weighted average cost of capital). To further explain the objective function, we can say that it has two main parts. The first part talks about the cost of the electricity consumed in each section of the configuration that we have. Consequently, in the first part with three terms, the first term only points out the cost for the electricity consumed by the electrolyzer at hour h . The second term refers to the cost of the electricity consumed by the compressor at hour h . However, the amount of electricity utilized here depends on the amount of Hydrogen produced by the electrolyzer at that hour and that is why first, this amount in Kg is calculated, and then, amount of electricity which the compressor requires for handling the produced Hydrogen is being computed. The third term refers to the cost of electricity needed for the distribution of demanded Hydrogen at hour h , which does not have anything to do with the Hydrogen produced at that hour. The demand needs to be provided by either the Hydrogen, which is just produced, or the amount of Hydrogen which is already stored in the storage from previous hours. So, the total demand of hour h is being handled by the distribution network. To further elaborate on the second part of the objective function, it is important to say that this part deals only with the economic arrangements of the problem in hand. In this second part, the first term refers to the amortization of the CAPEX for all equipment, electrolyzer, compressor, distribution, storage, in just one expression based on their lifetime of 20 years (long lifetime). The next three terms points out the cost of OPEX for the electrolyzer (which depends on the Hydrogen production capacity of the electrolyzer installed), the compressor

(which again depends on the Hydrogen production capacity of the electrolyzer installed), and the distribution network. OPEX is not amortized, and its costs are being implemented directly because it is not meant to be paid by debt. The last term of the second part of the objective function is related to the amortization of the CAPEX for stack replacement based on its lifetime, which is different from other equipment (10 years instead of 20 years).

As for the constraints, the initial conditions of the storage (constraint 34), the electrolyzer's state in terms of being on and off and also its rate (constraints 35 and 36) need to be defined. Then, it should be dictated to the model that the storage can contain only a specific amount of gas (constraints 37 and 38). Then, there is constraint 39, which is a very important constraint since it connects the state of storage at hour h with its previous hour of $h-1$, to find out the storage level at hour h by considering the amount of Hydrogen that has left the storage at hour $h-1$ and the amount of Hydrogen produced at hour h . After dealing with the storage, in constraints 40 to 42, the constraints impose the limitation on the electrolyzer that it can only operate up to its optimal capacity, a capacity that is going to fulfill the demand of Hydrogen throughout the year while pointing out that the final rate at which the electrolyzer is working at, should be in the permitted range. In the last four constraints of 43 to 47, the domain of each of the variables has been defined.

Objective Function Definition

$$\begin{aligned} \text{Min } \sum_{c \in \text{cap}} & ((\sum_{h \in \text{hour}} (sp_mwh_h \times x_p_h + sp_mwh_h \times (x_p_h \div cons_e \times \\ & cons_c) + sp_mwh_h \times (cons_d \times h_kg_h))) + (((C_dec \times e_C_c + c_C_c) \times x + s_C_c \times y + \\ & d_C_c) \times lwacc + (x \times C_dec \times e_C_c \times e_O_c) + (x \times c_C_c \times c_O_c) + (d_C_c \times d_O_c) + \\ & ((C_dec \times st_C_c \times x) \times shwacc)) \div tot_h) \end{aligned}$$

Equation 33

Subject to

$$y_p_0 = 200 \quad \text{Equation 34}$$

$$x_e_0 = 0 \quad \text{Equation 35}$$

$$x_p_0 = 0 \quad \text{Equation 36}$$

$$y_p_h \geq s_min \quad h \in \{ 1, \dots, end \} \quad \text{Equation 37}$$

$$y_p_h \leq y \quad h \in \{ 1, \dots, end \} \quad \text{Equation 38}$$

$$y_{p_h} = y_{p_{h-1}} - h_{kg_{h-1}} + (x_{p_{h-1}} \div cons_e)$$

$$h \in \{ 1, \dots, end \} \quad \text{Equation 39}$$

$$x_{p_h} \leq tot_h \times (1 - x_{e_h}) + x$$

$$h \in \{ 1, \dots, end \} \quad \text{Equation 40}$$

$$x_{p_h} \geq (-1) \times tot_h \times (1 - x_{e_h}) + e_{min} \times x$$

$$h \in \{ 1, \dots, end \} \quad \text{Equation 41}$$

$$x_{p_h} \leq tot_h \times x_{e_h}$$

$$h \in \{ 1, \dots, end \} \quad \text{Equation 42}$$

$$x_{e_h} \in \{ 0, 1 \}$$

$$h \in \{ 1, \dots, end \} \quad \text{Equation 43}$$

$$0 \leq x \quad \text{Equation 44}$$

$$0 \leq x_{p_h}$$

$$h \in \{ 1, \dots, end \} \quad \text{Equation 45}$$

$$0 \leq y \quad \text{Equation 46}$$

$$0 \leq y_{p_h}$$

$$h \in \{ 1, \dots, end \} \quad \text{Equation 47}$$

2.5.4 Model 4

Here, due to having hourly data for the Hydrogen demand and also the prices, we have two parameters of *start*, which is 0, and *end*, which is 8760 (in other words the hours of one year), and they are used as numerators for hourly data. As we have four main parts in our configuration, *eq* here works as a numerator for these parts and by using this numerator in $cons_{eq}$ we talk about the specific consumption in KWh per Kg of Hydrogen being handled of each of the equipment. To complete this explanation, it is needed to bear in mind that in *eq*, {'e', 'c', 's', 'd'}, each of the elements stand for the electrolyzer, the compressor, the storage, and the distribution network, respectively. Additionally, we have e_{kw} and e_{min} that are related to electrolyzer's feature, its Hydrogen production capacity (in KW) and the technical minimum rate (as a percentage of its Hydrogen production capacity) at which it can operate. Then, the characteristics of the storage need to be defined, s_{low_p} as its minimum amount of Hydrogen that should remain in the storage at any given point in time as a percentage of its Hydrogen storage capacity and s_{kg} as its Hydrogen storage capacity in Kg. The parameter of pcr_p is defined as the maximum allowable amount of primary containment reserve (PCR or FCR) as a percentage of the electrolyzer's capacity. Then

we have the hourly defined parameters, sp_mwh_h , pcr_mwh_h , h_kg_h , and $CO2_mwh_h$. For each hour, these parameters show the hourly spot price (price of electricity at the spot market), hourly remuneration of PCR, hourly Hydrogen demand of the refueling bus station, and the average hourly Carbon Dioxide content of the used electricity, respectively. The only important difference between Model 4 and Model 1 is the last defined parameter, RES_kw_h , which is the hourly RES electricity production in KW. This RES electricity is fully available to the electrolyzer to be utilized for Hydrogen production, with a priority of dispatch and use, compared to the electricity coming from the grid.

Parameter Definition

$start = 0$: the start of a year at point 0

$end = 8760$: the end of a year, when going from 0 to 1, hour 1 is done

$hour = \{start, \dots, end\}$: a set defined for going through the year hour by hour

$eq = \{ 'e', 'c', 's', 'd' \}$: numerator for our equipment which are electrolyzer, the compressor, the storage, and the distribution network

e_kw : Hydrogen production capacity of the electrolyzer in KW

e_min : minimum possible working rate of the electrolyzer as a percentage of its Hydrogen production capacity

s_low_p : minimum possible level of the storage as a percentage of its Hydrogen production capacity

s_kg : storage Hydrogen storage capacity in Kg, the mass of the storage has been defined as the Kg of Hydrogen that it can contain at the pressure coming out of the compressor

pcr_p : maximum allowed amount of the PCR as a percentage of the electrolyzer's capacity

sp_mwh_h : electricity price for hour h , known as spot price for hour h , in MWh, given for 8760 hours of the year

pcr_mwh_h : PCR remuneration price for hour h in MWh, given for 8760 hours of the year

h_kg_h : Hydrogen demand for hour h in Kg, given for 8760 hours of the year

$CO2_mwh_h$: average CO_2 content of the electricity consumed for hour h in Kg per MWh, given for 8760 hours of the year

$cons_{eq}$: specific electricity consumption of each of equipment eq in KWh per Kg of Hydrogen produced

RES_kw_h : RES electricity production for hour h in KW

Also in this part, just like Model 1, for completely defining our problem, we need to have the previous four variables, plus the fifth one which brings the RES electricity into our model:

1. x_{e_h} : This is a binary variable that takes 1 when the electrolyzer is on at hour h and 0 if otherwise.
2. x_{pg_h} which shows the rate at which the electrolyzer is working at hour h , which can take any amount between 0 and 1 (in other words, from 0% until 100%).
3. y_h is the variable related to the level of the storage, the amount of gas inside the storage in Kg at hour.
4. z_h is defined as a variable that shows the PCR allocated at hour h , as a percentage of the electrolyzer's capacity.
5. $0 \leq t_h$ which expresses the amount of RES electricity that the electrolyzer is using at hour h .

The objective function is defined in Equation 48. The target is to minimize the costs of consumed electricity while taking into account the only remuneration obtained by selling PCR to the grid. The important note here is that the cost of RES electricity is zero and only the electricity coming from the grid needs to be paid for. To further clarify the objective function, the first term only points out the price for the electricity consumed by the electrolyzer at hour h . The second term refers to the price of the electricity consumed by the compressor at hour h . However, the amount of electricity utilized here depends on the amount of Hydrogen produced by the electrolyzer at that hour and that is why first, this amount in Kg is calculated, and then, amount of electricity which the compressor requires for handling the produced Hydrogen is being computed. The third term refers to the price of electricity needed for the distribution of demanded Hydrogen at hour h , which does not have anything to do with the Hydrogen produced at that hour. The demand needs to be provided by either the Hydrogen, which is just produced, or the amount of Hydrogen which is already stored in the storage from previous hours. So, the total demand of hour h is being handled by the distribution network. The last term points out to the remuneration of PCR at hour h , the amount of which is determined through a variable as a percentage of the electrolyzer's Hydrogen production capacity.

As for the constraints, the initial conditions of the storage (constraint 49), the electrolyzer's state in terms of being on and off and also its rate (constraints 50 and 51), the PCR rate (constraint 52), and the initial amount of RES used (constraint 53) need to be defined. The amount of RES utilized at hour h always needs to be less than or equal to the total amount of RES produced (based on the RES production profile) at hour h (constraint 54). Then, it should be dictated to the model that the storage can contain only a specific amount of gas (constraints 55 and 56). Then, there is constraint 57, which

is a very important constraint since it connects the state of storage at hour h with its previous hour of $h-1$, to find out the storage level at hour h by considering the amount of Hydrogen that has left the storage at hour $h-1$ and the amount of Hydrogen produced at hour h . After dealing with the storage, it is time for regulating the PCR, which can take only specific amount, shown in constraints 58 and 59. In the next two constraints of 60 and 61, the connection between electrolyzer's working rate and the amount of PCR have been discussed while bearing in mind that a part of electricity also comes from RES. Again, here the general rule that the electrolyzer can only operate between its minimum and maximum allowed working levels applies. In the last five constraints of 62 to 66, the domain of each of the variables has been defined.

Objective Function Definition

$$\begin{aligned} \text{Min } \sum_{h \in \text{hour}} & (sp_mwh_h \times (e_kw \times x_pgh) + sp_mwh_h \times ((e_kw \times x_pgh \\ & \div cons_e \times cons_c) + (cons_c \times t_h \div cons_e)) \\ & + sp_mwh_h \times (h_kg_h \times cons_d) - pcr_mwh_h \times z_h \times e_kw) \end{aligned}$$

Equation 48

Subject to

$$y_0 = 1.5 \times s_low_p \times s_kg \quad \text{Equation 49}$$

$$x_{e_0} = 0 \quad \text{Equation 50}$$

$$x_{p_0} = 0 \quad \text{Equation 51}$$

$$z_0 = 0 \quad \text{Equation 52}$$

$$t_0 = 0 \quad \text{Equation 53}$$

$$t_h \leq RES_kw_h \quad \text{Equation 54}$$

$$y_h \geq s_low_p \times s_kg \quad h \in \{1, \dots, end\} \quad \text{Equation 55}$$

$$y_h \leq s_kg \quad h \in \{1, \dots, end\} \quad \text{Equation 56}$$

$$y_h = y_{h-1} - h_kg_{h-1} + (e_kw \times e_pg_{h-1} \div cons_e) + (t_{h-1} \div cons_e) \quad h \in \{1, \dots, end\} \quad \text{Equation 57}$$

$z_h \leq pcr_p$	$h \in \{ 1, \dots, end \}$	Equation 58
$z_h \geq 0$	$h \in \{ 1, \dots, end \}$	Equation 59
$x_pg_h + (t_h \div e_kw) + z_h \leq 1 \times x_e_h$	$h \in \{ 1, \dots, end \}$	Equation 60
$x_p_h + (t_h \div e_kw) - z_h \geq e_min \times x_e_h$	$h \in \{ 1, \dots, end \}$	Equation 61
$x_e_h \in \{ 0, 1 \}$	$h \in \{ 1, \dots, end \}$	Equation 62
$0 \leq x_pg_h \leq 1$	$h \in \{ 1, \dots, end \}$	Equation 63
$0 \leq y_h$	$h \in \{ 1, \dots, end \}$	Equation 64
$0 \leq z_h \leq 1$	$h \in \{ 1, \dots, end \}$	Equation 65
$0 \leq t_h$	$h \in \{ 1, \dots, end \}$	Equation 66

2.5.5 Model 5

It is safe to say that Model 5 is a combination of Model 3 and Model 4.

