Techno-economic assessment on hydrogen energy conversion systems for the Pulp and Paper and Metallurgical industries

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Thesis to obtain the Master of Science Degree in

Mechanical Engineering

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December 2021

Acknowledgments

The development of this thesis, which will result in the conclusion of my Master's Degree, has only been possible to archive with the support I receive. Thus, I would like to acknowledge those who have contributed to this achievement.

First and foremost, I would like to express my deepest gratitude to my mom and dad. Thank you for all of the opportunities you provide me. Your unconditional love and support will always be the foundation of all my successes, and my accomplishments will always be yours too.

I would also like to thank my supervisor, Dr. Rui Pedro da Costa Neto, for all the words of encouragement on the most difficult days, all the knowledge imparted, and the advice given over the last few months, that were essential for the development of this work.

To my incredible friends at IST, who have made these last five years so much more than an academic experience and provided me with memories that I will treasure for the rest of my life. And to my NBIST girls, with whom I have shared the court for the past few years and who have never failed to brighten my day.

I could not help but thank my lifelong confidants, my brother and sister, for all the support and patience. And to my grandmothers, who have always celebrated every little accomplishment of my life with immense pride.

Lastly, to all of my ever-lasting friends and family. I will always be grateful for you.

Resumo

O hidrogénio, um elemento muito abundante, surge como possibilidade de ser um vetor energético relevante para a descarbonização de muitos setores. Ter uma forma de armazenar energia local, sem necessidade de importar combustível, afigura-se uma solução muito apelativa, especialmente para processos industriais que não só podem beneficiar da utilização de hidrogénio como também consomem elevados valores de oxigénio altamente puro, tais como as indústrias de pasta e papel e metalúrgicas. São necessários avanços e escalabilidade das tecnologias do hidrogénio verde, para alcançar a competitividade com os métodos tradicionais, pelo que este trabalho propõe a identificação de variáveis que influenciam o seu custo, como substituto de gás natural. Neste contexto, com o desenvolvimento da economia do hidrogénio verde, e com base nas suposições assumidas neste trabalho, é demonstrado que a substituições do gás natural, por hidrogénio, ainda não é competitiva, considerando os preços atuais. No setor da pasta de papel, os preços da eletricidade necessários para ser alcançada a competitividade, com os métodos de produção tradicionais, teriam de variar entre 33-44 €/MWh, e para a indústria do aço, entre 44-54 €/MWh, em comparação com os 90 €/MWh utilizados como referência. Nas mesmas condições, ao considerar as taxas penalizadoras de emissões, estes preços teriam de aumentar para 236-265 €/$\mathrm{tCO_2}$ para a pasta de papel e 189-281 €/$\mathrm{tCO_2}$ para as aplicações do aço, comparativamente aos 60 €/$\mathrm{tCO_2}$ praticados hoje. Estes projetos têm o potencial de atingir um LCOH de 1,56 €/kg$\mathrm{H_2}$, quando o armazenamento e a compressão não são consideradas. Se existir procura de oxigénio na cadeia de valor, parte deste sub-produto pode ser consumido no local com valor acrescentado.

Palavras-chave: descarbonização; produção de hidrogénio; pasta de papel; aço; energia; análise económica

Abstract

Hydrogen, a very abundant element, has recently emerged as a relevant energy vector for the decarbonization of many sectors. Having a way to store energy locally, without the need to import fuel, seems a very appealing solution, especially for industrial processes that can not only benefit from the use of hydrogen, but also consume large amounts of highly pure oxygen, such as the pulp and paper and metallurgical industries. Advances and scalability of green hydrogen technologies are needed to achieve competitiveness with traditional methods, so this work proposes the identification of variables that influence its cost, as a substitute for natural gas. In this context, with the development of the green hydrogen economy, and based on the assumptions made in this work, it is shown that the substitution of natural gas, by hydrogen, is not yet competitive, considering the current prices. In the pulp industry, the electricity prices needed to achieve competitiveness with traditional production methods would have to range between 33-44 €/MWh, and for the steel industry, between 44-54 €/MWh, compared to the 90 €/MWh used as a reference. Under the same conditions, when considering the penalizing emission rates, these prices would have to increase to 236-265 €/$\mathrm{tCO_2}$ for pulp and 189-281 €/$\mathrm{tCO_2}$ for steel applications, compared to 60 €/$\mathrm{tCO_2}$ today. These projects have the potential to achieve a LCOH of 1.56 €/t $\mathrm{H_2}$, when storage and compression are not considered. If there is demand for oxygen in the value chain, part of this by-product can be consumed on-site with added value.

Keywords: decarbonization; hydrogen production; paper and pulp; steel; energy and economic analysis

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Nomenclature

AEL	Alkaline Electrolysis
ASU	Air Separation Unit
BF	Blast Furnace
BOF	Basic Oxygen Furnace
CAPEX	Capital expenditures
CCSU	Carbon Capture Sequestration and Utilization
CHP	Combined Heat and Power
DRI	Direct Reduced Iron
EAF	Electric Arc Furnace
ETS	Emissions Trading System
EU	European Union
FC	Fuel Cell
GHG	Greenhouse Gas
HHV	High Heating Value
IEA	International Energy Agency
IPCC	Intergovernmental Panel on Climate Change
LCOE	Levelized Cost of Electricity
LCOH	Levelized Cost of Hydrogen
LHV	Low Heating Value
LOHC	Liquid Organic Hydrogen Carriers
NG	Natural Gas
OBF	Oxygen Blast Furnace

OPEX	Operational expenditures
PCI	Pulverized Coal Injection
PEM	Polymer Electrolyte Membrane
RA	Reducing Agent
RE	Renewable Electricity
RES	Renewable Energy Sources
SMR	Steam Methane Reforming
SOEL	Solid Oxide Electrolysis
SOFC	Solid Oxide Fuel Cell

Chapter 1

Introduction

1.1 Motivation

Climate change and environmental degradation are, more than ever, a threat to our planet. In order to overcome these challenges, numerous proposals are being launched. In the light of the Paris Agreement of 2015, it is necessary to invest in the development of sustainable energy technologies in order to limit the temperature increase up to 2℃ above pre-industrial levels, while pursuing efforts to limit it even further to 1.5 ºC [1]. According to the Intergovernmental Panel on Climate Change (IPCC), if we wish to keep global warming below 1.5℃, the world will need be net zero by 2050 [2]. Failure to address the problem of greenhouse gas (GHG) emissions, comprehensively, puts all generations, current and future, at risk.

The European Commission has since adopted the European Green Deal, establishing a strategic approach that places the energy and green transition at the centre of political action with the ultimate aim to reduce $\mathrm{CO_2}$ emissions and transform the European Union (EU) into a modern, resource-efficient and competitive economy, where there are no net emissions of GHG, reaching carbon neutrality by 2050 [3]. Electrification, massive efficiency gains, and behavioral changes all play important roles in achieving these objectives, but the energy sector is confronted with two challenges: first, the global energy demand growth, and second, the rising environmental concerns.

The share of renewable energy in primary supply, worldwide, must grow from 14% in 2018 to 74% in 2050 in the 1.5℃ scenario [4]. European policy framework for the period 2020–2030 promotes increasing the share of renewable energy in the electricity sector to 45% by 2030 (so far, a 30.8% share has been reached [4]). However, renewable electricity alone will never be able to provide all our energy needs, and $\mathrm{H_2}$ will need to play a crucial complementary role, especially in countries with ambitious climate objectives [5]. For this reason, $\mathrm{H_2}$ popularity has been emphasized worldwide, as a competitive candidate for both energy storage, which allows it to be used for other purposes and at times other than immediately after its production, and supply. The macroeconomic (import reduction) and environmental impact will become increasingly important, at least according to the EU's vision (Green Deal), to which

Portugal appears to subscribe (EN-H_2) [6].

Such interest has been emphasized by the EU Hydrogen Strategy announced in July 2020 which aims to use green H_2 (produced from renewable energy) to fulfil up to 14 % of its final energy demand by 2050 [7]. A recent report published by the Hydrogen Council [8], suggests that the 92 companies involved are committed to deploying H_2 as a critical part of the solution to the climate challenge and more than 30 countries have already H_2-specific strategies and road maps, such as Portugal, Netherlands, Germany, Spain and France [6] [9] [10] [11] [12]. While traditional supply activities decline, these companies that deeply rely on the oil and natural gas (NG) want to take part in the change towards technologies such as carbon capture sequestration and utilization (CCUS), offshore wind and H_2 production that are needed to tackle emissions.

H_2, as an energy carrier, is still not competitive, especially green H_2, which production costs need to be drastically reduced in order to meet the established expectations. Even so, it is expected for H_2 to hold long-term promise applications in many sectors including transport, heating, power generation and energy-intensive industries, then forming a bridge between the power sector and industries where the direct use of electricity would be challenging, such as in the production of steel or large ships fuelling and aviation [13]. Whereas for the last couple of years, transport has been at the centre of all developments, the field of applications has recently broadened with much more emphasis on stationary applications in the industry and buildings sector, as well as feedstocks for chemical products [4]. However, the different sectors require a differentiated view, so it is necessary to consider the technological and economical contexts in which H_2 can act as a replacement to the already existing forms of energy and also the potential alternatives to its usage.

According to the International Energy Agency (IEA), it is crucial to decarbonize electricity generation and the industry. The industrial sector has been most difficult to decarbonize, especially due to the lack of clean available alternatives to compete with NG, which is the most commonly consumed gas [14]. NG dependence in the EU reached an all-time high of 89.5% in 2019, up from 83.8% in 2018 [15]. This numbers show that heat and power solutions are not yet fully integrated in the EU. The energy system mostly relies on technologies that convert a specific input fuel - gas, liquid or solid fuels, electricity - into heat, while the power needs are supplied by centralized power plants or decentralized power plants. To achieve deep emission reductions in the high temperature industry, in particular, synergies and interactions among the different energy carriers and energy uses need to be encouraged based on the multi-sectorial coupling, which implies the deployment of technologies that are able to convert between energy carriers and energy storage systems [16].

With the ambition for Portugal to achieve carbon neutrality in 2050, the National Energy and Climate Plan (PNEC 2030) was approved on 21 May 2020 [17]. Transportation and mobility, service and residential structures, industry, waste and wastewater, agriculture, land use, land change, and forestry are all covered by the PNEC 2020/2030. This established a set of ambitious goals in terms of energy and climate for the 2021-2030 horizon, such as the reduction of GHG emissions between 45% and 55%

compared to 2005, the reduction of primary energy consumption by 35% and the increase of the weight of renewable energies in the gross final consumption of energy to 47% [17] [18]. The aim is also to reduce the country's energy dependence from 74,2% in 2019, to 65% in 2030 and to values below 20% in 2050 [17]. To achieve these goals, and in the context of public policy agendas, an emphasis is given on the decarbonization of industry, the promotion of sustainable mobility and energy efficiency [18].

Industrial processes in industries like cement, iron and steel, and ceramics are very difficult, if not impossible, to electrify, both technically and economically. Green H_2 emerges in this context as a possible solution to help achieve substantial reduction of emissions in these sectors. It is a non-polluting fuel gas (its combustion generates only water vapor) that can possibly replace the NG currently used in industry, decarbonizing the respective production processes. Moreover, it can be obtained through the electrolysis of water using renewable electricity in its production, functioning as an inexhaustible fuel that also allows the storage of renewable electricity, giving the network the resilience and reliability that renewable energies alone do not ensure.

Portugal is focused to provide an integrated approach to profound decarbonization pathways for the energy system, driven by a transformation of the industrial sector towards being sustainable, efficient, and a low-carbon economy, the present work seeks fulfilment of this objective and aims to explore the potential use of green H_2 together with highly pure oxygen (O_2) production through electrolysis, by studying the advantages of having a local energy source, with no need to import fuel, especially for industrial processes that not only can benefit from the use of H_2 but also consume large values of highly pure O_2.

This study explores the potential in particular for the pulp and paper and metallurgical industrial sub-sectors and provides insights about the possible applications and benefits, both in economic and technical terms. The added value of this research will be the insights for potential decision-making tools that may be useful to legislators, as well as owners and investors, who wish to stay in business, with the long-term goal of achieving net zero economies.