Here, due to having hourly data for the Hydrogen demand and also the prices, we have two parameters of *start*, which is 0, and *end*, which is 8760 (in other words the hours of one year), and they are used as numerators for hourly data. Another numerator, *cap*, has also been defined here which is going to be used only when the one-time costs of CAPEX and OPEX need to be considered later in the objective function. As we have four main parts in our configuration, *eq* here works as a numerator for these parts and by using this numerator in $cons_{eq}$ we talk about the specific consumption in KWh per Kg of Hydrogen being handled of each of the equipment. To complete this explanation, it is needed to bear in mind that in *eq*, {'e', 'c', 's', 'd'}, each of the elements stand for the electrolyzer, the compressor, the storage,

and the distribution network, respectively. Additionally, we have e_{min} and s_{min} that are the technical minimum rates (as a percentage) of the Hydrogen production capacity of the electrolyzer and the Hydrogen storage capacity of the storage, respectively. In contrary to Model 1 and Model 2, the Hydrogen production capacity of the electrolyzer and the Hydrogen storage capacity of the storage are not known and figuring out the optimal capacities is one of the main goals of this model. Furthermore, PCR has been deleted in this model and it will not be implemented in Model 3 because of the findings of the previous Two Models. These findings will be discussed in the results chapter. Then we have the hourly defined parameters, sp_{mwh}_h , h_{kg}_h , and $CO2_{mwh}_h$. For each hour, these parameters show the hourly spot price (price of electricity at the spot market), and hourly Hydrogen demand of the refueling bus station, and the average hourly Carbon Dioxide content of the used electricity, respectively. Then, there is RES_{kw}_h , which is the hourly RES electricity production in KW. This RES electricity is fully available to the electrolyzer to be utilized for Hydrogen production, with a priority of dispatch and use, compared to the electricity coming from the grid. More parameters are defined in this model as well due to the one-time costs mentioned a few lines earlier. Model 3 considers all the CAPEX and OPEX related to the equipment and the WACC. So, $e_{C_{cap}}$, $st_{C_{cap}}$, $c_{C_{cap},s}$, $c_{C_{cap}}$, and $s_{C_{cap}}$ point out the CAPEX of the electrolyzer, the stack replacement, the storage, the compressor, and the storage while $e_{O_{cap}}$, $c_{O_{cap}}$, and $d_{O_{cap}}$ are the parameters inserted in the model for the OPEX of the electrolyzer, the compressor, and the distribution system. These parameters are all in euros. Also, to fully analyze the economics of the configuration and have a real-life case, $wacc$, $lwacc$, $shwacc$, and C_{dec} are also introduced into the model as well which are economic parameters.

Parameter Definition

$start = 0$: the start of a year at point 0

$end = 8760$: the end of a year, when going from 0 to 1, hour 1 is done

$hour = \{start, \dots, end\}$: a set defined for going through the year hour by hour

$eq = \{ 'e', 'c', 's', 'd' \}$: numerator for our equipment which are electrolyzer, the compressor, the storage, and the distribution network

$c = 1$: used for the another numerator for the one-time costs

$cap = \{1, \dots, cap\}$: numerator to be used only when the one-time costs of CAPEX and OPEX need to be considered.

e_{min} : minimum possible working rate of the electrolyzer as a percentage of its Hydrogen production capacity

s_{min} : minimum possible level of the storage as a percentage of its Hydrogen storage capacity

sp_{mwh_h} : electricity price for hour h , known as spot price for hour h , in MWh, given for 8760 hours of the year

pcr_{mwh_h} : PCR remuneration price for hour h in MWh, given for 8760 hours of the year

h_{kg_h} : Hydrogen demand for hour h in Kg, given for 8760 hours of the year

$CO2_{mwh_h}$: average CO₂ content of the electricity consumed for hour h in Kg per MWh, given for 8760 hours of the year

$cons_{eq}$: specific electricity consumption of each of equipment eq in KWh per Kg of Hydrogen produced

RES_{kw_h} : RES electricity production for hour h in KW

$e_{C_{cap}}$: the electrolyzer's CAPEX in euros

$st_{C_{cap}}$: the stack replacement's CAPEX in euros

$c_{C_{cap}}$: the compressor's CAPEX in euros

$s_{C_{cap}}$: the storage's CAPEX in euros

$d_{C_{cap}}$: the distribution network's CAPEX in euros

$e_{O_{cap}}$: the electrolyzer's OPEX as a percentage of its CAPEX

$c_{O_{cap}}$: the compressor's OPEX as a percentage of its CAPEX

$d_{O_{cap}}$: the distribution network's OPEX as a percentage of its CAPEX

$Lwacc$: amortization factor resulted from the weighted average cost of capital for the equipment with the longer lifetime of 20 years (unitless) which is 0.101852

$Shwacc$: amortization factor resulted from the weighted average cost of capital for the equipment with the longer lifetime of 10 years (unitless) which is 0.149029

C_{dec} : CAPEX decrease, presented as a percentage, an economic parameter that shows how much the CAPEX will increase throughout the years as a result of technological advancement, it can take the amounts of 1, 0.8, 0.6, and 0.4 .

$tot_h = \sum_{h \in hour} h_{kg_h}$: total demanded calculated for further computations in the objective function

$$h \in \{ start, \dots, end \}$$

The defined variables are:

1. x which is the Hydrogen production capacity of the electrolyzer in KW, and its optimal value needs to be found.
2. x_{e_h} : This is a binary variable that takes 1 when the electrolyzer is on at hour h and 0 if otherwise.
3. x_{pg_h} which shows the rate at which the electrolyzer is working at hour h in KW, which can take any amount above 0.
4. y which is the Hydrogen storage capacity of the storage (mass of Hydrogen getting stored) in Kg and its optimal value needs to be found.
5. y_{p_h} is the variable related to the level of the Hydrogen stored in the storage in Kg, or in other words, the mass of the of gas inside the storage in Kg at hour h .
6. $0 \leq t_h$ which expresses the amount of RES electricity that the electrolyzer is using at hour h .

The objective function is defined in Equation 67. The target is to minimize the costs of electricity consumed at each part (the cost of RES electricity is zero and only the electricity coming from the grid needs to be paid for) of the configuration while taking into account the economic considerations, including the CAPEX and OPEX of each of the equipment in their respective lifetime and the WACC (weighted average cost of capital). To further explain the objective function, we can say that it has two main parts. The first part talks about the cost of the electricity consumed in each section of the configuration that we have. Consequently, in the first part with three terms, the first term only points out the cost for the electricity consumed by the electrolyzer at hour h . The second term refers to the cost of the electricity consumed by the compressor at hour h . However, the amount of electricity utilized here depends on the amount of Hydrogen produced by the electrolyzer at that hour and that is why first, this amount in Kg is calculated, and then, amount of electricity which the compressor requires for handling the produced Hydrogen is being computed. The third term refers to the cost of electricity needed for the distribution of demanded Hydrogen at hour h , which does not have anything to do with the Hydrogen produced at that hour. The demand needs to be provided by either the Hydrogen, which is just produced, or the amount of Hydrogen which is already stored in the storage from previous hours. So, the total demand of hour h is being handled by the distribution network. To further elaborate on the second part of the objective function, it is important to say that this part deals only with the economic arrangements of the problem in hand. In this second part, the first term refers to the amortization of the CAPEX for all equipment, electrolyzer, compressor, distribution, storage, in just one expression based on their lifetime of 20 years (long lifetime). The next three terms points out the cost of OPEX for the electrolyzer (which depends on the Hydrogen production capacity of the electrolyzer installed), the compressor (which again depends on the Hydrogen production capacity of the electrolyzer installed), and the distribution network. OPEX is not amortized, and its costs are being implemented directly because it is not meant to be paid by debt. The last term of the second part of the objective function is related to the amortization of

the CAPEX for stack replacement based on its lifetime, which is different from other equipment (10 years instead of 20 years).

As for the constraints, the initial conditions of the storage (constraint 68), the electrolyzer's state in terms of being on and off and also its rate (constraints 69 and 70), and the initial amount of RES used (constraint 71) need to be defined. Afterwards, it should be noted that the amount of RES utilized at hour h always needs to be less than or equal to the total amount of RES produced (based on the RES production profile) at hour h (constraint 72). Then, it should be dictated to the model that the storage can contain only a specific amount of gas (constraints 73 and 74). Moreover, there is constraint 75, which is a very important constraint since it connects the state of storage at hour h with its previous hour of $h-1$, to find out the storage level at hour h by considering the amount of Hydrogen that has left the storage at hour $h-1$ and the amount of Hydrogen produced at hour h . After dealing with the storage, in constraints 75 to 77, the constraints impose the limitation on the electrolyzer (working with the electricity coming from both sources of the grid and the RES, hence 2 terms at the left sides of the expressions) that it can only operate up to its optimal capacity, a capacity that is going to fulfill the demand of Hydrogen throughout the year while pointing out that the final rate at which the electrolyzer is working at, should be in the permitted range. In the last four constraints of 80 to 84, the domain of each of the variables has been defined.

Objective Function Definition

$$\begin{aligned} \text{Min } \sum_{c \in \text{cap}} & \left(\left(\sum_{h \in \text{hour}} \left(sp_mwh_h \times x_pg_h + sp_mwh_h \times (x_pg_h \div cons_e \times \right. \right. \right. \\ & cons_c) + sp_mwh_h \times (cons_d \times h_kg_h) \left. \left. \left. \right) \right) + \left((C_dec \times e_C_c + c_C_c) \times x + s_C_c \times y + \right. \right. \\ & d_C_c) \times lwacc + (x \times C_dec \times e_C_c \times e_O_c) + (x \times c_C_c \times c_O_c) + (d_C_c \times d_O_c) + \\ & \left. \left. \left. \left((C_dec \times st_C_c \times x) \times shwacc \right) \right) \div tot_h \right) \end{aligned}$$

Equation 67

Subject to

$$y_p_0 = 200$$

Equation 68

$$x_e_0 = 0$$

Equation 69

$$x_{pg_0} = 0 \quad \text{Equation 70}$$

$$t_0 = 0 \quad \text{Equation 71}$$

$$t_h \leq RES_{kw_h} \quad \text{Equation 72}$$

$$y_{p_h} \geq s_{min} \quad h \in \{1, \dots, end\} \quad \text{Equation 73}$$

$$y_{p_h} \leq y \quad h \in \{1, \dots, end\} \quad \text{Equation 74}$$

$$y_{p_h} = y_{p_{h-1}} - h_{kg_{h-1}} + (x_{p_{h-1}} \div cons_e) \quad h \in \{1, \dots, end\} \quad \text{Equation 75}$$

$$x_{pg_h} + (t_h \div e_{kw}) \leq tot_h \times (1 - x_{e_h}) + x \quad h \in \{1, \dots, end\} \quad \text{Equation 76}$$

$$x_{pg_h} + (t_h \div e_{kw}) \geq (-1) \times tot_h \times (1 - x_{e_h}) + e_{min} \times x \quad h \in \{1, \dots, end\} \quad \text{Equation 77}$$

$$x_{pg_h} + (t_h \div e_{kw}) \leq tot_h \times x_{e_h} \quad h \in \{1, \dots, end\} \quad \text{Equation 78}$$

$$x_{e_h} \in \{0, 1\} \quad h \in \{1, \dots, end\} \quad \text{Equation 79}$$

$$0 \leq x \quad \text{Equation 80}$$

$$0 \leq x_{pg_h} \quad h \in \{1, \dots, end\} \quad \text{Equation 81}$$

$$0 \leq y \quad \text{Equation 82}$$

$$0 \leq y_{p_h} \quad h \in \{1, \dots, end\} \quad \text{Equation 83}$$

$$0 \leq t_h \quad h \in \{1, \dots, end\} \quad \text{Equation 84}$$

3 Results of Numerical Experiments

The mathematical formulation of each of the models explained in the previous chapter were introduced to CPLEX (version 20.10) for solving with the help of AMPL and the results are discussed in this chapter of the thesis.

As a general note, all the models were solved to optimality by CPLEX and solution time on average was 16.9 seconds.

3.1 Model 1 Results

First, the case of France is evaluated here. Generally, the data regarding two parameters of hourly Hydrogen demand and the maximum allowed allocation percentage of FCR have been changed by changing the amount of its parameter in the mathematical model for the main model and as a result, 12 versions (3 different numbers for PCR and 4 different demand profiles) of the output have been created.

The results show that with the same demand profile, as the maximum allowed percentage of FCR is increasing from 0% to 25%, the total cost of the configuration as well as the price of each kilogram of Hydrogen decrease as the share of the remuneration for FCR is helping the system as a revenue while having a constant yearly demand in all cases of 0%, 10%, and 25%. Below, Table 6 shows the price of each Kilogram of Hydrogen with different inputs:

Electricity Cost of 1 Kg of Hydrogen in a year (Euros/Kg)			
Cases	0% FCR	10% FCR	25% FCR
1a	2.161	2.151	2.132
2a	2.314	2.307	2.295
1b	2.157	2.147	2.128
2b	2.311	2.304	2.293

Table 6 Cost of 1 Kg of Hydrogen in different cases

This price for each kilogram of Hydrogen is actually the energy (electricity) cost used by the configuration throughout the year and it is obvious that there is a trade-off between the yearly number of operational hours and the electricity cost (demand profiles of 2a and 2b make the electrolyzer work more than the demand profiles of 1a

and 1b because of the higher demand that they ask for satisfying and as shown in the table above, the prices of each Kg of hydrogen is higher in those cases).

As it is clear to interpret, adding flexibility to the system in terms of allowing it to decide if it is wise to allocate FCR or not, does not have a notable effect on the price of each kilogram of Hydrogen although it is counted as a remuneration for the system.

The effect of a more distributed demand profile can be seen here by comparing the results of having demand profiles of 1a and 1b or 2a and 2b since each group have the same total weekly Hydrogen demand in Kg. The distributed demand throughout each week and in general throughout the year, only affects the price by 0.1%-0.2%. Also, in the case in hand, turning on the electrolyzer each time does not put any cost on the system and also, the decline of the electrolyzer's efficiency due to turning on and off have not been considered. Consequently, to decide if using a more distributed demand profile has benefits or not, these two later parameters can be influential due to negligible change in price.

The change in the total weekly Hydrogen demand (from 1a to 2a or from 1b to 2b) has also affected the price. Increasing the total weekly Hydrogen demand from 2130 Kg to 2640 Kg (around 25%) has increase the price around 8%. Not considering the decline in electrolyzer's efficiency due to being on for a longer period of time which can put extra costs on the system and lead to an extra alteration in the price, trying to get the most out of the capacity of the electrolyzer by forcing a higher the total weekly Hydrogen demand in Kg on the system makes sense considering these numbers.

For analyzing the hourly states at which the electrolyzer is working at as well as the amount of Hydrogen present in the storage, due to the high number of data (8760 sets of data available), the yearly analysis will not be really explanative. The solution for this matter is to define weekly, monthly, or quarterly profiles to divide the year into several comparable periods. This model is used later in this thesis. The following Fig.

21 describes how the electrolyzer setpoints throughout the year has changed by changing the maximum allowed amount of FCR allocated to have an overall idea:

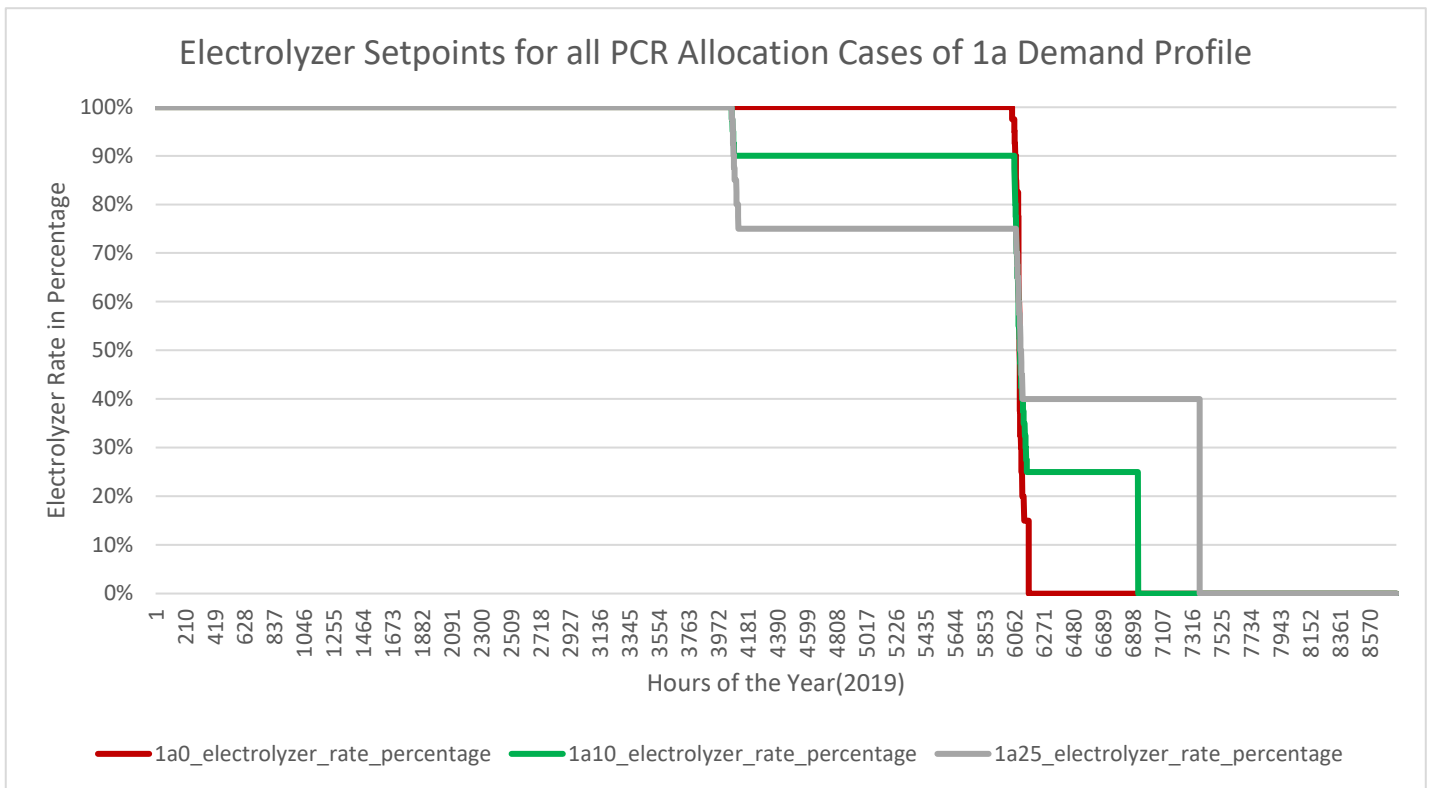


Figure 21 Electrolyzer Setpoints for all PCR Allocation Cases of 1a Demand Profile

The graph depicts that as the maximum allowed percentage of FCR allocation is increasing, the electrolyzer is working less at full rate because the configuration is dedicating a higher amount of electricity to Frequency Containment Reserve to increase the remuneration for the configuration and as a result, reduces the costs.

In this Model, since the aim of the optimization is to decide what the hourly electrolyzer's rates are to minimize the electricity costs, it is useful to see how these rates have changed with respect to the spot prices throughout the year. Below in Fig. 22, these changes have been depicted for demand profile 1a and 1b in 2019 for France. As expected, at lower prices as well as at hours with negative prices (negative prices work as remuneration for the system) throughout the year, the electrolyzer works at higher rates, 100% or as close as possible with taking into consideration the limitations for the storage and demand level, and as the prices increase, electrolyzer works at lower rates, in order to control the costs that it puts on the systems. This graph also conveys how the optimization has to take place, meaning that the system has to choose

to work in hours with less cost at full potential while restricting its function in hours with higher costs.

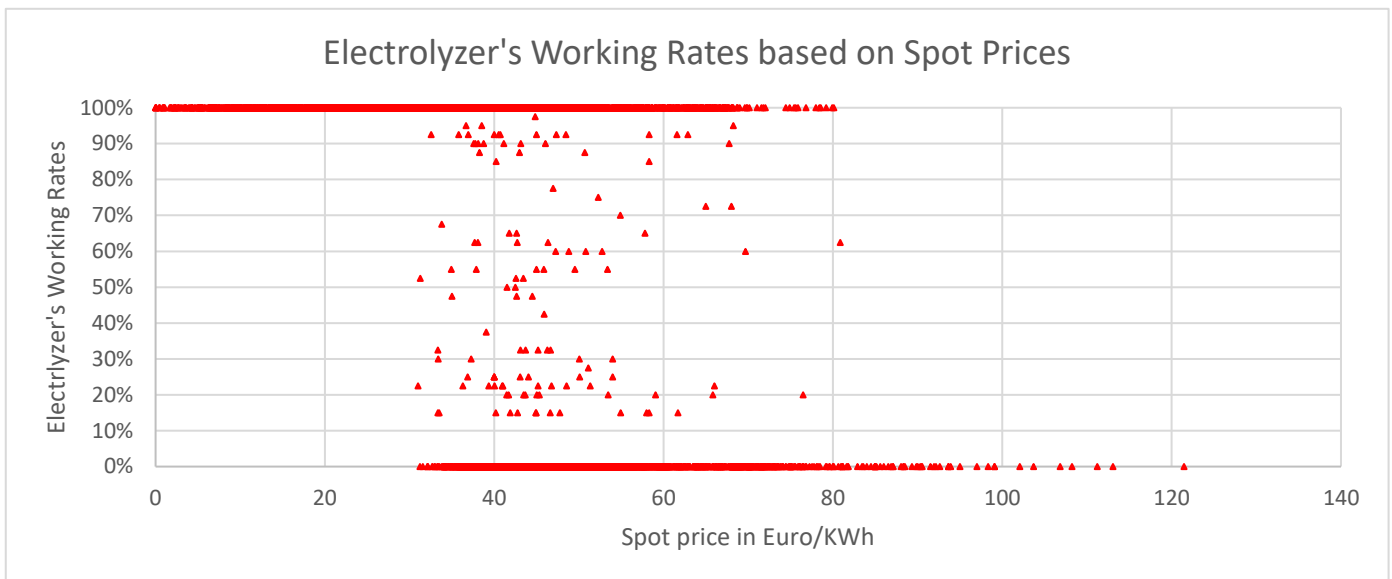


Figure 22 Electrolyzer's Working Rates based on Spot Prices

Another interesting analysis is comparing the CO₂ content of each Kg of Hydrogen in all these 12 scenarios which were discussed in this section. The numbers are stated in Table 7:

CO ₂ Content of 1 Kg of Hydrogen (Kg/Kg)			
Cases	0% PCR	10% PCR	25% PCR
1a	1.987	1.989	1.995
2a	2.551	2.554	2.558
1b	1.982	1.985	1.990
2b	2.544	2.547	2.552

Table 7 CO₂ content of 1 Kg of Hydrogen in different cases

The effect of a more distributed demand profile (comparison between 1a and 1b or 2a and 2b since each duo has the same total amount of demand throughout the year but the distribution of this demand in the days of each week is different between the members of each duo) and also allocating more FCR can be understood from the numbers in the above table. For the former matter, results show that a more distributed demand profile affects the CO₂ content of each Kg of Hydrogen by only around 0.25%. Consequently, it can be seen that CO₂ content is influenced by the total weekly

Hydrogen demand, and not the way that the demand profile is distributed throughout the year. As for the latter matter, by increasing the maximum allowed FCR percentage in all cases, the CO₂ content of each Kg of Hydrogen only changes by around 0.3%, which is negligible and due to the analysis of the price, done previously, that has shown that the prices won't change notably, it is advised not to allocate a higher amount of FCR. This is because in these calculations, the aging of the components has not been taken into consideration. Consequently, it will considerably affect the lifetime of the plant and decrease the efficiency in the long run while it doesn't have any economic added value.

As briefly explained previously, to get into the details of one set of input data, average time profiles are introduced to the analysis and consequently, two known periods of time, spring and fall, have been chosen and the graphs below (Fig. 23) have been depicted in their respective months (spring has been considered to be from the beginning of March until the end of May and fall has been considered to be from the beginning of September until the end of November).