1.2 Objectives

This dissertation intends to analyze the technological and economic competitiveness of the integration of H_2 in certain industrial sectors, while also exploring the possibilities of having a local energy source and integration of the O_2, produced as a by-product, in operations along the value chain or exploring its possible markets. To achieve the objectives of the present study, the following deliveries are proposed:

- Explore the state-of-art of different green H_2 production technologies, summarizing their working principles and characteristics (costs, efficiencies, competitiveness etc.);
- Explore the state-of-art of the current fossil fuels consumption and energy dependency, in the European and Portuguese industrial contexts, while summarizing the potential applications of H_2

and its importance in this particular sector, as well as the industrial processes, value chains and mature technologies;

- Estimate the levelized cost of H_2 (LCOH) from different scenarios and applications as well as their investment costs, and their final share in the cost of H_2;
- Assess how different variables would affect the LCOH and the viability of the project;
- Understand the interdependence on the feasibility of investments in technical innovations, emission penalties, mass deployment of renewable electricity and technological advances in electrolysis and how they will affect competitiveness with current methods;
- Obtain the values required for these new solutions to compete with current production processes;

1.3 Thesis Outline

Chapter 1 describes the current state of our energy systems, highlighting the importance of decarbonization, which is becoming increasingly important as the year 2050 approaches, with some policy-making and political action aiming for the EU to achieve neutrality targets and become resource-efficient. Improvements in efficiency, a higher share of renewable electricity, and a transition to electrification are the primary steps to take. However, it is difficult to electrify various sectors in our society, both technically and economically. Therefore, the significance of H_2 as the only energy vector capable of decarbonizing our society's difficult-to-abate sectors emerges.

Chapter 2 the state-of-the-art of the different H_2 production technologies and potential markets is covered, providing an overall approach of the competitiveness of this green H_2 in different applications. This section provides insights about the current situation of H_2 as an energy vector, some projects that are being developed and an overview of the potential use of green H_2 in the industry is covered. With the aim established by the PNEC 2030 to reduce the country's energy dependence from 74,2% in 2019, to 65% in 2030, a review of the primary energy sources is given, with an emphasis on NG which represents the biggest share in the Portuguese industrial sector and has been increasingly important over time. Carbon pricing as a decarbonization policy is reviewed, with the recent market trends and future ones covered. Finally, an overview of the manufacturing systems, methods and procedures used in the industries under consideration is provided.

Chapter 3 provides different pathways and scenarios elaborated in order to study the competitiveness of the different application methods for H_2 are defined. In this section, the different pathways are described and the values used for the economic analysis are stated for every case. In addition, the modelling approaches are shown and the way results will be presented is explained. Two scenarios are explored, the first one considers an evolution based on the technology learning curve that H_2 is expected to follow until 2030, according to different studies. The second scenario follows the EU Commission optimistic intentions of increasing the pace of H_2 deployment, both by improving economies of scales but also by boosting innovation.

Chapter 4 demonstrates the work's outcomes in terms of the economical assessment. CAPEX and OPEX breakdowns and a LCOH, are provided. Furthermore, the significance of selling the O_2 generated as a by-product is demonstrated by calculating the projects' NPVs. The impact on emissions, electricity, and NG prices is given and discussed. Significant cost savings are possible in both of the scenarios presented, particularly in Scenario 2, where the achieved LCOH becomes competitive, and all projects begin to become profitable.

Chapter 5 introduces the main conclusions of the study. The dependencies found on the availability of low-cost clean electricity or higher carbon emissions prices are summarized. Also technological advancements in H_2 storage and electrolysis are addressed to be critical to the process's competitiveness. The O_2 market is emphasized as crucial for the projects' attractiveness, as NPV becomes positive in almost all the implementations due to the revenue generated by the commercialization of this gas. Among the studied pathways, if the EU support is successful these industries may have potential green routes profitable until 2050. Because the long-term assumptions contain substantial uncertainty, the absolute outcomes of the models are less useful than the dependencies found.

Chapter 2

State of the Art

2.1 Hydrogen Production

In 2020, the global dedicated $\mathrm{H_2}$ production was around 90 million tonnes (Mt) [19]. As a consequence, $\mathrm{H_2}$ production was responsible for $\mathrm{CO_2}$ emissions of around 900 Mt, equivalent to the $\mathrm{CO_2}$ emissions of the United Kingdom and Indonesia combined [19] [20] .

$\mathrm{H_2}$ can be produced using a variety of energy sources and technologies. It is used in many industrial applications, such as fertilizers, petroleum refining processes, petrochemical, fuel cells (FC), and chemical industries. The primary uses of $\mathrm{H_2}$ are ammonia $(\mathrm{NH_3})$ and oil refining, which account for two-thirds of total consumption, as shown in Figure 2.1, for a breakdown of it use trends.

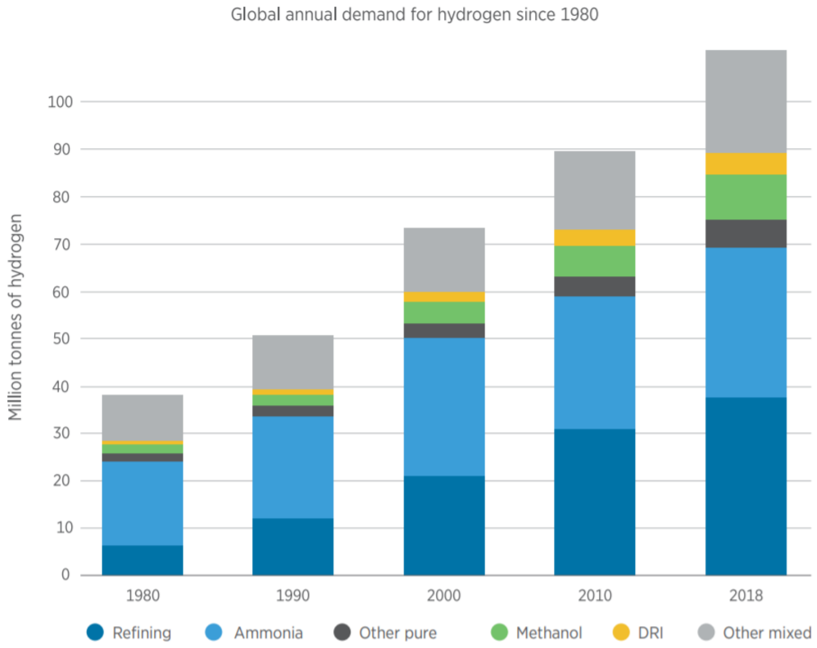


Figure 2.1: $\mathrm{H_2}$ use trends from 1980 - 2018 [21]
DRI stands for Direct Reduced Iron

Its production is mostly still provided by fossil fuels without CCUS, with NG currently being the primary source of production, followed by coal and a small fraction is produced from the use of oil and electricity [19]. Around 96% is generated from NG and coal, and around 4% is generated as a by-product from chlorine production [22]. In order to sort the different $\mathrm{H_2}$ production methods and its carbon footprint, the following nomenclature is used:

Grey $\mathrm{H_2}$ is produced using fossil fuels. It is mostly obtained from NG in an energy-guzzling process that is known as steam methane reforming (SMR). In SMR, steam (water vapour) is mixed with NG, which reacts with the methane ($\mathrm{CH_4}$) and breaks the gas down into carbon monoxide (CO) and $\mathrm{H_2}$ [23].

Blue $\mathrm{H_2}$ is produced using non-renewable energy sources. In this process, fuel is decarbonized with CCUS solutions. Because blue $\mathrm{H_2}$ is not inherently carbon-free, the production requires $\mathrm{CO_2}$ monitoring, verification, and certification [23].

Turquoise $\mathrm{H_2}$ is made from NG pyrolysis, with pure carbon being produced as a by-product that can be sold on the market. It is still in its early stage of development, but it has the potential to become a cost-effective method [24].

Green $\mathrm{H_2}$ is produced using renewable energy sources (RES).

According to the IEA, global $\mathrm{H_2}$ need will expand from 90 Mt in 2020 to more than 200 Mt in 2030, resulting in a rise of the proportion of low-carbon $\mathrm{H_2}$ from 10% in 2020 to 70% in 2030, with around half of the low-carbon $\mathrm{H_2}$ produced coming from electrolysis and the remaining from coal and NG with CCUS (this ratio varies substantially between regions) [20].

Replacing all grey $\mathrm{H_2}$ in the world will require 3,000 TWh/year from renewable electricity which is equivalent to the current demand of Europe [19]. Even so, grey $\mathrm{H_2}$ is expected to progressively become green or blue [25]. In Portugal, $\mathrm{H_2}$ will be produced essentially via alkaline electrolysis using electricity from RES and in 2050, 5% to 8% of total electricity produced will be used for $\mathrm{H_2}$ generation, resulting in a global contribution of 4% in the national final energy consumption [6].

Green $\mathrm{H_2}$, has now become the focus of the strategies to achieve neutrality, due to its decarbonization potential, generated through a eletrochemical process known as electrolysis (Section 2.1.1) powered by RES. However, the role of other low-carbon $\mathrm{H_2}$ production processes such as blue $\mathrm{H_2}$, are not yet ruled out in a primary transition phase, being considered as bridge solutions that can help decarbonize the economies, mostly in regions with low-cost NG resources and available $\mathrm{CO_2}$ storage [3] [26]. In fact, according to a 2020 KPMG supported study [25], blue $\mathrm{H_2}$ remains the most cost effective low-carbon $\mathrm{H_2}$ technology through 2030s, becoming cost competitive with gas only by 2040 (predominantly driven by the carbon price). Inherently, and most importantly, blue $\mathrm{H_2}$ can not be cost competitive with NG in the absence of a carbon pricing, due to the efficiency losses that occur while converting it to $\mathrm{H_2}$.

The cost of $\mathrm{H_2}$ varies significantly from region to region, as it depends massively on the prices and availability of energy inputs. Costs are indeed falling but green $\mathrm{H_2}$ is still 2-3 times more expensive than grey H_2 and further cost reductions are needed [4]. In Figure 2.2, the production costs by technology predicted by the IEA in the Sustainable Development Scenario of 2019 and 2050 are presented.

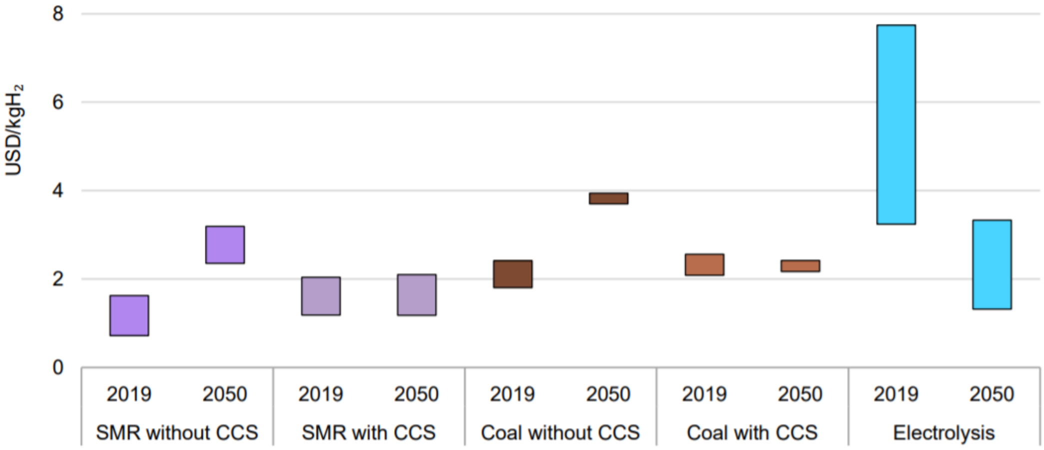


Figure 2.2: H_2 production costs by technology in the Sustainable Development Scenario, 2019 and 2050 [26]

The average cost of producing green H_2 today is around 2.5-5.5 €/kgH_2, according to the European Parliament's H_2-policy released on April 2021 [24], while H_2 produced from NG would cost around 2.0 €/kgH_2, depending on whether CCUS is used or not [27], assuming that the methane prices will not rise. This production process results in emissions of about 9.3 kgCO_2/kgH_2 [24]. Even so, the general cost of clean H_2 production is predicted to drop by up to 70% over the next decade especially due to the deployment of RES, decrease of the electrolyzer CAPEX investment and the increasing price of CO_2 [4]. Consequently, the prices could even drop to 0.8 - 2.5 €/kgH_2 in 2050 – essentially about the same as the cost of the producing with NG with CCUS [20].