In Fig. 23, the first set of graphs show the setpoints for the storage in springtime at each hour in Kg for different cases of FCR. As it is shown, the amount of Hydrogen in the storage in all cases has followed a similar pattern and the amount of stored Hydrogen doesn't really get affected by the amount of FCR allocated.

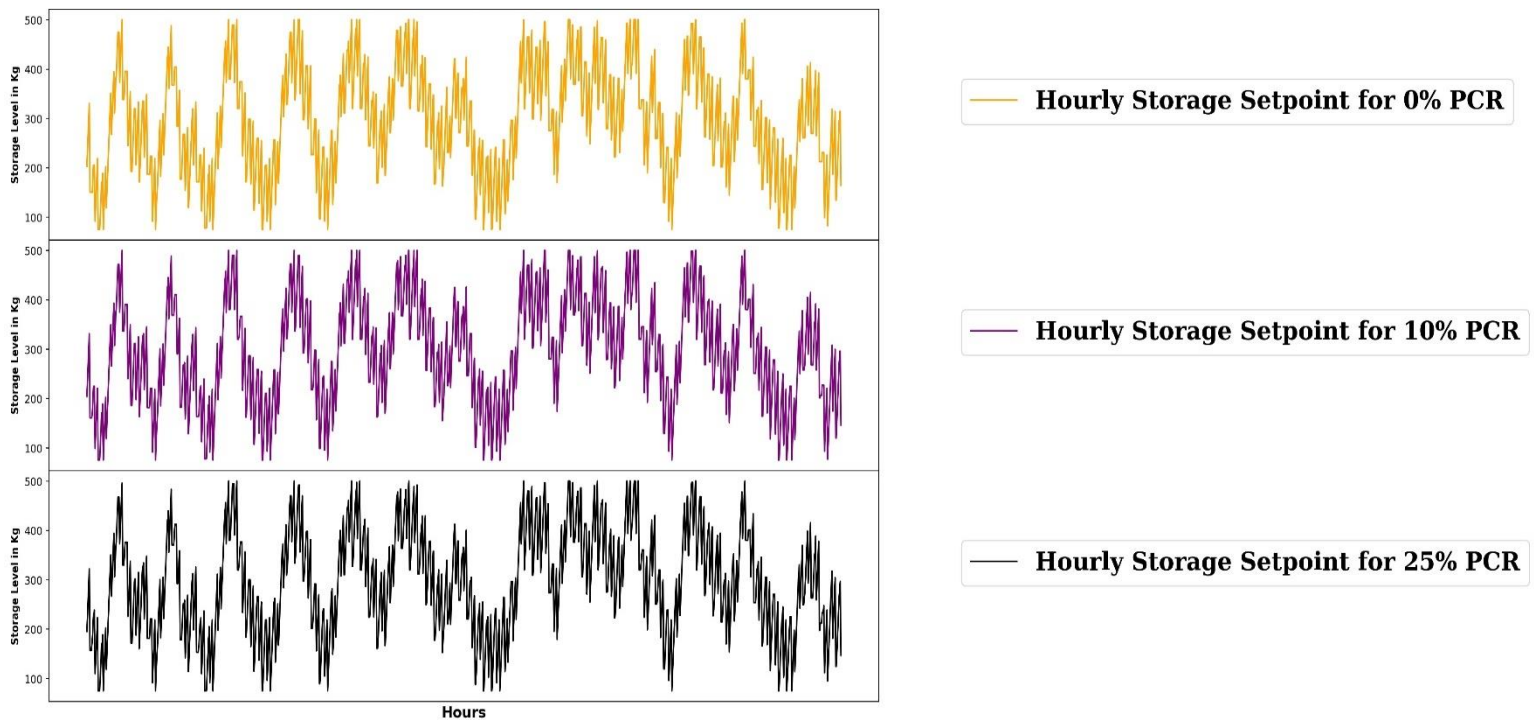


Figure 23 Hourly storage setpoints in springtime for different FCR allocations

Analyzing storage under different circumstances in terms of input and throughout different models presented in the thesis has shown that due to having a storage with

not extremely high volume for storing Hydrogen and due to not setting a buffer of 24-48 hours in order to further push the storage to accommodate more Hydrogen (something that can be in place in the case of actual market), the storage analysis does not show any an added value or promising result since no notable changes in the setpoints are seen between different models.

In the next set of graphs presented in Fig. 24, the setpoints of the storage in fall and spring have been compared while having the amount of FCR fixated at 0%. These patterns, on the other hand, compared to the previous analysis, follow different trends due to the difference in the price of electricity which is the only input changing between these two cases.

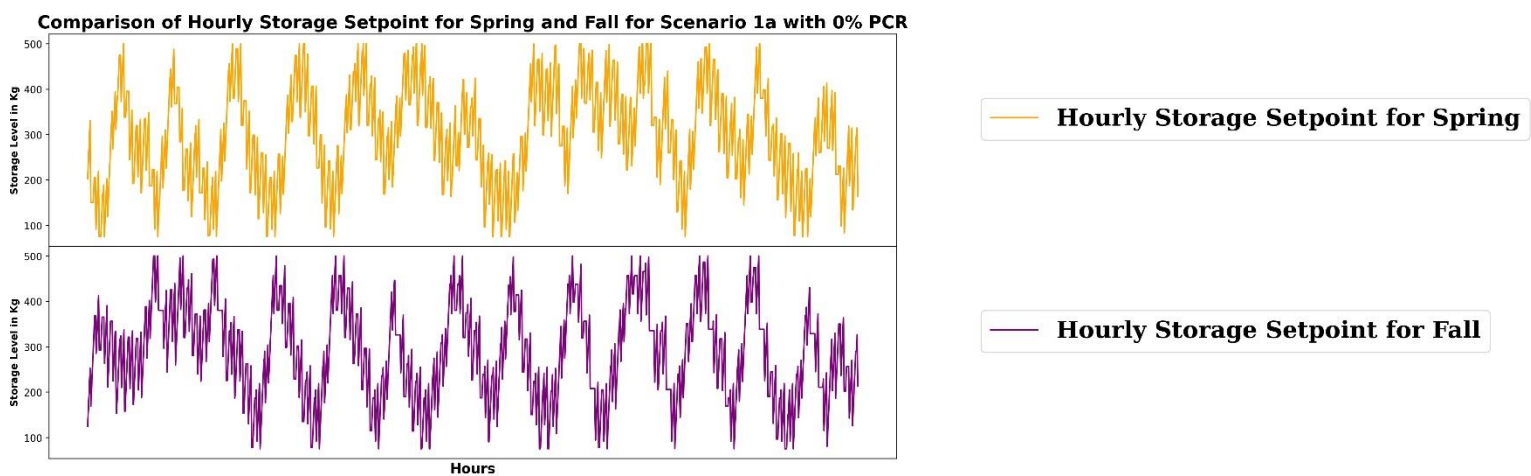


Figure 24 Comparison of hourly storage setpoints for spring and fall for all approach 1a and 0% FCR allocation

As explained in the last point of the input section, the same optimization program has been carried out with the input data of Germany, considering 0% FCR allocated and the 1a demand profile. The energy price related to each Kg of Hydrogen for Germany in 2019 is 2.003 Euro/Kg which is 7% lower than the energy price of each Kg of Hydrogen in France for the same reference year. This slight change in the price is due to the slight changes that exist in the hourly price of electricity throughout the year in these two countries. The average prices of electricity throughout the year (39.45 Euro/MWh in France and 37.67 Euro/MWh in Germany) confirm this matter as well. Consequently, due to the hourly electricity prices being almost similar, the behavior of the electrolyzers for France and Germany are similar as well.

3.2 Model 2 Results

The CO₂ content of 1 Kg of H₂ production in both Germany and France are found, below, in the table. The final amount of CO₂ associated with production of one kilogram of Hydrogen in Germany in 2019 is about ten times of this number in France,

as expected, since the average hourly CO₂ content per 1 MWh of electricity in Germany is about ten times of this number in France (416.36 Kg/MWh for Germany and 34.15 Kg/MWh for France, Table 8):

CO ₂ content of 1 Kg of Hydrogen in a year (Kg/Kg) - 0% FCR	
France	1.91
Germany	23.39

Table 8 CO₂ content of 1 Kg of Hydrogen

There is a specific point which needs to be mentioned in this model. Model 2 aims for reaching the desired demand profile while minimizing the CO₂ related to this demand. Consequently, the energy (electricity) price is not an influential parameter here. However, there is a correlation between the spot price and the CO₂ content per 1 MWh at each hour. This correlation has been shown in Fig. 25. Clearly, the higher the average CO₂ content of each MWh is, the higher the spot price will be regardless of the country this analysis is targeting.

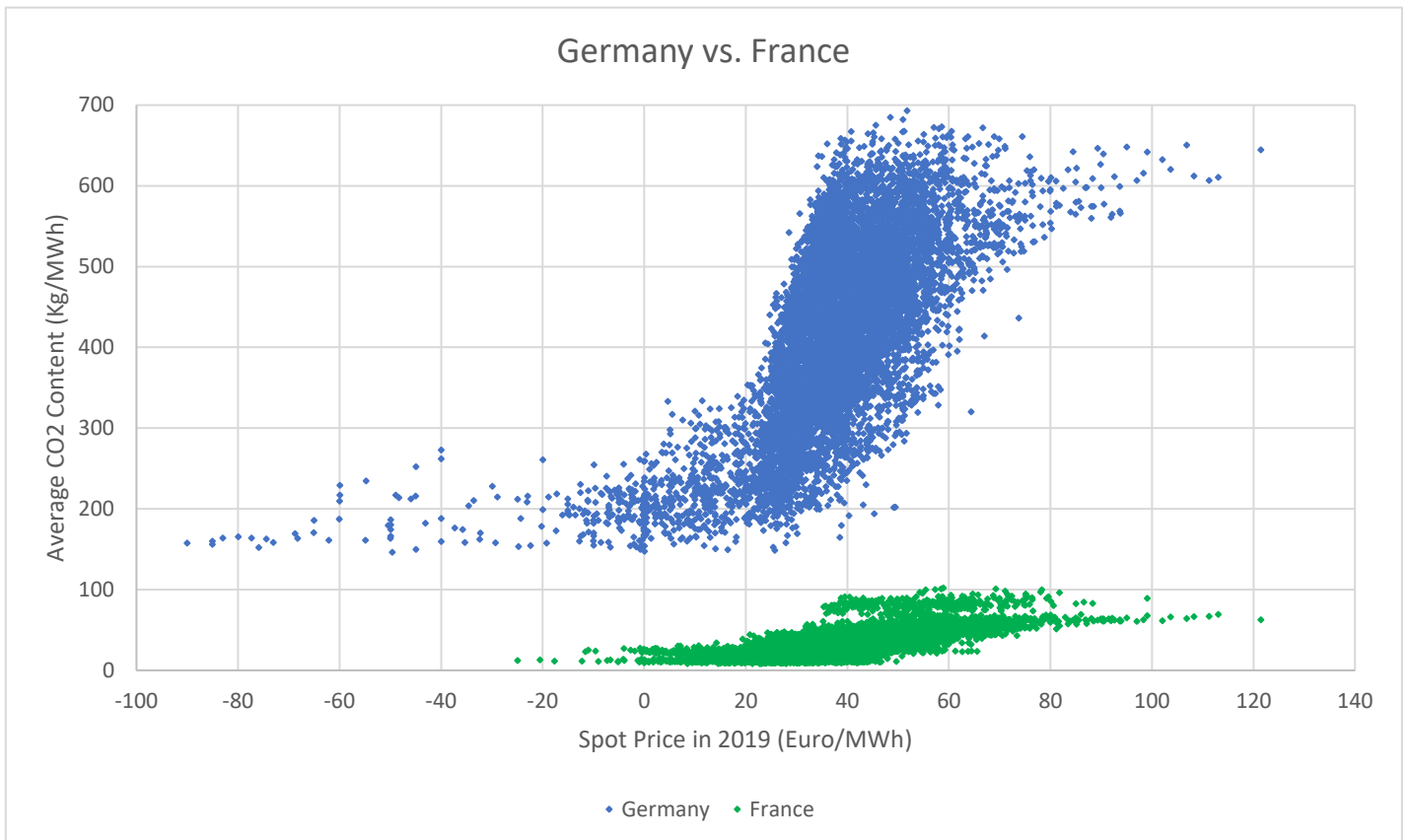


Figure 25 Correlation between the spot price and the CO₂ content per 1 MWh, France vs. Germany

Another beneficial comparison which needs to be done here is to see whether the present model of CO₂ minimization is really useful for emission reduction or not by significantly reducing the CO₂ content of each kilogram of Hydrogen and to see how this matter has affected the price of Hydrogen. Table 9 has summarized these two matters for France in 2019.