Fuel cost (electricity) is by far the largest component in the cost breakdown of producing green H_2 using a water electrolyzer, accounting for approximately 45-75% of production costs [28]. The OPEX is dictated by the availability of a low-carbon electricity source meaning that as investments in wind and solar increase, so does the chance for offtake of low-cost electricity for green H_2 production [28].

For industrial H_2 production, there is significant need of water. The use of sea water can become an appealing alternative in coastal areas. Today the direct use of sea water in electrolysis leads to corrosive damage and chlorine production [29], for this reason several researchers are working in finding efficient ways to use sea water. In this context, water desalination, which is a widely known technology, can be applied in order to obtain useful feedstock with relative low costs. The most common method for purifying the sea water is to use reverse osmosis, demanding 3-4 kWh/m^3 and having costs around 0.63-2.25 €/m^3 of water [30]. However, this aspect is expected to have only a minor impact on the total costs H_2 production which increase by 0,009-0,018 €/kgH_2 [31]

The major problem associated with H_2 gas utilization as a fuel is its unavailability in nature in its molecular form (H_2), as it is mainly found in water molecules (H_2O) and organic biomass, and also the need for inexpensive production methods [32]. Nevertheless, the possibility that H_2 offers to decarbonize specific sectors that would not be easily addressed with direct electrification, the so-called hard-to-abate sectors, accentuates that efforts shall be made in order to foster its adoption in the energy systems.

In the Sustainable Development Scenario, H_2 and hydrogen-based fuels account in 2070 for 13% of all final energy needs. Figure 2.3 shows the global CO_2 avoided emissions in a future where Paris Agreement targets are achieved, where H_2 is expected to tackle around 8% of the total CO_2 reductions in order to achieve net zero targets by 2070 [26].

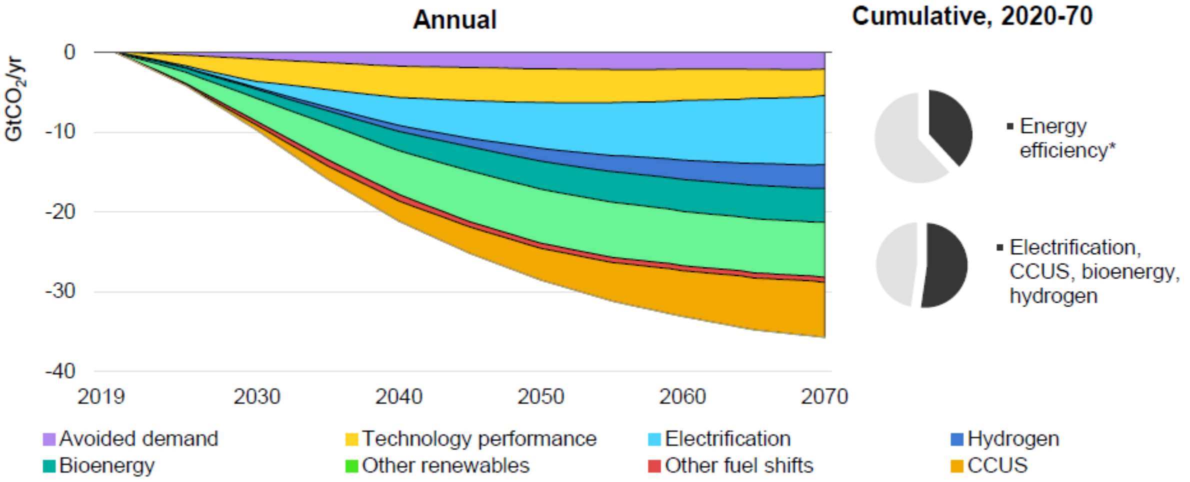


Figure 2.3: Global CO_2 reductions avoided by the adoption of each sustainable alternative related to the stated policies scenario forecast [26]

2.1.1 Electrolysis

Water electrolysis based on electricity derived from RES is the most environmentally friendly process to produce H_2, using the electricity to split water molecules into H_2 and O_2 as by-product. At the moment, it is still a more expensive method than SMR with less than 0.1% of global production in 2020, coming from water electrolysis, mainly due to economic issues [27].

Green H_2 produced from electrolysis depends greatly on the electricity input costs, which may account for 60-90% of the LCOH [27]. Therefore, the declining costs in electricity production using RES (in particular solar PV and wind) and the sustainable environmental targets established are opening a window of opportunity for this technology [27]. Electrolyzers are scaling up quickly, from megawatt to gigawatt-scale, as technology continues to evolve. For instance, several companies have already announced big projects using electrolysis and it is expected that the total capacity of electrolyzers should expand to almost 5000 GW until 2050, from 0.3 GW today [33].

In order to split the water molecule, the reaction has to be induced, which means that energy is required. An 100% efficient electrolyzer would consume around 33.3 kWh or 120 MJ to produce 1 kg of

H_2 [21]. However, the inefficiencies of the used systems increase this value to ranges between 45-55 kWh/kgH_2 depending on the electrolyzer system operation point. With full power, 55 kWh/kgH_2 corresponds to 60% efficiency and with low power, 55 kWh/kgH_2 corresponds to 74% efficiency, depending on the point of operation. The main chemical reaction occurring is:

$$2H_2O \rightarrow 2H_2 + O_2 \tag{2.1}$$

Approximately 9 kg of water are needed to produce 1 kg of H_2 and 8 kg of O_2 [34]. H_2 obtained with this technology has a high purity once the H_2 has been dried and O_2 impurities have been removed, which is a critical characteristic in several applications such as in industrial feedstock and those using low temperature FC [35].

Currently, three water electrolysis technologies are commercially available or under development: Alkaline Electrolysis (AEL), Proton Exchange Membrane Electrolysis (PEMEL), and Solid Oxide Electrolysis (SOEL). The three principles will now be discussed:

AEL is a mature technology that has been undergoing research for decades and great progress has been achieved [34]. For this reason, AEL devices are the most commonly used H_2 generators for industrial-scale applications [36].

AEL is formed by an anode and a cathode, which operate with a liquid electrolyte solution $(KOH/NaOH)$ with 25-30% concentration [37]. Anode and cathode are separated by a diaphragm or membrane with the dual purpose of carrying electric charge between the electrodes and separating the products formed at each electrode [36], which allows the flow of hydroxyl ions (OH^-) formed in the cathode to the anode, in order to obtain H_2 or O_2 at the cathode and anode respectively [21]. The membrane must have high chemical and physical stability with a high ionic conductivity [37].

The process principle of an alkaline electrolyzer is shown in Figure 2.4 and the reactions occurring at each side of the cell are shown in Equation 2.2 and Equation 2.3 .

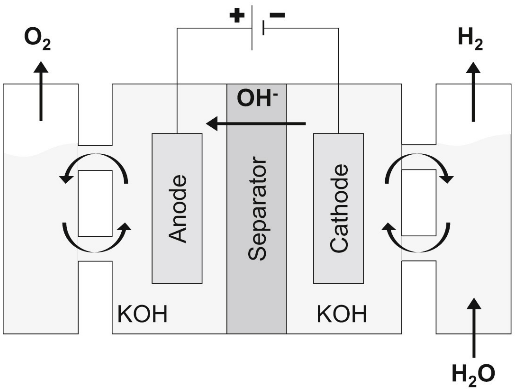


Figure 2.4: AEL process illustration [38]

$$Anode: 2OH^- \rightarrow H_2O + \frac{1}{2}O_2 + 2e^- \tag{2.2}$$

$$Cathode : 2H_2O + 2e^- \rightarrow H_2 + 2OH^- \tag{2.3}$$

These systems have a lower capital cost compared to the other existing technologies and are already considered a well established technology. However, the corrosive environment inside the stack, low current densities (0,2-0,4 A/cm^2) and the required low operational pressures create issues that affect system size and production costs [39]. The start-up time and fluctuations in power input are weaknesses that limit the system efficiency and gas purity [36]. Hence, most development around this technology focuses on improving current density and operating pressure to enable dynamic operations such as working with renewable sources. Currently, alkaline electrolyzers costs are in the range of 450 to 1.260 €/kWe and future cost reductions are expected due to large scale production [36].

PEMEL was idealized in the early fifties and in 1966 started being developed in an attempt to overcome the drawbacks of AELs [40]. In terms of sustainability and environmental impact, PEM water electrolysis is one of the favorable methods for conversion of renewable energy to high pure $\mathrm{H_2}$. They are mainly used for small-scale operations [37].

PEMEL is accrued by pumping of water to the anode where it is spilt into $\mathrm{O_2}$, protons (H^+) and electrons (e^-). These protons travel via proton conducting membrane to the cathode side. The electrons exit from the anode through the external power circuit, which provides the driving force (cell voltage) for the reaction [37]. At the cathode side the protons and electrons re-combine to produce the $\mathrm{H_2}$ as illustrated in Figure 2.5 and by the following equations 2.4 and 2.5.

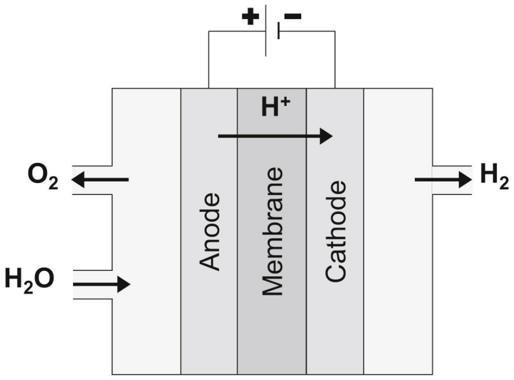


Figure 2.5: PEMEL process illustration [38]

$$Anode : H_2O \rightarrow 2H^+ + \frac{1}{2}O_2 + 2e^- \tag{2.4}$$

$$Cathode : 2H_2O + 2e^- \rightarrow H_2 \tag{2.5}$$

The high current density, cell efficiency, fast response, highly compressed and ultrapure $\mathrm{H_2}$, compact design are its main benefits [37]. This comes at a cost though, with disadvantages such as a higher price of components with expensive catalyst and fluorinated membrane materials and a high complexity due to a high pressure environment requirement [41]. It also has lower durability when compared with AELs system. Therefore, one of the main challenges in this technology is to reduce the production cost and to maintain the high efficiency [39]. As a result, current development efforts are being developed with the aim to reduce the complexity of the system in order to scale it and reduce capital costs through cheaper materials and more sophisticated stack manufacturing processes [42]. Currently, PEM electrolyzers costs are in the range of 990 to 1620 €/kWe.

SOEL is the least developed electrolysis technology. It is not yet widely commercialised, but systems have been developed and demonstrated on laboratory scale and have attracted attention. SOELs use solid ion-conducting ceramics as the electrolyte, enabling operation at high pressure and high temperatures and utilizes the water in the form of steam [43]. The electrical energy is converted into the chemical energy while producing ultra-pure H_2. These types of electrolyzers work under high temperatures (650-1000℃), which offers better electrical efficiency in the H_2 generation ($>$ 85%). As the temperature of the water (steam) increases, so does the kinetics of the reaction, offering a possibility to take advantage of waste heat [40].

Unlike the previously discussed systems, the high temperature at which SOEL systems work, reduces the required electrical energy for the electrolysis process [44]. This is because, based on Gibbs free energy, the minimum required electrical energy is equal to:

$$\triangle G = \triangle H - T\triangle S \tag{2.6}$$

In the above equation, $\triangle$G is the minimum required electrical energy and, as seen in Figure 2.6, it decreases with increasing temperature while total energy demand remains almost constant. On the other hand, electrical and thermal energy are highly dependent upon temperature. When operating temperature of the cell increases, electrical energy decreases and the required thermal energy increases. This behaviour is very beneficial because producing electrical energy is more costly than producing thermal energy [43]. Therefore, by increasing temperature of the cell, one could reduce required electrical energy and instead use more thermal energy to do the electrolysis process [44].