	The CO ₂ Content of 1 Kilogram of Hydrogen (Kg/kg)	The Cost of 1 Kilogram of Hydrogen (Euro/kg)
Model 1 (Minimizing the Energy Costs)	1.987	2.161
Model 2 (Minimizing the CO ₂ Content)	1.913	2.330

Table 9 Comparison between Model 1 and 2

The data above explains that using the CO₂ minimization model has only decreased the CO₂ content of one kilogram of Hydrogen by 4% while increasing its final price around 8%. Moreover, the almost similar way that the electrolyzer has behaved in these two models, which is shown in Fig. 26, confirms that implementing this model to decrease the final footprint of Hydrogen production on the environment does not seem a competitive choice considering these numbers.

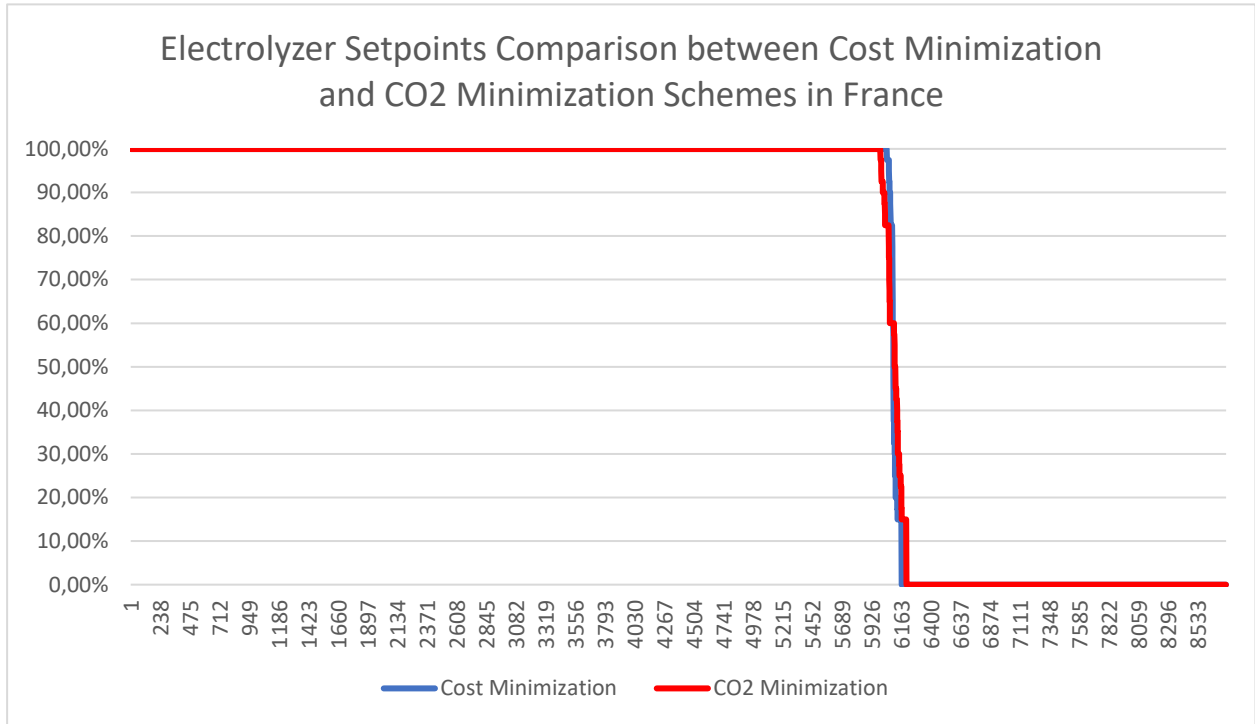


Figure 26 Electrolyzer Setpoints Comparison between Cost Minimization and CO₂ Minimization Schemes in France in 2019

To further complete the analysis above, the cost of each ton of CO₂ avoided for each Kg of Hydrogen needs to be calculated.

$$(2.330 - 2.161) \div (1.987 - 1.913) \times 1000 = 2284 \text{ Euros}$$

The numbers mentioned in the previous table as well as the following procedure are used in the calculations and the acquired amount of money above is significant which should be taken into consideration in the change of strategies from minimizing the cost to minimizing the CO₂ footprint. To further analyze if this amount of expenditure as rational one or not, economic-wise, the number above should be compared with the current value for CO₂ quota in European Union's Emissions Trading System (or ETS, which is a Cap & Trade system to trade emission allowances). This framework has been set up in 2005. According to this system, each year, a certain number of greenhouse gases and emissions are allowed to be produced by the plants which are under the observation of this system, which is also called cap. This number of caps is decreasing each year to promote going green. However, the plants in this framework have the possibility to trade the permits that they have in their possession with the price set by ETS. Currently, this value is 63.12 Euro/ton of CO₂. In consequence, choosing Model 2 to minimize the amount of CO₂ produced by the plant is not reasonable at all while the expenditure for each ton of CO₂ in this model is almost 37

times of the price of CO₂ allowance in Europe. (European Energy Exchange AG, 2021) (European Commission for EU Emissions Trading System, 2021)

3.3 Model 3 Results

The price of each kilogram of Hydrogen in France in 2019 and its respective storage and electrolyzer capacities have been mentioned in the table below. As it is clear, as the electrolyzer and stack replacement CAPEX are decreasing (from 100% to 40%), the proposed capacity of storage is decreasing as well while the proposed capacity of the electrolyzer is slowly increasing. Also, as the CAPEX costs of a big part of the configuration is dropping, the price of each kilogram of Hydrogen is declining too (Table 10):

Storage Initial Condition	CAPEX Costs %	Electrolyzer Capacity	Storage Capacity	Price of 1 Kg of Hydrogen in the Model (Euros/Kg)
200KG	100%	727.163	297.644	4.351
	80%	727.64	296.925	4.114
	60%	733.333	288.333	3.874
	40%	756.25	253.75	3.638

Table 10 Proposed capacities and their respective prices of Hydrogen

This set of results show that the price of each kilogram of Hydrogen is affected by electrolyzer's CAPEX costs (the cost of each kilogram of Hydrogen has decreased almost 20% by CAPEX decrease to 40%), however, the optimum sizing of the electrolyzer and the storage is not derived by electrolyzer's CAPEX costs (the installed electrolyzer power variation around 4% and the installed storage capacity variation around 15%). Consequently, considering technological advancements regarding electrolyzers, which result into CAPEX reduction in the next upcoming years, is not going to make massive changes in the configuration in terms of electrolyzer and storage capacity used. On the other hand, these advancements can be noteworthy for the final price of each kilogram of Hydrogen in the market.

To have a brief overview of the prices of the most common electrolyzer used in industry, the CAPEX costs for an alkaline electrolyzer is around 750 EUR/kW which by 2025 is expected to drop (based on the economic and market predictions) to a number of 500 EUR/kW. (Noussan, 2020)

As previously explained, the final price of each Kilogram of Hydrogen consists of three parts: Energy cost, CAPEX cost, and OPEX cost. The pie chart of Fig. 27 shows the composition of the price of 1 kilogram of Hydrogen for the 1st case of the table above (CAPEX implemented completely):

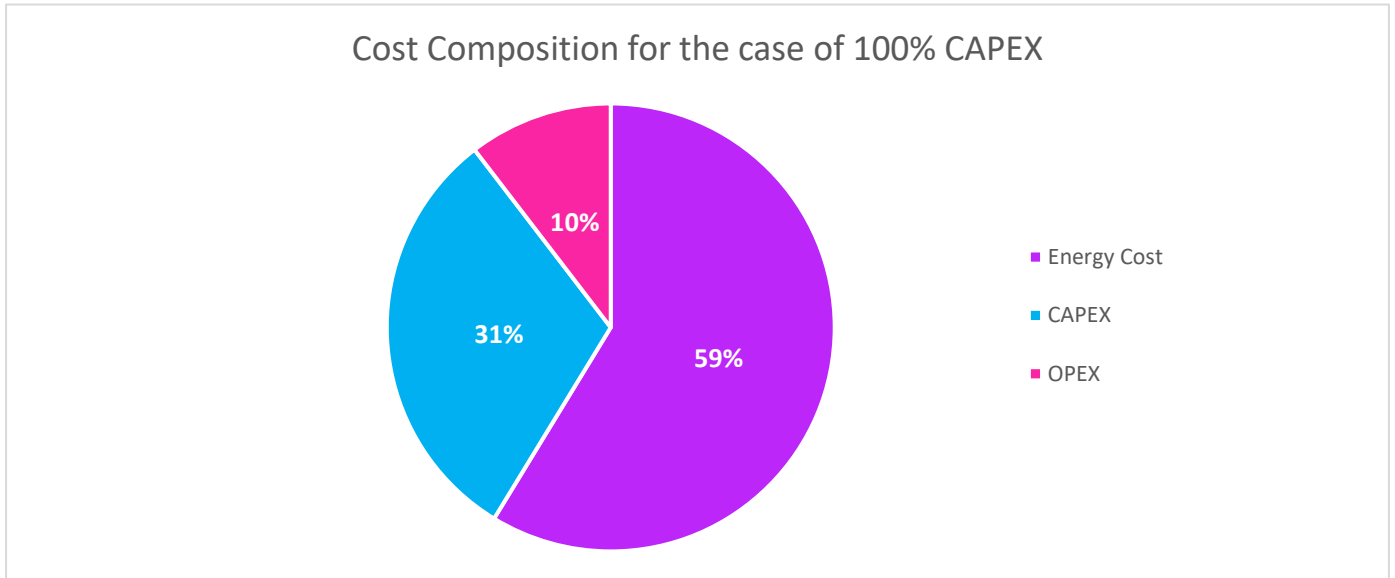


Figure 27 Cost Composition for the case of 100% CAPEX

The percentages change as the input of the data changes for the optimization model (the CAPEX decreases, shown in Table 11):

	Percentage of each part of the total cost			
	COST Percentage for 100% CAPEX	COST Percentage for 80% CAPEX	COST Percentage for 60% CAPEX	COST Percentage for 40% CAPEX
Energy Cost	56%	59%	62%	66%
CAPEX	33%	31%	28%	25%
OPEX	11%	10%	10%	9%

Table 11 Composition of the total costs in different cases of Model 3

An interesting comparison can be done comparing the CO₂ content of each kilogram of Hydrogen in Model 2 and 3, when the objective is to minimize the amount of CO₂ content of each kilogram of Hydrogen and the total cost of the configuration (energy costs as well as OPEX and CAPEX costs), respectively. This comparison can be done

using the optimum installed capacity of electrolyzer and storage found in the first run of Approach 3 model (the case of 100% of CAPEX and OPEX implemented) and the fixed configuration presented in Model 2 since the input data and the conditions for these two cases are the same in terms of country, year, and demand profile. The numbers can be found in Table 12.

The amount of CO ₂ per Kilogram of Hydrogen (Kg/kg)	
CO2 Minimization Model	1.913
CAPEX Minimization Model	2.090

Table 12 Comparison of the CO₂ content of each Kg of Hydrogen in Model 2 and 3

As it is clear, in Model 3, because the focus was on minimization of the total cost and not decreasing the environmental impacts of each kilogram of Hydrogen, the CO₂ content of each kilogram of Hydrogen is higher in the case of Model 3 which is the total cost minimization case.