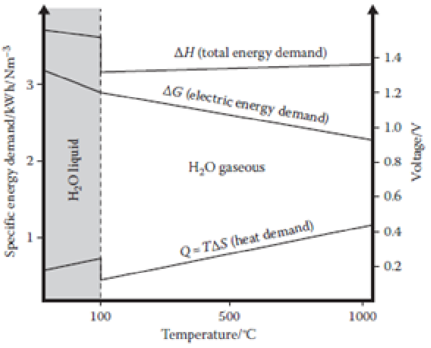


Figure 2.6: SOEL operation principles [45]

Water is fed to cathode and O^{2-} ions are transported to the anode side through the electrolyte while H_2 is produced at the cathode side. The reactions at the electrode are as indicated in Equation 2.7 and

2.8. The process principle is shown in Figure 2.7.

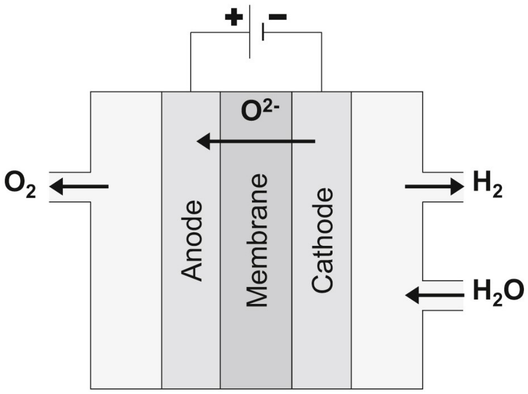


Figure 2.7: SOEL process illustration [38]

$$Anode : O^{2-} \rightarrow \frac{1}{2}O_2 + 2e^- \tag{2.7}$$

$$Cathode : H_2O + 2e^- \rightarrow H_2 + \frac{1}{2}O_2 \tag{2.8}$$

The main advantages of this system are low material cost, a possibility to operate in reverse mode as a FC or in co-electrolysis mode producing syngas from water steam and $\mathrm{CO_2}$ and its high electrical efficiency [46]. A key challenge and one of the main disadvantages is the rapid material degradation as a direct consequence of high operational temperatures [38]. Ongoing research is focused on stabilizing existing component materials and also developing new materials. Furthermore, research is being conducted to try and bring down the operating temperature to enable commercial operations [46]. Currently, SOEL electrolyzers costs are in the range of 2520 to 5040 €/kWe [43].

SOEL plays a minor role as it is still in an early stage of development, whereas AEL and PEM are well-established technologies up to the megawatt scale and commercially available [47]. Gaps in cost and performance are expected to narrow over time as innovation and mass deployment of different electrolysis technologies, drive convergence towards similar costs. The costs could be cut by more than 50% in the long term [32], due to larger scale of the manufacturing processes and optimization of these. In many cases, government subsides should start to create economies of scale that will drive down costs and will help to scale up the supply chain of the electrolyzer industry.

The high heating value (HHV) of $\mathrm{H_2}$ is frequently used to calculate electrolyzer efficiency. However, in some circumstances, it may be more convenient to calculate the electrolyzer's efficiency coefficient using the LHV. In an alkaine and PEM electrolyzer, the water is in the liquid state, so the correct way of calculating the efficiency should be based on the LHV [48]. According to the European Commission [49], for electrolysis systems, the aim is to report system energy efficiency on LHV, which will be the case for the development of this dissertation. In the following Table 2.1, a quantitative comparison of the different electrolysis technologies is presented alongside with their technological and economic characteristics. In Tables 2.2, 2.3 and 2.4 are the projections for the evolution of these technologies.

Table 2.1: Main characteristics and proprieties of electrolyzer systems today [36] [37] [40] [49] [50] [47]

	AEL	**PEMEL**	**SOEL**	**Unit**
Electrolyte	Aq. potassium hydroxide	Polymer Membrane	YSD	
Cathode	Ni, Ni-Mo alloys	Pt, Pt-Pd	Ni/YSD	
Anode	Ni, Ni-CO alloys	RuO2, IrO2	LSM/YSZ	
Current Density	0.2-0.4	0.6-2.0	0.3-2.0	A cm^{-2}
Operating Temperature	60-80	50-90	500-1000	C
Operating Pressure	1-30	15-30	$<$30	bar
Stack Lifetime	$<$90000	$<$90000	$<$40000	hour
System Lifetime	20-30	10-20	-	year
Efficiency (LHV)	63-70	56-63	74-81	%
Cold Start Time	$>$15	$>$10	$>$60	min
Gas Purity	$>$99.993	99.999	99.999	%
Maturity	Mature	Commercial	Demonstration	
CAPEX	450-1260	990-1620	2520-5040	€/kW
OPEX	3	1.5	-	% of CAPEX

Table 2.2: AEL production pathways cost and properties projections [49]

AEL	Today	2030	2050	Unit
Efficiency	63-70	63-72	70-80	%
Stack Lifetime	50-90	73-100	100-150	thousand hours
CAPEX	450-1260	360-765	180-630	€/kW
OPEX	3	3	3	% of CAPEX

Table 2.3: PEMEL production pathways cost and properties projections [49]

PEMEL	Today	2030	2050	Unit
Efficiency	56-63	61-69	67-74	%
Stack Lifetime	30-90	60-90	100-150	thousand hours
CAPEX	990-1620	585-1350	180-810	€/kW
OPEX	1.5	1.5	1.5	% of CAPEX

Table 2.4: SOEL production pathways cost and properties projections [49]

SOEL	Today	2030	2050	Unit
Efficiency	74-81	74-84	77-84	%
Stack Lifetime	10-30	40-60	75-100	thousand hours
CAPEX	2520-5040	720-2520	550-900	€/kW
OPEX	-	-	-	% of CAPEX

2.1.2 Oxygen as a by-product

O_2 is produced as a by-product of several industrial processes [51]. This substance can help to optimize industrial performances, such as in combustion, gasification processes, process heaters, industrial fermentation and boilers to enhance productivity [52].

As previously mentioned, 9 kg of water produce 1 kg of H_2 and 8 kg of O_2 at standard conditions of 25 ℃ and 1 atm [52]. This presents an opportunity to use this O_2 commercially, by selling the by-product to the industries that inevitability need it, reducing the cost for H_2 production by electrolysis technology, thus helping to bring down the capital costs of electrolysis.

The cost of producing this substance for different purposes such as medical and industrial is high, which makes it an expensive chemical, therefore affecting the growth of its market. Selling prices of O_2 are difficult to access and vary according to literature, depending on proprieties such as purity and final uses. The price range is usually between 0.85-1.10 €/kgO_2 in Portugal for medical purposes and 0.10-0.30 €/kgO_2 for industrial purposes [53] [54].

The global industrial O_2 market size is expected to gain market growth in the forecast period of 2020 to 2025, with a compound annual growth rate (CAGR) of 6.5% according to [55]. Some of the applications where O_2 is used are shown in Table 2.5.

Table 2.5: O_2 demand by its purity [56]

Low-purity O_2	- Steel industry - Metallurgical industry - Chemical industry - Cement industry - Sewage treatment - Ozone production - Food packaging in a modified atmosphere
High-purity O_2	- Microelectronics industry - Fibre optic industry - Preparation of breathable atmospheres - Analytical instrumentation
Medicinal O_2	- Hospitals - Home treatments

With the increasing environmental concerns, demand for O_2 is rising for processes glass melting. This substance, when produced in large production rates, uses an cryogenic distillation for Air Separation Units (ASUs) process through liquefaction of atmospheric air and separation of the O_2 by continuous cryogenic distillation [57]. Depending on the unit site and needed O_2 purity, the specific power demand for cryogenic O_2 generation ranges from 200 to 550 kWh/tO_2 [58]. It can be transported either in liquid form or in gas cylinders. The base containers for liquid O_2 are available in various quantities varying from 31 to 41 litres [52], with pressures typically up to 200 bar. Electrolysis of water is another method of producing pure O_2, but it is not yet economical for large volume of production.

Oxy-fuel Combustion

Oxy-fuel combustion is the process of burning fossil fuels with a pure O_2 gas mixture, totally replacing air as the source of oxidizer for combustion, increasing the O_2 content in boiler inlet from the 21% in plain air. Having only O_2 in the combustion chamber boosts combustion efficiency [59]. A schematic of a typical oxy-fuel combustion system can be seen in Figure 2.8.

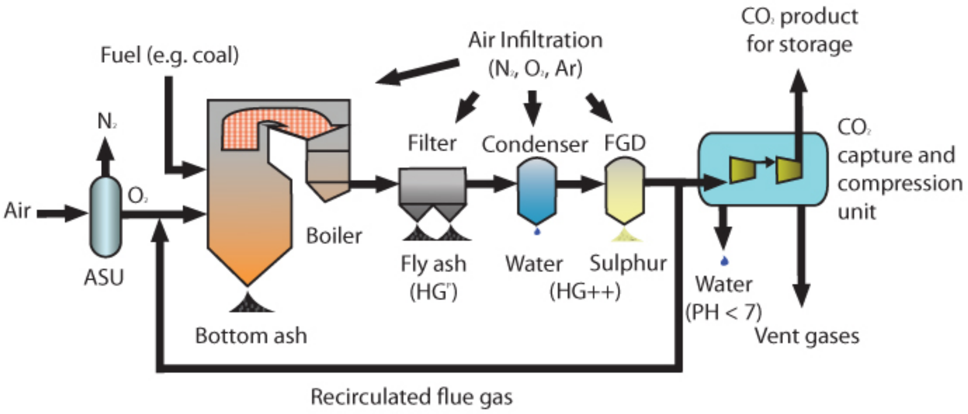


Figure 2.8: Oxy-fuel combustion system [60]

When the nitrogen (N_2) component of air is avoided with the use of O_2, thus not heated, fuel consumption is reduced and higher flame temperatures are possible. Therefore, not only the combustion itself is more efficient but also the heat transfer [57]. This process also increases the thermal efficiency due to the reduced exhaust gas volume, a result that is fundamental and valid for all types of oxy–fuel burners [61]. Additionally, the concentration of the highly radiating products of combustion, CO_2 and H_2O, is increased in the furnace atmosphere. For heating operations, these factors lead to a higher heating rate, fuel savings, lower CO_2 and nitrogen oxide (NO) emissions, which are harmful to both humans and the environment [55] [59].

In order to attain equivalent combustion properties, air-fuel combustion requires less dilution and more fuel [62]. As a result, oxy-fuel combustion has been widely regarded as a viable way to improve the performance of fossil fuel combustion processes while lowering pollution emissions, particularly CO_2. By employing nominally 25% of O_2 (O_2 enhanced combustion), this new technology has been found to boost a boiler's black liquor dry solids burning capacity by around 10% to 20% above the prior capacity [58]. Moreover, according to a study developed by Wu et al., which aim was to investigate the influence of 21–30% O_2 concentration on the heating rate, emissions, temperature distributions, and NG consumption in the heating and furnace-temperature fixing tests, it was found that when the O_2 concentration was increased from 21% to 30%, the heating rate was increased by 53.6% in the heating test and the fuel consumption was reduced by 26.1% in the furnace-temperature fixing test.

Figure 2.9 resulted from a study conducted by the U.S Department of Energy and can be used to calculate energy savings in NG fuel consumption for commonly used process heating applications. O_2 enhanced combustion is used primarily in the glass-melting industry, but other potential applications can be found in Table 2.6.

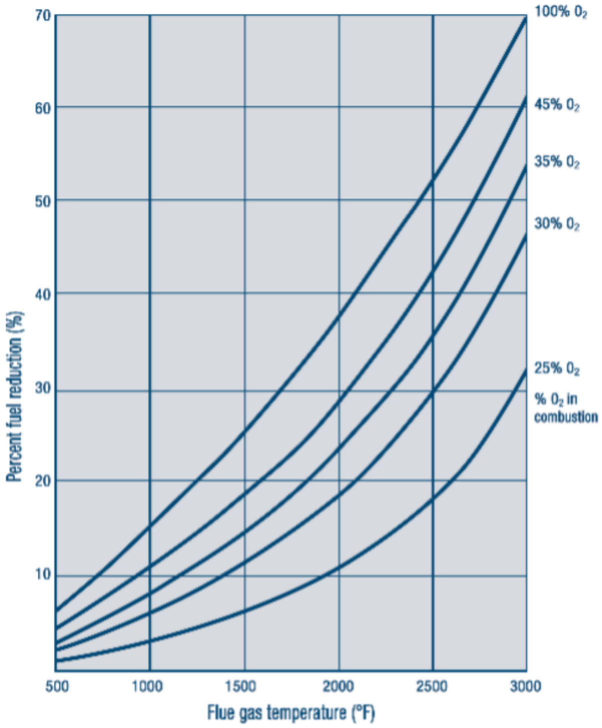


Figure 2.9: Energy savings from O_2 injection - Temperature inside the furnace material [64]

Table 2.6: Potential Applications for Oxygen-Enhanced Combustion

Industry	Applications
Steel	Reheat, soaking pits, ladles
Aluminium	Melting
Copper	Smelting and melting
Glass	Melting
Pulp and Paper	Lime kilns, black liquor boilers
Petroleum	Process heaters, crackers
Power	Production Coal-fired steam boilers
Chemical	Sulphur

The major advantages of this process are considered the fact that it produces a highly concentrated CO_2 stream (this makes it easy to further concentrate the exhaust gas to an almost pure stream of CO_2) and capturing can be applied without additional material or solvent, low NOx production and increases both the convective and radioactive heat transfer [59]. The main disadvantage of this process is requiring approximate pure O_2, which may result from electrolysis. Therefore, as oxy-fuel combustion offers a greater potential for integration with the major emitters of CO_2, such as power plants or the cement sector [55], this shows the relevance it can have in the electrolysis by-product market.

2.1.3 Coupling with Wind/Solar

The Portuguese Renewable Energy Association (APREN) data shows that from January to May 2021, from all the electricity generated in Continental Portugal, 71,6% came from RES [65], with hydro energy dominating (38.4%) followed by wind (23.7%) and solar energy coming sixth in the ranking with only 2.7% [66].

With the arising need to produce green $\mathrm{H_2}$, it is important to understand the technical and economical conditions of coupling electrolyzers to green power sources such as wind and solar. As previously mentioned in Section 2.1, declining costs for solar PV and wind generation are important factors when considering building electrolyzers alongside RES as they may become a low-cost supply option for $\mathrm{H_2}$. The levelized cost of electricity (LCOE) of solar PV has fallen 85% since 2010, onshore wind at 56% and offshore wind at 48%, while the LCOE of more mature technologies such as biomass, geothermal and hydropower has remained stable [65] [67], even after taking into account the transmission and distribution costs of transporting it from remote locations to the end users. When wind and solar are abundant, electrolyzers can use some of that energy to create $\mathrm{H_2}$, which can be stored or converted into $\mathrm{H_2}$ carriers (see Section 2.1.4) and previously transported. The storage and later use of the energy generated by the RES, enabling the control of the energy supplied at any moment independently of the strength of the wind or solar radiation, is a very attractive option.

Solar may become the largest source of low-carbon electricity capacity by 2040 [68]. Solar PV energy has gained attention due to the fact that it does not emit pollutants and does not jeopardize the appropriate forest management necessary for carbon storage as happens with the use of biomass for burning, it does not have noise problems nor location requirements as demanding as wind energy and, above all, it has the lowest costs, not implying extensive maintenance. Solar projects now offer some of the lowest cost electricity ever seen being even cheaper than new coal [27]. In Portugal, the global weighted-average LCOE of utility-scale PV plants declined from 0.270 €/kWh in 2010 to 0.049€/kWh in 2020 [67]. However, the biggest limitation is that they depend on solar radiation and therefore, energy demand cannot always be provided since its power production rate change with periods.

Solar energy represented only 2.7% of the generated electricity in May in Portugal [69]. This number has remained relatively unchanged since at least 2019 [65]. Portugal is one of the countries in Europe with the highest incidence of solar radiation. The average annual number of hours of sunshine is approximately 2500 hours (varies between 2200 and 3000 hours in mainland) [69], which makes it a great candidate to lead in the field of this technology. However, Portugal still doesn't take fully advantage of the potential of this technology, considering all the sunny days it benefits from. In comparison, Germany, which does not have this benefit, at least like Portugal (this number is between 1200 and 1700 hours), has 4.8 GW of solar energy installed, being the largest solar energy market in Europe [69]. According to the PNEC 2030, a total installed capacity of 2 GW operating in 2020 was predicted. However, the current installed capacity is of 1.03 GW.

Electrolysis systems are mostly expected to be installed onshore/inland. **Onshore wind** is a proven, mature technology with an extensive global supply chain and offshore wind is also expected to grow rapidly as for 2021. It is predicted a further worldwide acceleration worldwide of wind additions to 68 GW (7.3 GW being offshore) [70] [71].

In May, wind represented 23.7% of the total electricity produced in Portugal. A total of 256 parks (237 in mainland, 9 in R.A Açores and 10 in R.A Madeira) are installed with a capacity in onshore wind farms of 5.4 GW [72]. Most of the Portuguese wind capacity is located in the north-northeast districts. Viseu is the district with the largest installed capacity, followed by Coimbra, Vila Real and Castelo Branco [71]. The central region is responsible for around 48% of the national wind power production [72]. Adding the North region, this weight rises to 88%, as it can be seen in Figure 2.10. The installed capacities are 2234 MW in the north, 2613 MW in the centre, 103 MW in Lisbon, 222 MW in Alentejo and 225 MW in the south [72].

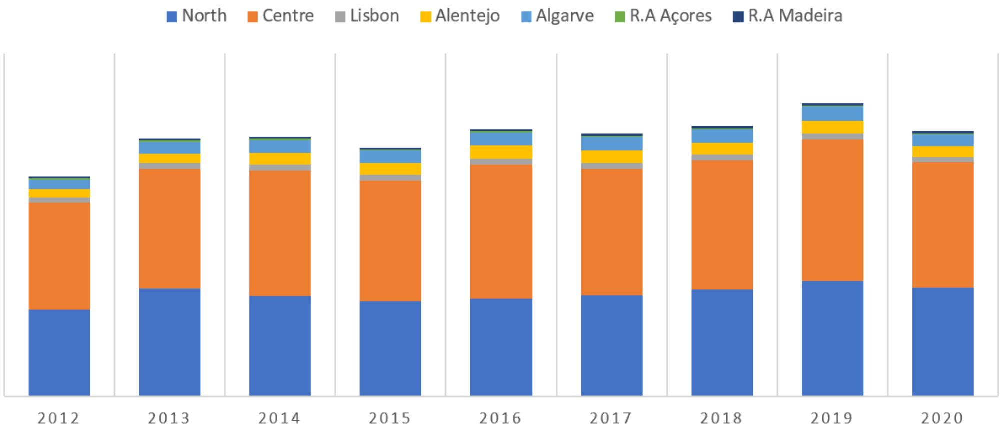


Figure 2.10: Wind power production in Portugal [72]

Offshore wind farms are set for a large growth in the EU, with current policies aiming to multiply its capacity by 4 over the next decade [73]. Having into consideration that today approximately 40% of the world's population lives within 100 km of the coast [31] and that in Portugal 60% of the country's population lives at within 25 km from the coast, this numbers represent an important aspect to be considered in favours when considering offshore wind farms, as RES could power a high share of the world economies without long transmission distances.

Achieving the aimed CO_2 emission reduction goals will require a total capacity of 560 GW of offshore wind by 2040, compared to the 20 GW in 2018 [73], as stated by the IEA. Consequently, a rapid growth in this industry is predicted, with Europe and China as the main leaders. The potential of offshore relies on the possibility of taking advantage of better resources in areas where there are no obstacles and wind energy is more constant. Adding to the list, are technological improvements and turbine sizes (as they can be much bigger in the sea) [31]. These tend to be more expensive and more difficult to build in comparison to onshore, which is a more mature technology and implies less logistics (i.e., weather windows, vessel availability) and specialized work forces [70] [73].

According to IRENA, the global weighted-average LCOE of **onshore** wind fell from 0.071€/kWh in 2010 to 0.032€/kWh in 2020 (56% fell) and the LCOE of **offshore** wind fell from 0.140 to 0.072 €/kWh (48% fell) [67]. Results suggest that from 2023, the cost of electricity will fall to between 0.041 €/kWh and 0.082 €/kWh and can be achieved even in relatively new markets [4]. Despite the development of these new technologies, the price of electricity remains volatile.

2.1.4 Distribution and Transportation

Centralized and decentralized production facilities are expected to play a role in the evolution and long-term use of $\mathrm{H_2}$ as an energy carrier. The different resources and processes used to its production may be suitable to one or more of these scales of production.

$\mathrm{H_2}$ can be produced in small units where it is needed. Decentralized production may be the most viable approach for introducing $\mathrm{H_2}$ in the next few years, mainly because the initial demand will be low. In these situations, such as vehicle refuelling stations, the $\mathrm{H_2}$ production technologies that may offer potential for development are small-scale water electrolysis. Also intermediate-size $\mathrm{H_2}$ production facilities (production of around 5-50 t/day) located in close proximity (40-160 km) to the point of use may play an important role in the long-term [74]. These facilities can provide not only a level of economy of scale but also minimize $\mathrm{H_2}$ transport costs and infrastructure.

Large centralized $\mathrm{H_2}$ production facilities (production of around 750 t/day) that take advantage of economies of scale will be needed in the long term to meet the expected large $\mathrm{H_2}$ demand [74]. These applications will require more capital investment as well as a substantial $\mathrm{H_2}$ transport and delivery infrastructure. Although the importance of these methods is significant in order to improve the transportation of $\mathrm{H_2}$ and therefore $\mathrm{H_2}$ production itself, decentralized production is the most viable approach in the scope of this thesis with the objectives scaled to the specific objectives of the study. Therefore, only a brief inside of transportation methods will be given, as centralized production may be applied in a more future spectrum with transport becoming an important factor.

The production of $\mathrm{H_2}$ is not the only concern, in addition several challenges add up to the $\mathrm{H_2}$ supply chain and its posterior transportation. Any gas must be compressed in order to be transported economically. And this represents the biggest issue with $\mathrm{H_2}$ distribution and why most of $\mathrm{H_2}$ generated in Europe, for example, goes a short distance to where it is consumed, produced on the same site or next door. Three main options exist for $\mathrm{H_2}$ distribution, them being trucking, shipping and the use of pipelines, while using a range of different carriers. Currently, liquid $\mathrm{H_2}$, liquid organic $\mathrm{H_2}$ carriers (LOHC) and $\mathrm{NH_3}$ are the solutions with the most emphasis [25]. As some of these are very innovative processes and the associated technologies and costs are still very uncertain and challenging, they are being explored in multiple pilot studies [75] [76] [77] [78]. However, the decision of which distribution option to pursue will differ from case to case, based on the demand profile and the distance from supply.

Pipelines

H_2 pipeline delivery for distribution is considered a cost-effective way to move H_2 from its production location to end users without major changes, but only at large volumes and long distances. The cost to build a large-scale, dedicated H_2 pipeline system is very high, and completion could take several years. Alternative delivery pathways will be employed during the early market growth phase, such as tank trucks or onsite production, and these alternatives may even endure alongside pipeline delivery in a mature H_2 infrastructure. Transport of H_2 via existing and refurbished gas pipelines are being explored with several pilot studies [79] [80] [81] [82]. The use of the current existent NG pipelines may reduce new infrastructure investment costs and help to accelerate the transition. However, these costs of retrofitting versus building new pipelines depend on a variety of factors such as diameter and pressure, the quality of the materials used, the pipeline's overall condition, the existence of cracks, the social costs of construction.

To move to 100% H_2, most appliances and end-use equipment such as boilers, gas turbines and cook stoves, as well as most of the transmission and part of the distribution system for NG, will need major upgrades and, for now, can only sustain a gradual transition in volumes of 10-20% without major investments [42]. Introducing a global average blend of 15% of H_2 in volumetric terms would reduce CO_2 emissions from gas consumption by around 6% and would significantly boost demand for H_2 and consequently drive down costs [27] [42]. Gradually increasing the share of H_2 that can be accommodated by the gas infrastructure can provide reliable long-term signals for large-scale deployment of electrolysis.

The first pilot project of this kind in Portugal, called the Green Pipeline Project [83], led by Galp Gás Natural Distribuição (GGND), will cost half a million euros to be developed in two years. The project includes the construction of a 1.4 km pipeline that will transport 100% H_2, between the producer, to the mixing point with NG. GGND in Portugal is committed to decarbonizing its entire NG infrastructure, of almost 13,000 kilometres through the injection of decarbonized gases, or low-carbon gases, such as H_2 or biomethane. The project will first inject a small percentage and in a confined network, which serves about 80 customers, mostly residential [84].