3.4 Model 4 Results

This analysis starts with the comparison between the price of one kilogram of Hydrogen between Model 1 (only having electricity from the grid) and Model 4 (having electricity from the grid and from the RES, which is a wind turbine here) has been done to clarify the effect of RES on the pricing. However, in the mathematical model, the energy (electricity) costs calculations have not taken into account the total expenditure for the Hydrogen (the price of RES which is wind, or any other renewable resource has been set to 0 to implement the concept of priority of dispatch for the electrolyzer as discussed in the beginning of this section). After reaching the optimum hourly utilization rate at which RES should be harnessed and the electrolyzer should be operated at, the actual price of wind (levelized cost of electricity coming from onshore wind in the case of this section) needs to be added to the price of each kilogram of Hydrogen. In total, 4265.144 MWs of RES have been harnessed for providing 111090 Kgs of Hydrogen throughout the year. Based on the reports published by IRENA, the LCOE in case of having onshore wind in EU in 2019 is 0.067 USD/KW (= 56.28 Euro/MW) (The International Renewable Energy Agency, 2019). Consequently, the results are reported in Table 13:

The price of 1 Kilogram of Hydrogen (Euro/kg)	
Model 1 (Minimizing the Energy Costs Utilizing Grid)	2.161
Model 4 (Minimizing the Energy Costs Utilizing Grid + RES)	2.960

Table 13 Comparison between Model 1 and 4 for the price of 1 Kilogram of Hydrogen (Euro/kg)

When using RES as a source for providing electricity, the price of Hydrogen has increased around 37% which is notable in terms of economic considerations. It is crucial to remember that the point of having RES as the electricity provider is not to necessarily decrease the costs of production, but to decrease the carbon emission of each kilogram of Hydrogen. Comparing Model 4 and 1, which have the same input conditions, the CO₂ content of each kilogram of Hydrogen decreases when using RES (around 76%) which shows that integrating RES with Hydrogen production is definitely one of the most influential methods to mitigate emission production and the numbers in the Table 14 show the results of the analysis:

The CO₂ content of 1 Kilogram of Hydrogen (Kg/kg)	
Model 1 (Minimizing the Energy Costs Utilizing Grid)	1.987
Model 4 (Minimizing the Energy Costs Utilizing Grid + RES)	0.534

Table 14 Comparison between the CO₂ content of 1 Kilogram of Hydrogen (Kg/kg)

Consequently, reductions in RES price can heavily contribute to make the RES Hydrogen competitive in the market. This can happen because of the improvements in the equipment technology line, reduction in O&M costs (due to the integration of autonomous inspections as well digital and improved data analytics), implementation of economies of scale (with scaling up the production which directly affect the installation and O&M costs), as well as switching to schemes that support the competitive auctions and procurement that can be really influential as it is obvious in the reported price of electricity. As an example, the data related to the electricity coming from onshore wind in 2019 and then 2020 by Irena which are 0.067 USD/KW (= 56.28 Euro/MW) and 0.045 USD/KW (= 37.8 Euro/MW), respectively. The decline in the weighted LCOE of commissioned onshore wind projects in France and Germany from 1984 to 2020 has been shown in the graphs of Fig. 28, confirming this matter. (The International Renewable Energy Agency, 2019) (The International Renewable Energy Agency, 2020)

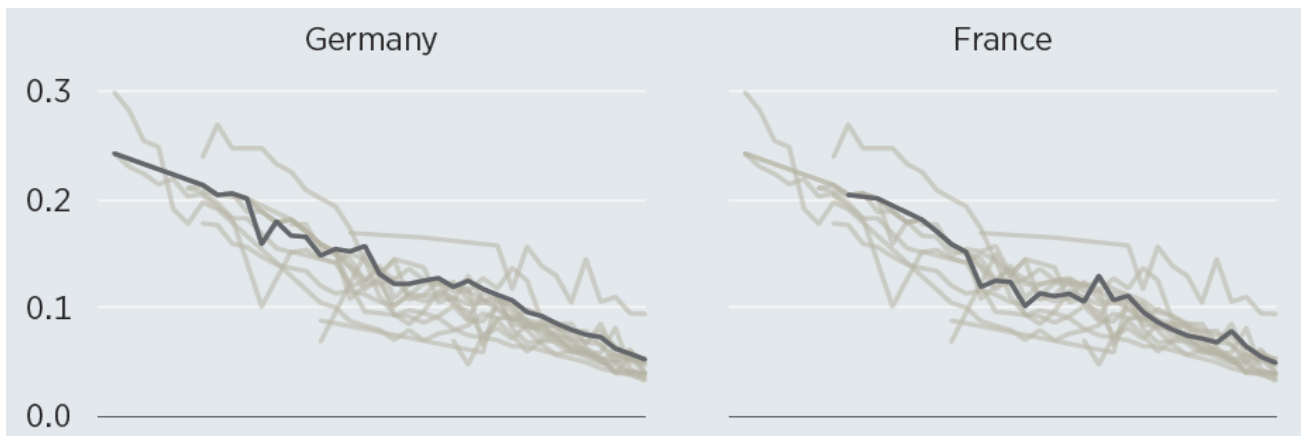


Figure 28 Weighted LCOE of commissioned onshore wind projects in France and Germany from 1984 to 2020 in USD/KWh (source: (The International Renewable Energy Agency, 2020))

In Europe, although the Hydrogen production by the help of renewable resources through electrolysis avoids costs like general taxes or network costs, the capacity of the renewable resource (being wind or solar) is usually limited. Yet, the final price if each kilogram of Hydrogen coming from the renewable resources is considered to be competitive in most EU countries.

In EU Member States as well as UK and also Norway, with the current documented rate (Hydrogen Europe Intelligence Department, 2020) of average solar irradiation and wind conditions, the price of each kilogram of Hydrogen produced with a configuration directly connected to the renewable resource ranges from €3.5/kg (from solar PV located in Portugal) to €6.5/kg (from onshore wind located in Luxemburg). The prices for other countries in EU is depicted in Fig. 29. Solar PV in southern European countries and onshore wind for northern European countries are the cheapest resources which can be used to produce Green Hydrogen. Germany and Belgium are exception here because offshore wind is considered to be the cheapest pathway on average. The fact needed to be stressed here is that these the costs mentioned have been calculated and reported on the basis of having an average wind and solar profile for each country throughout the year. This strategy and the advantages it brings in terms of decreasing the stress on the grid for balancing the supply and demand as well as the RES operator being able to use all the capacity of the plant and participating in the demand side program will lead to having a market in which the price Green Hydrogen, coming from RES, having the possibility to compete with Grey Hydrogen, coming from fossil fuels. (Hydrogen Europe Intelligence Department, 2020)

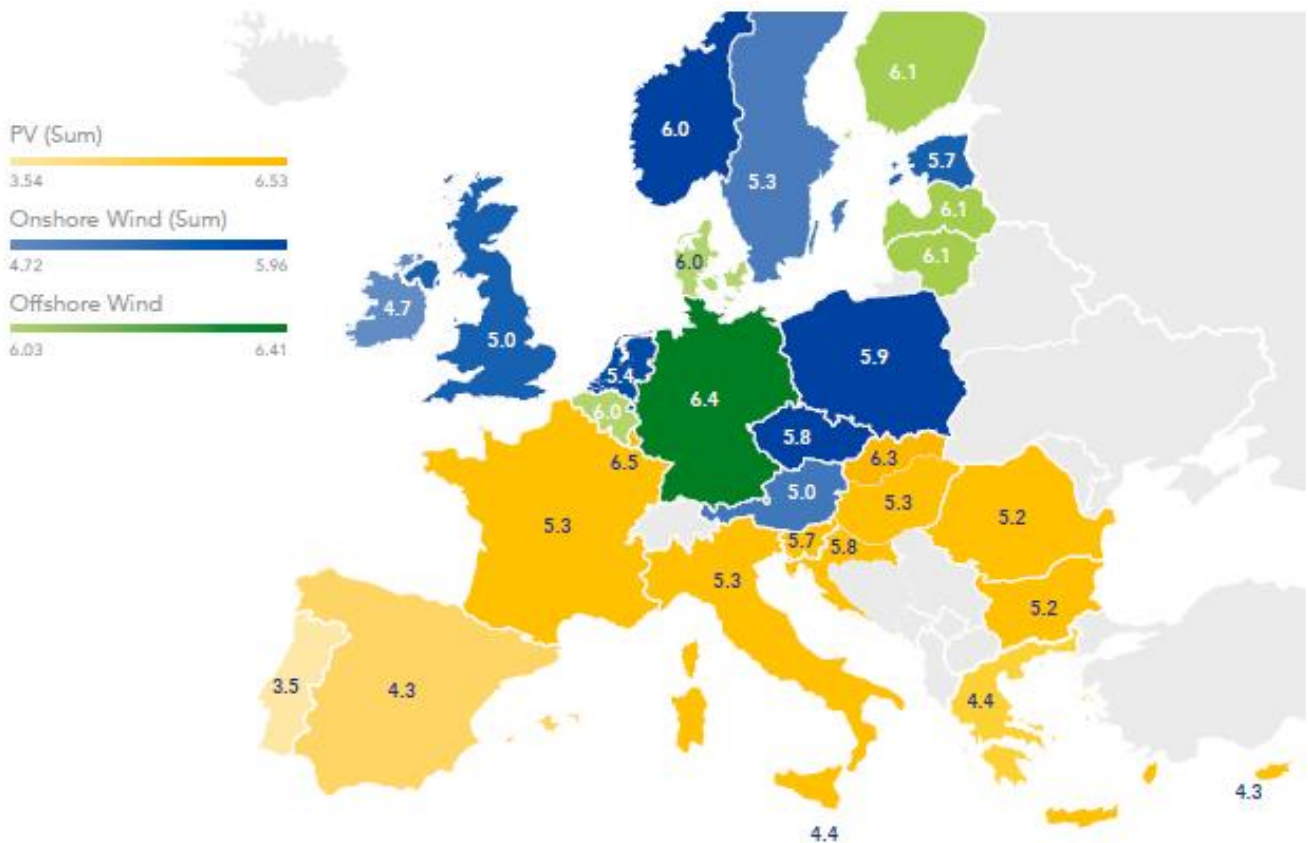


Figure 29 Green Hydrogen prices (costs) in EU countries in 2019 (Euro/Kg) (source: (Hydrogen Europe Intelligence Department, 2020))

To further complete the analysis above, the price of each ton of CO₂ avoided for each Kg of Hydrogen needs to be calculated using the price and CO₂ footprint of each Kg of Hydrogen.

$$(2.960 - 2.161) \div (1.987 - 0.534) \times 1000 = 550 \text{ Euros}$$

This number shows that switching to a configuration that has integrated RES electricity will put a reasonable cost on the system considering the decline in the CO₂ footprint. Therefore, this integration is definitely a logical choice to go forward with. Moreover, comparing this number (550 Euros) with the price of each ton of CO₂ avoided for each Kg of Hydrogen for Model 2 (2284 Euros), in which the strategy was directly to minimize CO₂, the importance of integrating RES is evident from an economic point of view.

The next figure, Fig. 30, shows how much RES has been utilized by the configuration throughout the year. As expected, the RES has been harnessed as much as possible considering the facts that first the electrolyzer's capacity can make use of maximum 1MWh of electricity at each hour (in the hours that the RES produced was more than 1000KW, only 1000KW has been harnessed and not more), and second, the cycle of the demand has an effect on the amount of RES used to produce Hydrogen. In the end, in total, 4265.144 MW out of total RES production of 4763.432 MW have been used by the configuration (89.54%).

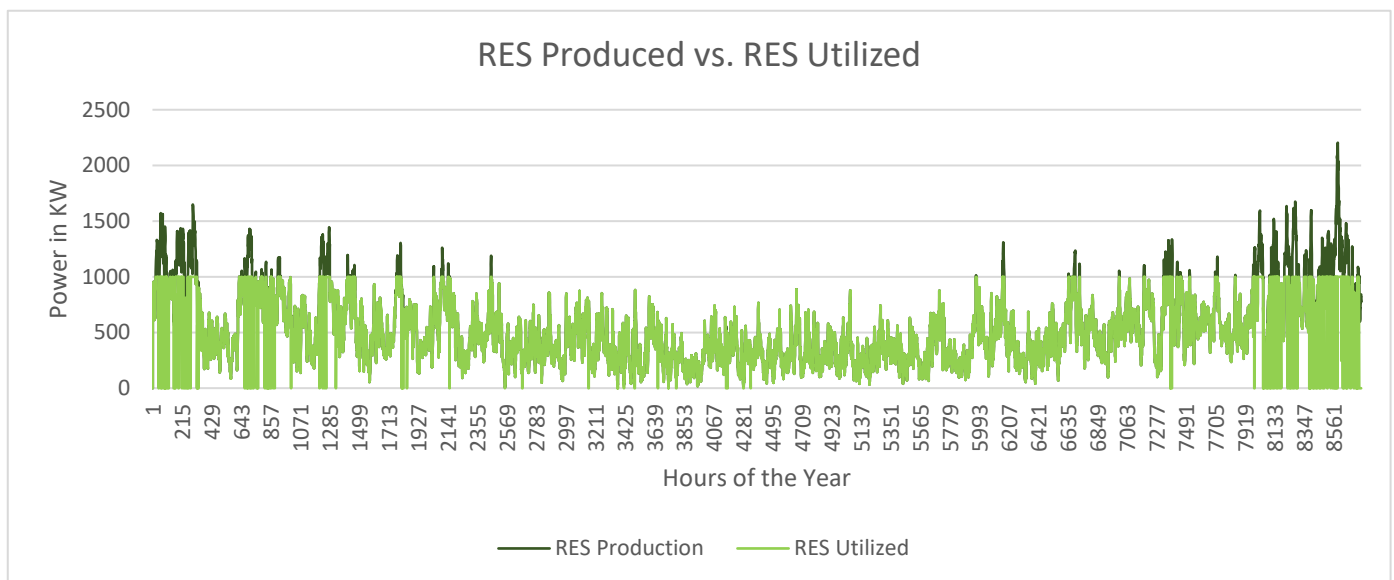


Figure 30 RES Produced vs. RES Utilized

In Model 4, there are two different types of Hydrogen produced based on the origin of the electricity that the electrolyzer is using. 70% of the Hydrogen produced in this model to satisfy the demand is Green Hydrogen, with the electricity coming from renewables, and the rest is considered to be Grey Hydrogen since the origin of the electricity coming from the grid is not known and it is safer to assume that it does not have a renewable or nuclear origin. The percentages are shown in the pie chart of Fig. 31:

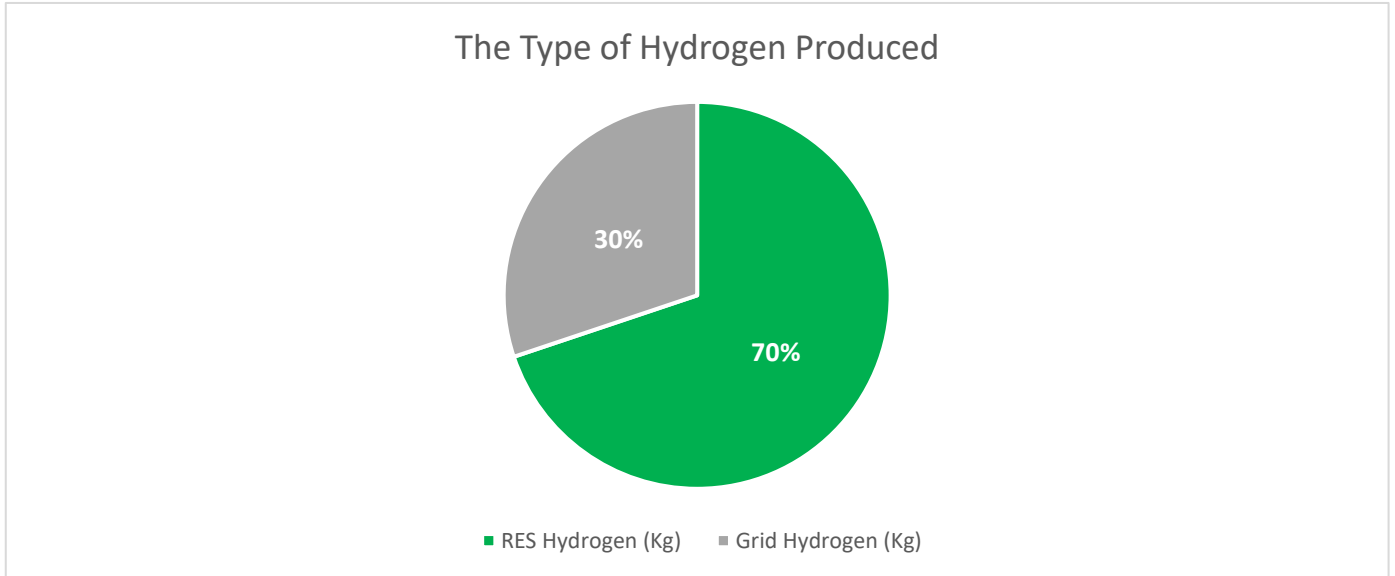


Figure 31 Percentage of Green and Grey Hydrogen

3.5 Model 5 Results

Again, just as the previous model, it should be noted that the prices reported from the models are not the real price of each kilogram of Hydrogen and in order to find the correct price, the price of electricity coming from RES has to be added to the final numbers coming from the models. With the same methodology used in the previous case, the calculations have been done and the complete results have been reported in Table 15:

Storage Initial State	CAPEX impact	Electrolyzer Capacity (KW)	Storage Capacity (Kg)	Amount of RES Utilized (Out of 4763.432 MW)	Cost of RES for Each Kg of H2 (Euro/Kg)	Cost of Each Kg of H2 from the Model (Euro/Kg)	Final Price of Each Kg of H2 (Euro/Kg)
200 Kg	100%	710.61	291.324	4088.391	2.0712	2.843	4.914
	80%	711.114	290.428	4089.835	2.0720	2.611	4.683
	60%	719.193	276.085	4095.765	2.0750	2.378	4.453
	40%	733.291	259.14	4105.047	2.0797	2.14	4.220

Table 15 Model 5 detailed results

Here as well as Model 3, the advancements in electrolyzer technology which result in the decline in the related CAPEX from 100% to 40% has only affected the optimum capacity of electrolyzer used around 4%. Due to this change in the effect of the CAPEX of electrolyzer and stack replacement the amount of RES used has changed slightly as well, but due to the mechanism of the model which sets the RES price as zero, the models has tried to take advantage of the RES available as much as possible.

The price of Hydrogen, however, has declined by about 15% while decreasing electrolyzer and stack CAPEX terms which can be considered as a driver for focusing more on improving the electrolyzer technology and also, reducing the price of each MW of the electricity coming from the RES. This is because the RES price made up around 40%-50% of the final price which is notably high. Of course, the price of each MW of RES electricity has been declining in the recent decade as it is shown in the graphs of Fig. 32 for the two sources of Onshore Wind and Solar Photovoltaic, however, more focus in this field can massively affect (much more than the technology advancements in electrolyzer production line) the price of Hydrogen in the market:

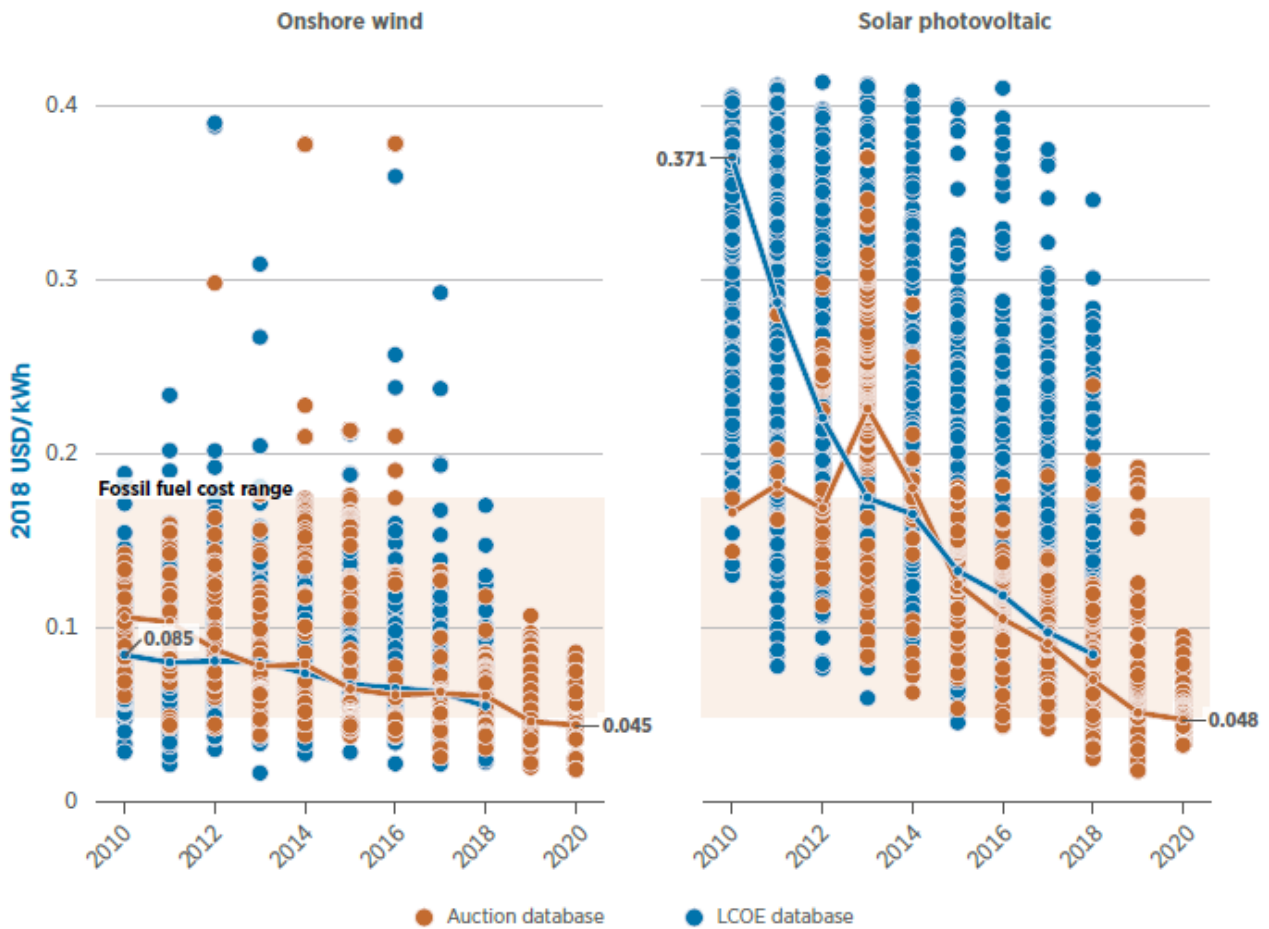


Figure 32 The price of each KW of electricity coming from two types of RES (source: (The International Renewable Energy Agency, 2019))

To wrap up this section of the analysis, it is safe to say that the decline in RES electricity prices, in the first place, and the reductions in electrolyzer’s CAPEX (coming from both the economy of scale and advancements in electrolyzer technology) in the second place, are the main drivers for reaching a cheaper Hydrogen in the next ten years ahead.

Comparing Model 3 and 5 in terms of the change in the price of each kilogram of Hydrogen by implementing RES can assist in defining whether RES penetration can be of any help in economic matters as well as environmental ones, which has been done in Table 16.

Model 3 and Model 5 Comparison							
CAPEX impact	Model 3 Price of 1 Kg of H2 (Euro/Kg)	Model 5 Price of 1 Kg of H2 (Euro/Kg)	Change in Price (%)	Percentage of Green Hydrogen Produced	CO2 Content of Each Kg of H2 (Kg/Kg) in Model 3	CO2 Content of Each Kg of H2 (Kg/Kg) in Model 5	Change in Amount of CO2 Content (%)
100%	4.351	4.914	11.46	85.83	2.108	0.674	68.03
80%	4.114	4.683	12.16	85.86	2.109	0.673	68.09
60%	3.874	4.453	12.99	85.98	2.109	0.67	68.23
40%	3.638	4.220	13.79	86.18	2.117	0.666	68.54

Table 16 Model 3 and Model 5 Comparison

After all the analysis that has been done on the price of each kilogram of Hydrogen, it is important to evaluate how the future prices look as well. Based on the analysis, the production costs from all types of Hydrogen (coming from both RES and fossil fuels) are going to decline, but not with the same rate. The graph in Fig. 33 shows the trends for all types of Hydrogen: (The International Renewable Energy Agency, 2019)

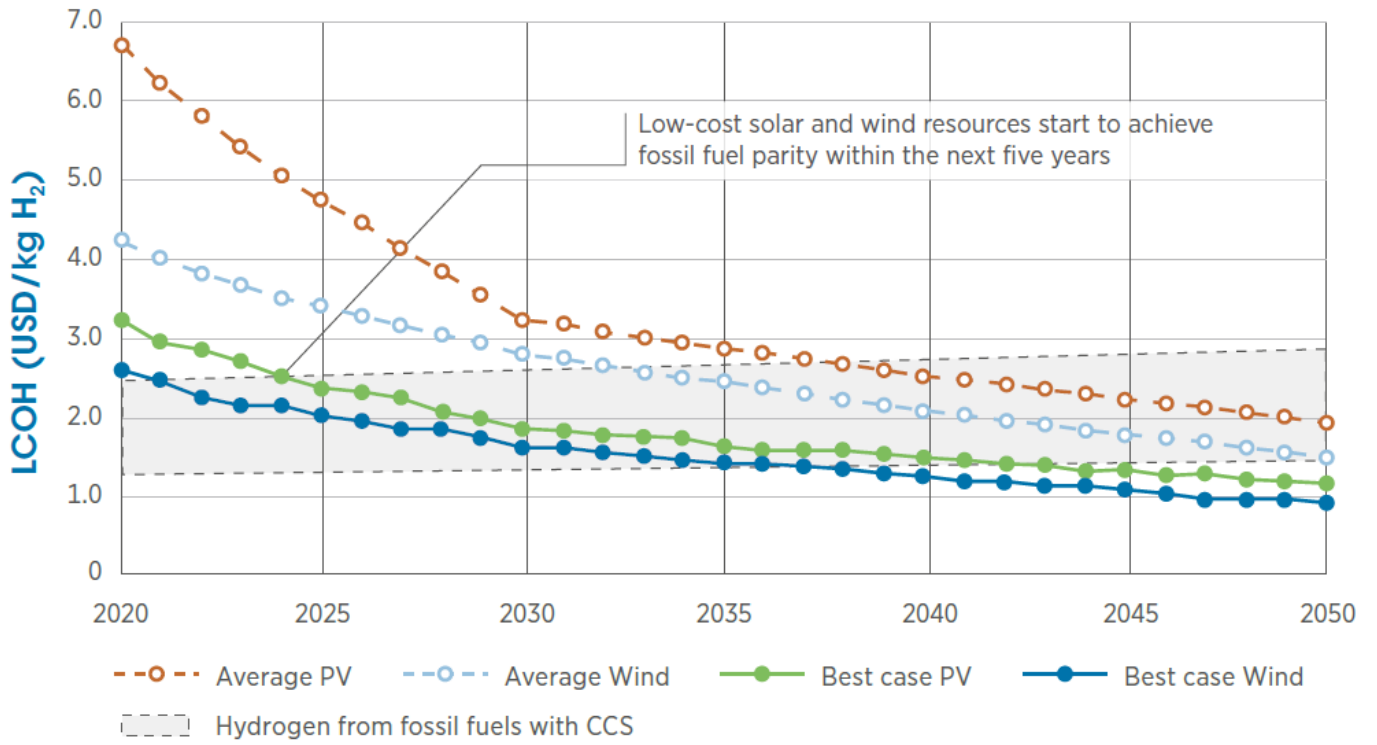


Figure 33 Estimated production cost trends for different production routes in the upcoming years (source: (The International Renewable Energy Agency, 2019))