Moving these substances across the network at scale is one of the big challenges as we move toward net zero. The work undertaken by such projects will inform how quickly it will be possible to transition to a cleaner, integrated energy system. According to the released report by the Hydrogen Council in January 2021, distribution pipelines most likely will only become relevant near 2040, when demand for H_2 in residential and commercial buildings exceeds the threshold that the blending of up to 20% H_2 into the NG grid can supply [8]. For this reason, national roadmaps are extremely helpful to understand what will be needed for a shift from NG to 100% H_2 in existing infrastructure, what blending levels trigger the need for major investments, and what the whole transition would look like in terms of investments, volumes of H_2 required, timelines and regulatory changes.

H_2 Carriers

Large-scale renewable energy production systems should be located in regions that can efficiently utilize local available renewable energies. Although batteries are capable of storing electrical energy efficiently, they are not cost-effective for large-scale or long-term storage and have material constraints. Subsequently, this energy has to be converted into H_2 energy carriers in synthesis plants on-site. Afterward, the H_2 energy carrier can be transported on ships and stored for on-site, on-demand energy allocation. The use of carriers, this is, molecules that can be combined with H_2 in order to form larger and more stable compounds, can benefit from the already existing infrastructure for transportation and storage. In general, H_2 can be compressed (CH_2), liquefied (LH_2) or blinded into solid or liquid storage materials for later use in turbines, in internal combustion engines (ICEs), in high-efficiency FCs or for chemicals [85], as outlined in Figure 2.11.

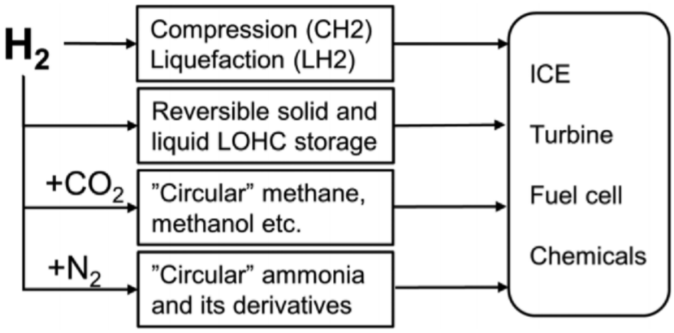


Figure 2.11: Utilisation of the renewable energy through hydrogen storage pathways [85]

When comparing the LHV of H_2 per mole to the LHV of NG per mole, it was found that NG is about 2.6 times as energy dense in molar units [86]. Another way to put it, is that it takes approximately three times as much energy to compress a MJ of heat energy when it is supplied as H_2, as it does when it is supplied as NG. This explains, again, why pipelines are not yet commonly used to transport H_2. Rather, NG is transported to areas where H_2 is required and a H_2 plant is constructed there.

Despite the energy density increase when H_2 is liquefied or compressed, the transportation as a pure molecule implies several challenges. To begin with, its energy density remains low when compared to other fuels or H_2 transportation options. Both CH_2 and LH_2 methods demand a large upfront expenditure because H_2 requires a cryogenic temperature of - 253 ℃ in liquid form or a container capable of enduring pressures of up to 70 MPa when compressed at room temperature [87]. Furthermore, the construction of new infrastructure can be highly costly due to its flammability, diffusivity, and corrosivity/embrittlement on various surfaces. Transporting and managing H_2 as a pure substance is still problematic. This is why H_2 carriers are being investigated in order to enable transport on a big scale. These carriers rely on the reaction of H_2 with molecules to generate larger, more stable compounds with greater transit and storage properties. The H_2 carriers with most emphasis are NH_3, methane (CH_4), methanol (CH_3OH) and LOHC [86].

2.1.5 Competitiveness in the industry

H_2 is already widely used in some industries, but it has not yet realized its potential to support clean energy transitions [27]. Although industry produces about one-quarter of global GDP and employment, it also produces 28% of the world's GHG emissions [22], a number that is expected to climb in 2050 if no action is taken [26]. Emissions from the use of fossil fuels to generate heat can be abated by switching to furnaces, boilers, and heat pumps that run on zero-carbon electricity [14]. However, electrifying heat can involve an expensive change in the production processes and in that specific situations H_2 will have an important role as the only viable option to decarbonize the industrial heating [22].

The most promising ways to reach industrial decarbonization are energy-efficiency improvements, the electrification of heat, the use of H_2 made with renewable electricity as a feedstock or fuel, the use of biomass as a feedstock or fuel, and CCSU. The chosen decarbonization option will vary from facility to facility, even within the same sector, as local factors determine which ones are most practical or economical. According to the IEA, every month from 2030 on, the world will equip 10 new and existing heavy industry plants with CCUS, add 3 new H_2-based industrial plants and 2 GW of electrolyzer capacity at industrial sites [27].

Low-temperature processes such as food and drink are expected to be among the first to electrify, with steel, cement and other high-temperature, energy-intensive businesses trailing behind. For low-grade heat, electrification is the lowest-cost decarbonization option. Therefore, H_2 will likely not play a significant role. However, when it comes to mid and high-grade heat, biomass is an option, but faces supply constraints in several regions. CCSU, for example, only is applicable in regions with access to CO_2 storage. In places where biomass or CCSU are not options, H_2 and electric heating are the only two low-carbon solutions for mid-and high-grade heat. These integrated systems could also help regions increase their energy autonomy and reduce industry-related emissions of fine particulate matter and other pollutants.

CCUS is a technology currently under development and it could offer better efficiencies and costs in the years to come. Once captured, concentrated CO_2 can be transported (most economically by pipeline) to places where it can be used as an input - for example, cured in concrete or as a feedstock to make synthetic jet fuel - or simply stored underground. The most attractive alternative would appear to be storage, given the immense geologic storage reservoir potential and the sophisticated technologies involved. However, because there are no legal incentives to offset the installation of capture technology and a storage infrastructure, storing it at scale is not yet economically viable. Current costs of CO_2 capture range 450 €/tCO_2 when it is extracted from air or 50 €/tCO_2 when a high purity stream is used, typically from power plants, steam reformers or cement facilities [88]. It is believed that CCS technology has an important role to play in enabling a net-zero economy and in the medium term, while awaiting for sufficient amounts of clean energy to produce green H_2.

Carbon pricing is a very effective decarbonization policy, as it makes low and zero carbon energy more competitive compared to high carbon alternatives, encouraging emitters to find and use economical ways of cutting emissions. This is considered to be the most effective way of shifting for a green transition in the industrial sector and will be further discussed in Section 2.1.5.

Figure A.1 summarizes an analysis that assesses in what markets H_2 would be the best solution for decarbonization by 2030 and Figure A.2 provides a timeline on when H_2 is expected to be cost competitive with low-carbon options [25]. These can be found in Appendix A.

2.2 Current state of the industry in Portugal

The energy dependence (ED) is a parameter that characterizes the extent to which an economy relies upon imports to meet its energy needs. The indicator is calculated as net imports of primary energy importations (IMP) minus exportation (EXP) divided by the sum of gross inland energy consumption (GIC) plus international maritime bunkers (IMB),as shown in Equation 2.9 [89].

$$ED(\%) = \frac{IMP - EXP}{GIC + IMB} \times 100 \tag{2.9}$$

Both the Portuguese and the EU-27 energy import dependence are shown in Figure 2.12:

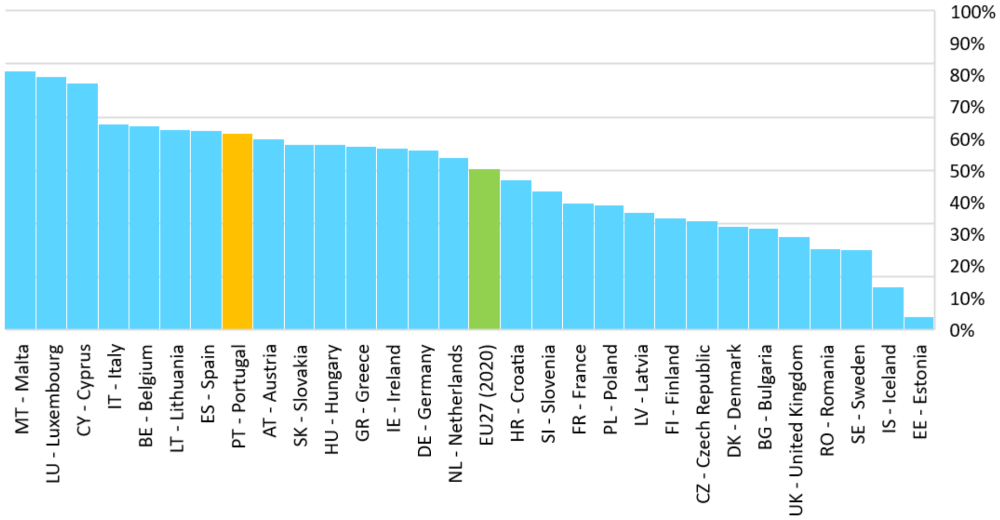


Figure 2.12: Energy import dependency in 2020 [89]

The current value of the EU-27 is 60.6% and none of the countries had a negative energy dependence, which means that all depended on primary energy imports to satisfy their energetic needs [89]. Portugal had the eight highest energy dependence among EU-27. For the last 20 years, Portugal has presented values between 70% and 90%, a consequence of the non-existent sources, such as oil or NG, which account for a large proportion of the overall primary energy consumption. In the last decade, the focus on renewable energies and energy efficiency has allowed Portugal to lower its energy dependence to levels below 80% [18], as shown in Figure 2.13.

The path to carbon neutrality will necessitate a significantly greater use of endogenous RES and

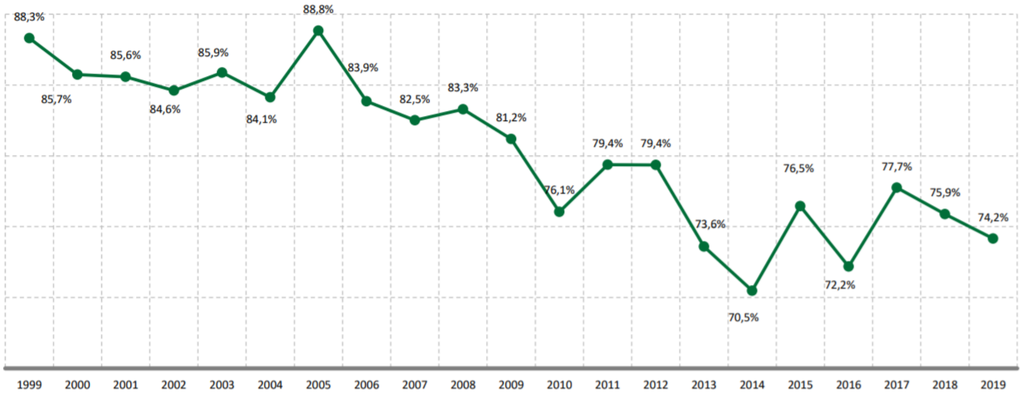


Figure 2.13: Evolution of Portugal's energy dependency [18]

alternative energy vectors that rely on these resources, such as H_2. The national energy system will shift in a more pronounced way over the next decade, from an essentially fossil base to an essentially renewable base by 2050, with positive consequences in terms of reducing energy dependence, which the established aim delivered by the PNEC 2030 is to reduce it to values of 65% in 2030 from the 74,2% in 2019 [17] [18]. Table 2.7 depicts the consumption of the major primary energy sources over the last 20 years in Portugal.

Table 2.7: Primary energy consumption (ktoe) by source [90]

Year	Total	Coal	Petroleum	NG	Electricity (Importer Balance)	Industrial Waste (Non Renewable)	RE
2000	25254	3813	15569	2064	80	87	3641
2005	27087	3349	15877	3761	587	121	3392
2010	23102	1657	11241	4507	226	150	5321
2016	22302	2848	9161	4340	-437	186	6205
2019	22470	1248	9454	5304	292	172	5999

The weight of oil in primary energy consumption has been falling in recent years, as a result of the introduction of NG in 1997 and the expansion and diversity of RES [6]. In fact, while this value decreases, the weight of NG and RE registered an increase, which is consistent with what was previously stated. Because Portugal has no NG resources, all is imported, contributing significantly to our energy dependence. In 2020, Portugal imported 66331 GWh of NG, at a total value of 1.2 billion € [18]. Figure 2.14 depicts the countries from which it was imported. Nigeria was the largest provider, accounting for 54.4% of total imports, followed by the United States with 16% [18]. Around 64% of the supplies were received through a pipeline, while the remaining part, liquefied, was transported to Portugal in ships that unload at the Sines terminal, on the southern part of the country [91].

According to a recent consumption forecast, of April 2021, published by DGEG [92], the industry sector consumes the most NG (about 65%), mainly due to a lack of competitive clean alternatives. This sector is followed by households (23%), services (11%) and the remaining 1% is used in agriculture and transports [92]. As a result, the possibility of its removal from the national grid by 2040 [17] is a concern

Figure 2.14: Imports of NG by country of origin in 2020 [18]

to all of the sector's companies. The consumption across the different industrial sub-sectors is listed in Table 2.8.

Table 2.8: NG consumption (ktoe) by the Portuguese industry [93]

INDUSTRY	2019	2018	2017	2016	2005
Iron and Steel	50.0	48.1	40.9	40.0	41.4
Chemical Petrochemical	175.8	181.3	168.4	147.5	64.4
Non-ferrous metals	16.0	16.8	17.3	16.2	7.6
Non-metallic minerals	456.2	447.8	446.0	438.5	516.6
Transport equipment	25.4	23.2	18.6	16.7	28.8
Machinery	35.5	36.8	32.9	32.5	21.3
Mining and Quarrying	2.6	1.6	1.8	2.5	6.3
Food, Beverages and Tobacco	161.8	152.5	157.4	151.6	66.5
Paper and Pulp	157.8	156.1	158	109.2	38.1
Wood and wood products	9.3	13.3	10.1	7.9	9.7
Construction	14.0	13.6	15.4	15.2	5.8
Textile and Leather	141.4	145.3	137.1	134.3	128.6
Non specified	12.1	10.8	10.2	8.3	20.9
Total	1258.1	1247.1	1214.1	1120.2	956.1

The above presented data shows how NG has been increasingly important over time. In fact, annual consumption has increased in 8 of the 13 industrial activities since 2005. Amongst them, the paper and pulp, chemical and petrochemical, and food and tobacco industries stand out. NG usage climbed around 31.6% between 2005 and 2019, indicating once more its growing importance. One of the goals of the H_2 focus is to replace the consumption of NG and other petroleum derivatives, thereby significantly reducing the import of this source of energy, accelerating the reduction of energy dependence, the energy bill and contributing to the intensification of certain energy consumption, difficult to electrify.

The NG end-consumer price corresponds to the sum of the three main components: the energy and supply component, the network component (transmission and distribution) and the component that includes taxes, fees, levies and charges. This last component includes taxes such as VAT, subsoil occupancy rate, among others. Regarding Portugal, in 2020 the weight of energy for the industry (Band I5: $>$1000000 GJ per year) was 60.8%, the network represented 14.9% and finally, taxes and fees represented 24.3% of the sale price to the final consumer final consumer [18]. Table 2.9 shows how NG prices have been fluctuating for the past 5 years.

Table 2.9: NG price evolution in Portugal with taxes and fees - Band I5 [94]

Year	2016 S1	2016 S2	2017 S1	2017 S2	2018 S1	2018 S2	2019 S1	2019 S2	2020 S1	2020 S2	2021 S1
€/MWh	32.67	26.64	28.37	27.4	27.14	32.54	32.68	28.33	26.17	19.98	23.04

The fact that this gas is a low-polluting option - often viewed by the industry as a medium-term “bridging fuel”, many industries might use it in the process of attempting to reduce some of the emissions and avoid being overly exposed to the growth of emission rates.

Figure 2.15 below depicts how the price of NG has been increasing in the Iberian Gas market during the present year 2021, according to data taken from MIBGAS.

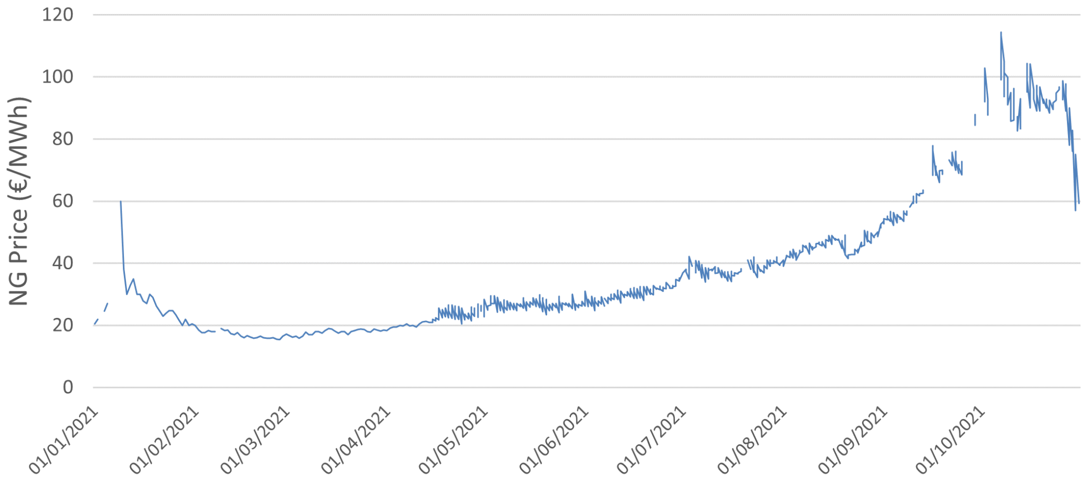


Figure 2.15: NG price trend 2021 (source: MIBGAS)

This graph shows how prices have been fluctuating until October 2021. This increase is a result of three situations: strong diplomatic tensions between Algeria (represent 9.1% of NG imports for Portugal) and Morocco, lower availability of Russian gas (represent 6.9% of NG imports for Portugal) for Central Europe, and increased purchases of NG by emerging countries [95].

Another important factor to consider in the fuels future prices is the carbon pricing. The price of fossil fuels is expected to remain relatively low for the next upcoming years. A carbon price will help to align the market return on clean-energy innovation with its social return by rising relative demand for clean energy sources. This will encourage the improvement of existing technologies as well as the creation of new ones. Low fossil fuel prices do not accurately indicate to markets the true social profitability of clean energy until they are adjusted by an appropriate carbon price.

The European Emissions Trading System (ETS), as explained by the European Environment Agency on its official website, is a mechanism for regulating GHG in activities that are responsible for about 45% of GHG emissions in the EU (such as fuel combustion, mineral oil refining, metallurgy, ceramics or paper pulp, among others) being considered the sector's most important climate change mitigation strategy. In the beginning of 2021, the price of $\mathrm{CO_2}$ was in the range of 20-25 €/$\mathrm{tCO_2}$. Figure 2.16 depicts how the price of emissions have been increasing during the year of 2021.

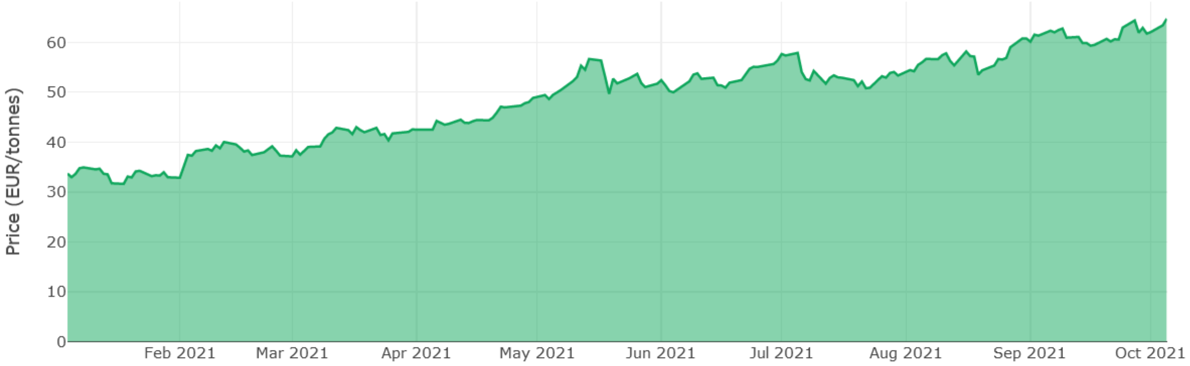


Figure 2.16: $\mathrm{CO_2}$ emission tax trend 2021 [96]

There are expectations of a gradual increase over the next decade [97], and that in the next year, prices could rise up to 100 €/$\mathrm{tCO_2}$, especially after considering that this value has already reached 60 €/$\mathrm{tCO_2}$ in September 2021, rising by approximately 50% since the beginning of the year [98]. This value has reached a long-term escalation towards the levels needed for investments in innovative clean technologies to be triggered. This increase also helps to explain the high prices of NG depicted in Figure 2.15. There is no stipulated trend for the growth of this price, as observed in Figure 2.16, however it is expected that it will grow sharply in the next few years and that after 2030 it will start to have a smoother growth, eventually stabilizing somewhere around the year 2050.

The EU-ETS covers a large amount of the industry sector and, because emissions from sectors covered by the ETS are already regulated by this EU instrument, the others that are not yet covered, such as the foundry industry, in the particular case of Portugal, the value stipulated for the year 2021 was 23.921 €/$\mathrm{tCO_2}$ without the values of the addition on emissions [98], which apply to certain products such as petrol, diesel, gas oil, LPG and NG used as motor or heating fuel, fuel oil, petroleum coke and coal [99], increasing this value. Which means that when the combusted fuel is NG, this value increases to around 38 €/$\mathrm{tCO_2}$.

This emission price, however, may have consequences in other not-so-predictable sectors. Table

2.10 shows how electricity prices for the industry in Portugal has been fluctuating, with no declining or specific trend. This is believed to happen, in part, due to the fact that there is still a lot of electricity produced using fossil fuels that goes to the national grid, requiring a compensation for the emissions penalties in the overall price of electricity.

Table 2.10: Electricity Price Evolution in Portugal with taxes and fees - Band IG [66]

Year	2016 S1	2016 S2	2017 S1	2017 S2	2018 S1	2018 S2	2019 S1	2019 S2	2020 S1	2020 S2
€/kWh	0.082	0.100	0.092	0.089	0.083	0.097	0.091	0.094	0.082	0.083

Portugal is supporting decarbonization through a wide variety of measures. A carbon tax that supports emissions reductions (a fee that has been increasing annually). Coal-fired generation was phased out in 2021. Portugal is further developing its large hydropower fleet, including additional capacity of pumped hydro storage. Currently is an international leader for integration of wind generation, and auctions introduced in 2019 are driving deployment of PV and battery storage and is pushing for better electricity interconnections with the rest of Europe with set ambitious goals for clean H_2 [17].

In 2018, the industry sector represented 30% of the final energy consumption [6]. Consequently, the decarbonization of industry has been a national priority in order to tackle emissions, with a few projects already in discussion, such as the optimization of combustion in industrial units (e.g. cement, incineration of solid urban waste, glass, paper pulp, steelworks, among others) through the injection of locally produced H_2. Therefore, it is important to understand the contribution of each sub-sector of the industry and their potential to reduce emissions in the next years, which is summarized in the following Table 2.11. These values represent the expectations from the RNC2050 [100], the long term strategy for carbon neutrality of the Portuguese economy in 2050.

Table 2.11: Expectation of the evolution of emissions in the industry sector (Mt CO_2) [100]

INDUSTRY	2005	2015	2020	2030	2040	2050	△ 2050/2005
	18.34	12.74	12.46	9.46|8.72	7.34|7.6	4.99|5.11	-72%|-73%
Iron and Steel	0.23	0.25	0.19	0.21|0.22	0.23|0.26	0.25|0.26	14%|10%
Chemical	3.25	1.76	2.13	1.9|1.83	1.75|1.54	1|0.74	-77%|-69%
Paper Pulp	0.66	1.17	1.75	0.72|0.43	0.2|0.18	0.09|0.09	-85%
Food, beverages and other	0.91	0.81	0.74	0.75|0.68	0.54|0.61	0.01|0.01	-99%
Mineral Industry *	10.18	6.83	6.24	4.97|4.7	4.22|4.25	3.21|3.53	-65%|-68%
Electrical and electronic equipment	2.87	1.73	1.23	0.8|0.75	0.33|0.61	0.38|0.45	-84%|-87%
Solvents	0.23	0.19	0.20	0.12|0.11	0.08|0.05	0.05|0.03	-89%|-79%

The main drivers of decarbonization for the sector that will potentially lead to these reductions, will be the improvement in the use of renewable energy (particularly solar thermal and biomass), energy efficiency audits, massive electrification and the emergence of new energy vectors such as H_2 [100]. It is also expected that the penalties associated with the emission of GHG will become increasingly severe so the sectors will have to fight alongside viable energy solutions.