4 Conclusions

We studied the problem of optimizing the production procedure of the needed Hydrogen for a refueling bus station utilizing a specific configuration. This thesis was investigated the working conditions and economics of this onsite production through electrolysis depending on different optimization objective functions (minimizing the cost, minimizing CO₂ footprint) and under different CAPEX assumption in 5 different models. To model the desired configurations of the Hydrogen production plant, mixed integer programming using CPLEX was chosen.

To conclude the findings on the previous section and summarize them, allocating FCR does not affect the Carbon Dioxide content of each Kg of Hydrogen and also the price of Hydrogen notably. This matter points out that because FCR allocation does not have any added economic value and considering the extra risk of aging that it puts on the equipment, it is recommended that FCR allocation does not take place.

As for the case of France and Germany, the price results are mostly similar (for instance, only 7% difference in the price of each Kg of Hydrogen produced in Model 1) which is due to the similar hourly electricity prices from their markets. On the other hand, the CO₂ content of each Kg of Hydrogen produced in Germany is around 10 times of this number in France. This is due to fact that the average hourly CO₂ content per 1 MWh of electricity in Germany is about ten times of this number in France.

Technology advancements regarding electrolyzers, which result into CAPEX reduction in the upcoming years, is not going to make massive changes in the configuration in terms of electrolyzer and storage capacity used. However, these technology advancements can be impactful for the final price of each kilogram of Hydrogen in the market.

Integrating the electricity coming from renewable energy sources can have several effects on the Hydrogen market. This integration will heavily reduce the CO₂ footprint of each Kg of Hydrogen produced, although it will increase the price distinctly. RES electricity makes of a huge part of the RES Hydrogen price, hence, small reduction in RES price matters and it can contribute to make the RES Hydrogen competitive in the market in the future.

To have the cost of each ton of CO₂ avoided for each Kg of Hydrogen in a competitive range compared to the price of CO₂ allowance in EU Emission Trading System (ETS). In all the cases examined in chapter 3, the cost of each ton of CO₂ avoided for each Kg of Hydrogen is not low. This is another matter to back up the aforementioned point that small changes in the price of RES and also putting incentives in place can help

move towards environmentally responsible Hydrogen production methods to reduce the CO₂ footprint of each Kg of Hydrogen.

As for future work, further studies on the implementation of a cluster of electrolyzers for onsite production, investigation of the electrolyzer's setpoint and its efficiency, and the effect of equipment aging on the results can be discussed in more detail.

Bibliography

- Abad, A. V. (2020). Green hydrogen characterisation initiatives: Definitions, standards, guarantees of origin, and challenges. *Energy Policy*, 138, 111300.
- Agora Energiewende. (2021, 07 16). *Agora Energiewende - About Us*. Retrieved from Agora Energiewende: <https://www.agora-energiewende.de/en/about-us/agora-energiewende/>
- Alighieri, D. (1321). *Comedia*. Firenze: Goose Feather Press.
- AMPL Inc. (2021, 06 16). *WHY AMPL?* Retrieved from AMPL: <https://ampl.com/>
- ATCO Corporate. (2021, 6 13). *ATCO.com*. Retrieved from ATCO.com: <https://www.atco.com/en-au.html>
- Atilhan, S. P.-H. (2021). Green hydrogen as an alternative fuel for the shipping industry. *Current Opinion in Chemical Engineering*, 31, 100668.
- Austria's independent transmission system operator (TSO), APG. (2021, 06 20). *GRID REGULATION - Primary control*. Retrieved from APG POWER GRID CONTROL: <https://www.apg.at/en/Energiezukunft/Glossar/Primaerregelung>
- Bertuccioli, L. C. (2014). *Study on development of water electrolysis in the EU*. Fuel cells and hydrogen joint undertaking.
- Burmistrz, P. C.-G. (2016). Carbon footprint of the hydrogen production process utilizing subbituminous coal and lignite gasification. *Journal of Cleaner Production*, 139, 858-865.
- Dincer, I. (2012). Green methods for hydrogen production. *International journal of hydrogen energy*, 37(2), 1954-1971.
- Droege, T. (2021, 07 02). *What are the colors of hydrogen?* Retrieved from Williams: <https://www.williams.com/2021/04/23/what-are-the-colors-of-hydrogen/>
- ENTSO-E. (2021, 05 10). *ENTSO-E Mission Statement*. Retrieved from ENTSO-E: <https://www.entsoe.eu/about/inside-entsoe/objectives/>
- European Alternative Fuels Observatory. (2021, 07 18). *H2 REFUELLING STATIONS*. Retrieved from European Alternative Fuels Observatory: <https://www.eafo.eu/alternative-fuels/hydrogen/filling-stations-stats>

- European Commission for EU Emissions Trading System. (2021, 09 10). *EU Emissions Trading System (EU ETS)*. Retrieved from European Commission : Energy, Climate change, Environment: https://ec.europa.eu/clima/policies/ets_en
- European Commission for Green Deal. (2021, 05 05). *EU climate action and the European Green Deal*. Retrieved from European Commission: https://ec.europa.eu/clima/policies/eu-climate-action_en
- European Energy Exchange AG. (2021, 09 10). *Spot Market*. Retrieved from European Energy Exchange (EEX): <https://www.eex.com/en/market-data/environmental-markets/spot-market>
- Fraunhofer-Institut für Solare Energiesysteme ISE. (2013). *WASSERSTOFF-INFRASTRUKTUR FÜR EINE NACHHALTIGE MOBILITÄT*. Fraunhofer.
- Fuel Cells and Hydrogen Joint Undertaking. (2019). *HYDROGEN ROADMAP EUROPE*.
- Garbarino, G. P. (2020). A study on CO₂ methanation and steam methane reforming over commercial Ni/calcium aluminate catalysts. *Energies*, 13(11), 2792.
- Greene, D. L. (2020). Challenges in the designing, planning and deployment of hydrogen refueling infrastructure for fuel cell electric vehicles. *ETransportation*, 6, 100086.
- Hosseini, S. E. (2016). Hydrogen production from renewable and sustainable energy resources: Promising green energy carrier for clean development. *Renewable and Sustainable Energy Reviews*, 57, 850-866.
- <https://support.microsoft.com/en-us/word>. (n.d.).
- Huang, J. &. (2014). Parametric analysis and assessment of a coal gasification plant for hydrogen production. *International journal of hydrogen energy*, 39(7), 3294-3303.
- Hydrogen Council. (2020). *Path to hydrogen competitiveness, A cost prospective*. Hydrogen Council.
- Hydrogen Europe Intelligence. (2020). *Clean Hydrogen*. Hydrogen Europe.
- Hydrogen Europe Intelligence Department. (2020). *Clean Hydrogen Europe Monitor*.
- IEA. (2019). *The Future of Hydrogen*. Japan.
- IRENA. (2018). *Hydrogen From Renewable Power*. Abu Dhabi: International Renewable Energy Agency.
- ISO. (2021, 07 18). *Gaseous hydrogen — Fueling stations — Part 2: Dispensers*. Retrieved from Online Browsing Platform (OBP) for ISO: <https://www.iso.org/obp/ui/#iso:std:iso:19880:-2:dis:ed-1:v1:en>
- J. Watson, F. Cric. (1953). Molecular structure of nucleic acids: a structure for deoxyribose nucleic acid. *Nature*, 171, 737–738.

- Kakoulaki, G. K.-W. (2021). Green hydrogen in Europe—A regional assessment: Substituting existing production with electrolysis powered by renewables. *Energy Conversion and Management*, 113649, 113649.
- Kramer, G. J. (2006). Clean and green hydrogen. *16th World hydrogen energy conference*. 13-16, pp. 13-16. Lyon: 16th World hydrogen energy conference.
- Kurtz, J. S. (2019). Review of transportation hydrogen infrastructure performance and reliability. *International Journal of Hydrogen Energy*, 44(23), 12010-12023.
- Liu, W. Z. (2021, January). The production and application of hydrogen in steel industry. *International Journal of Hydrogen Energy*, 46(17), 10548-10569.
- Matthew Farmer. (2021, 07 01). *What colour is your hydrogen? A Power Technology*. Retrieved from Power Technology: <https://www.power-technology.com/features/hydrogen-power-blue-green-grey-brown-extraction-production-colour-renewable-energy-storage>
- Navarro, R. M.-S.-G. (2009). Hydrogen production from renewable sources: biomass and photocatalytic opportunities. *Energy & Environmental Science*, 2(1), 35-54.
- Next Virtual Power Plant Operator & Power Trader. (2021, 06 20). *What is Frequency Containment Reserve (FCR)?* Retrieved from next kraftwerke: <https://www.next-kraftwerke.com/knowledge/frequency-containment-reserve-fcr>
- Nikolaïdis, P. &. (2017). A comparative overview of hydrogen production processes. *Renewable and sustainable energy reviews*, 67, 597-611.
- Noussan, M. R. (2020). The role of green and blue hydrogen in the energy transition— A technological and geopolitical perspective. *Sustainability*, 13(1), 298.
- Prometheus. (300.000 BC). *Olympus Patent No. 1*.
- Reuter, D. B. (2017). *New Bus ReFuelling for European Hydrogen Bus Depots*. Echterdingen: Fuel Cells and Hydrogen Joint Undertaking.
- RTE. (2021, 06 20). *RTE in brief*. Retrieved from RTE: <https://www.rte-france.com/rte-en-bref>
- Schmidt, O. G. (2017). Future cost and performance of water electrolysis: An expert elicitation study. *International journal of hydrogen energy*, 42(52), 30470-30492.
- Sharma, S. &. (2015). Hydrogen the future transportation fuel: From production to applications. *Renewable and sustainable energy reviews*, 43, 1151-1158.
- The Council Of The European Union. (2020). *Towards a hydrogen market for Europe*. European Commission.
- The International Renewable Energy Agency. (2019). *HYDROGEN: A RENEWABLE ENERGY PERSPECTIVE*. The International Renewable Energy Agency (IRENA).

- The International Renewable Energy Agency. (2019). *Renewable Power Generation Costs In 2019*. The International Renewable Energy Agency (IRENA).
- The International Renewable Energy Agency. (2020). *Renewable Power Generation Costs In 2020*. The International Renewable Energy Agency (IRENA).
- U.S. Department of Energy. (2021, 08 09). *Energy Systems*. Retrieved from GREET Model: https://greet.es.anl.gov/publication-smr_h2_2019

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List of symbols

Variable	Description
HRS	Hydrogen Refueling Station
FCR	Frequency Containment Reserve
RES	Renewable Energy Source
TRL	Technology Readiness Level
CAPEX	Capital Expenditure
OPEX	Operating Expenditure
PEMEL	Proton Exchange Membrane Electrolyzer
PEM	Proton Exchange Membrane
AEL	Alkaline Electrolyzer
SOEC	Solid Oxide Electrolyzer
SMR	Steam Methane Reforming
PV	Photovoltaic
CCUS	Carbon Capture Usage and Storage
FCEV	Hydrogen Fuel Cell Electric Vehicle
WACC	Weighted Average Cost of Capital

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