In the spectrum of intentions to drastically, and as quickly as possible, reduce emissions in this sector, the potential to explore the integration of this new energy vector as a potential strategy emerges. The advantage of having a local energy source, with no need to import fuel, can be an appealing solution, especially for industrial processes that not only can benefit from the use of $\mathrm{H_2}$ (including sale to the transportation and industrial gas markets, internal use for combustion replacing NG and blending in the NG network) but also consume large values of highly pure $\mathrm{O_2}$. These gases are already widely used in some industries, so these may have special potential and interest in implementing local production of green $\mathrm{H_2}$. Ensuring carbon-free electricity and sufficient biofuel resources is crucial for limiting GHG emissions in the supply chain. It is therefore important to consider the geographical locations where production takes place because, if necessary, and in order to guarantee electricity from RES, it may be necessary to buy electricity directly from solar or wind farms instead of from the national grid, which becomes more expensive or even impractical in locations far from these sources.

For the purposes of this study, it is critical to comprehend the potential that this energy vector may have in each sub-sector with local production via electrolysis, as discussed further below.

2.3 Paper and Pulp

Today, more than 38.1 million tonnes of paper are produced in about 891 pulp (151) and paper (740) mills in the EU [101]. The Confederation of European Paper Industries (CEPI) [101] is working on a plan for a competitive low-carbon economy in 2050. CEPI targets to cut $\mathrm{CO_2}$ emissions by 80% compared to 1990, lowering them to 12 million tons (10 million tons direct) from 49 million tons (32 million tons direct) in 2015 [102]. As for Portugal, according to Table 2.11, which reflects the RNC2050 intentions/predictions, an 85% decrease of emissions, compared to 2005, is expected.

The paper and pulp sector is considered one of the oldest and most significant industrial sectors in Portugal currently being the third largest pulp producer in Europe, representing 7.2% of the total pulp produced [103]. The value of sales, in 2019, of Portuguese Paper Industry Association (CELPA) members corresponded to 1.3% of that year's GDP [103]. These numbers show the importance this sector has for the Portuguese economy. The process chain, is further bellow described [104]:

Firstly, the mills produce pulp using eucalyptus wood that is collected in certified forests. Then, the wood arrives at the mills in the form of roundwood with bark, roundwood without bark or in chips. In some cases, the alkaline kraft process is used, in other cases the process used is the magnesium sulphite. After a screening process, the chips are fed together with white liquor to a continuous digester. The chemicals dissolve the lignin, the substance responsible for binding the fibres together, freeing them, resulting in the so-called unbleached pulp. After, the raw pulp resulting from cooking is washed to remove residual organic and inorganic waste products resulting from the cooking process and submitted to screening operations, to remove uncooked particles and other impurities. The unbleached pulp is submitted to an $\mathrm{O_2}$ delignification, from which results a yellow pulp which is sent to the bleaching plant.

The process of chemical recovery and energy production varies according to the type of pulp produced. On entering the bleaching plant, the pulp contains residual compounds, which are gradually removed, mostly through chemical reactions with bleaching agents until it becomes a thick, white suspension pulp. Lime is employed as a coagulant in colour removal, a filter conditioner, and, to a lesser extent, a neutralizing agent in the treatment of pulp and paper mill liquid wastes. The paste is then pressed and dried using a system for drying with hot air or steam and the final sheet is cut into smaller pieces, which are stacked in bales that are then sent to the warehouses [104].

Over the years, this sector has adapted to new technologies with the inclusion of cogeneration systems and through biomass. Although the industry has started to reduce its $\mathrm{CO_2}$ emissions, a significant emission reduction opportunity remains. When considering modern pulp production, the lime kiln is typically the only user of fossil fuels during normal operational process, mainly fired with NG.

Lime kilns are critical components of pulp and paper mills because they convert calcium carbonate ($\mathrm{CaCO_3}$), a by-product of the pulping process, to lime (CaO) [105]. The lime then returns to the pulping process, completing the loop used by mills that use the kraft-pulping process. To assist this reaction, the $\mathrm{CaCO_3}$ must be heated to temperatures above 850, usually in the range of 900-1000 °C in order to release $\mathrm{CO_2}$ gas [106]. Rotary lime kilns are commonly employed because they had the maximum thermal efficiency possible at the time, given the production quantities necessary at a normal pulp mill [105]. $\mathrm{H_2}$ can substitute NG without significant modifications in the combustion equipment [58].

Pulp mills could now be ideal sites for $\mathrm{H_2}$ production as they have access to significant energy infrastructure with concentrated demand for a gaseous heating fuel and $\mathrm{O_2}$. Moreover, in some cases, as renewable electricity at the pulp mill is already produced in biomass power plants, meaning that the $\mathrm{H_2}$ produced would already be a green fuel. However, this is not always the case. If this $\mathrm{H_2}$ is then burned in the lime kiln, even if only injected at a small percentage, the main source of fossil fuel based emissions at the pulp mill can be replaced. This would represent a significant decrease in the national NG consumption because, as previously seen in Table 2.8, this sector represents a great share of the yearly total consumption that has been increasing overtime. At some pulp mills, $\mathrm{H_2}$ has already been burned in lime kilns as a supplement to NG. For example, in the Stora Enso Oulu mill in Finland, 2000 tons of $\mathrm{H_2}$ are used annually, according to Kuparinen et al.

There has been an increase in the $\mathrm{O_2}$ demand in this sector in recent years [107], worldwide. Lower production costs, greater paper quality, increased wood mass output, and environmental measures to eliminate chlorine compounds from pulp bleaching operations and replace them with environmentally friendly bleach solutions are the reasons for this. It is used for purposes such as pre-bleaching (also known as $\mathrm{O_2}$ delignification) as it reduces the volume of effluents and the consumption of more expensive chemical bleaches. It is also be used to produce ozone ($\mathrm{O_3}$) as a way to bleach pulp and achieve the necessary level of brightness, or hydrogen peroxide ($\mathrm{H_2O_2}$) that is largely used in cellulose delignification and bleaching, pulp bleaching, and waste paper recycling to reduce or even replace the chlorine dioxide stage [107]. Lastly it can also be used for $\mathrm{O_2}$ enrichment for lime kilns. $\mathrm{O_2}$ also eliminates the drawbacks of buying more lime and the costs associated with dumping excess lime mud. Therefore, this substance, is either produced at the mill or purchased, and this means that having a suitably sized electrolysis plant, a separate $\mathrm{O_2}$ production plant would not be need.

This study is of particular interest given the recent intentions in Portugal of companies linked to paper pulp to explore this market. Altri's (Celbi, Caima and Celtejo) management team has been outlining a plan to attack renewables that extends the group's presence to other clean energy businesses than just biomass, where the installed capacity does not reach 100 MW. This plan should integrate biomass, solar energy and even green $\mathrm{H_2}$ projects.

In fact, in August 2020, Altri group was one of the companies that received a favourable opinion in the list of national projects to be included in a Portuguese application for Important Projects of Common European Interest (IPCEI) status, projects of special interest in the $\mathrm{H_2}$ sector, a kind of certification that will facilitate future applications of these projects (with IPCEI status) to public funding. Altri submitted to the evaluation committee a project for decarbonization of pulp production using green $\mathrm{H_2}$. However, the details of this project are not yet publicly known. Competitor Navigator also had a similar project approved with recourse to green $\mathrm{H_2}$.

The Portuguese P&P sector consists of 4 companies with 6 mills. From the 9 industrial facilities belonging to CELPA represented in Figure 2.17. According to the CELPA, the paper and pulp production capacity and structure are not particularly equal. In Table 2.12 the volumes distribution is presented.

Table 2.12: Distribution of production volumes (kton) [108] [109] [110] [111]

	Company	Location	Pulp	Paper	Tissue
1	The Navigator Company	Cacia	323.9	-	-
2	The Navigator Company	Figueira da Foz	572.7	649.2	-
3	Celulose Beira Industrial (CELBI)	Figueira da Foz	800.0	-	-
4	Celtejo	Vila Velha de Ródão	260.0	-	-
4	The Navigator Company	Vila Velha de Ródão	-	-	106.0
5	Renova	Torres Novas	-	-	35.0
6	Caima Indústria de Celulose	Constância	125.0	-	-
7	The Navigator Company	Setúbal	467.5	646.3	-
8	DS Smith Paper Viana	Viana do Castelo	-	425.0	-

While Celbi, Caima and Celtejo are associated with the production of paper pulp, Greenvolt, that is also a part of Altri, is dedicated to the production of electricity from forest biomass. The operational stations are shown in the following Figure 2.18.

Figure 2.17: Location Pulp and Paper [109]

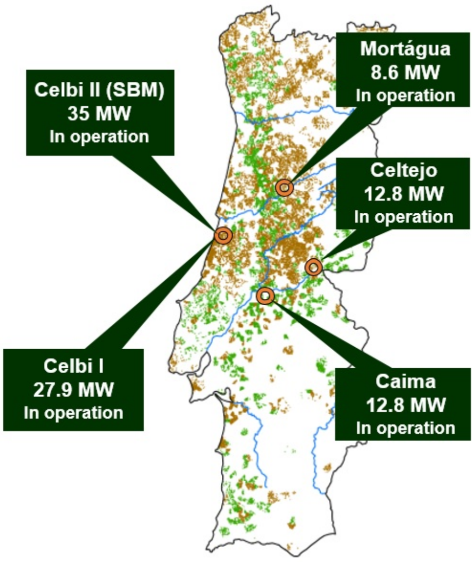


Figure 2.18: Location of Greenvolt's biomass power plants in operation [104]

2.4 Metallurgical

Steel is one of the most important engineering and construction materials, that can be found in many aspects of our lives. However, the industry is now under pressure to reduce its carbon footprint from both an environmental and economic standpoint. $\mathrm{CO_2}$ emissions from iron and steel production account for about 4-5% of total anthropogenic emissions and 22% of the industrial emissions in Europe [112]. Because iron and steelmaking processes rely on the reduction of iron ore, a process that is currently not directly electrified on a large scale and is fuelled mostly by fossil fuels, huge amounts of $\mathrm{CO_2}$ are released into the environment [113]. As the Table 2.11 indicates, this is the one of the most difficult industrial sectors to decarbonize, with lower expectations for mass emission reductions in the near future. Steel has the potential to be made without carbon emissions, but that will not happen without the right policy.

Steel is typically produced in two stages: iron ore is first converted into iron and then, in a subsequent step, the iron is converted into steel. It can be produced using one of two methods: an integrated blast furnace (BF) with a basic $\mathrm{O_2}$ furnace (BOF) process or through an electric arc furnace (EAF). For a more illustrative breakdown, see Figure A.3 in Appendix A.

The conversion of iron oxide to liquid iron is the basic process of BF iron production. It necessitates the use of a reductant to reduce iron oxide, as well as heat to carry out the reduction reaction and melt the smelting products. Pulverized coal injection (PCI), oil, NG, or a combination of these, are the most frequent supplemental reducing agents (RA) today, all of which produce $\mathrm{CO_2}$. The RA reacts with/burns the $\mathrm{O_2}$ to mainly produce CO and heat. The CO reduces the iron ore to metal iron, producing $\mathrm{CO_2}$. The BF gas exits at the top of the furnace, while the molten metal and slug are both expelled at regular intervals through the bottom. Later, the BOF (the most common process for producing steel) is the process of refining iron from the BF into steel with the injection of high purity O_2 at twice the speed of sound [114]. The high-carbon hot metal generates a slag, which eliminates undesired impurities such as carbon, silicon and phosphorus, resulting in liquid steel.

Instead, EAF manufacturers use cold steel scrap as their primary raw material, making it one of the world's largest recycling processes. Electrical energy is supplied via the graphite electrodes and heat generated by this powerful electric current, melts the steel scrap [114]. It is predicted that EAF-based goods will grow their market share in the future, as EAF remains the most feasible short-term approach to address the pressure to decarbonize. However, even though major locations are expected to increase their scrap utilization over time, the rate of change will be largely controlled by scrap availability [113]. This technology is heavily reliant on the availability of end-of-life steel, reason to support other advancements in steelmaking and not focusing only on EAF to address the decarbonization challenge. It should be noted that when converting to EAF-based production, emission-free power will also play a significant role in the future [114].

The direct reduction of iron (DRI) is produced from the direct reduction of iron ore (in the form of lumps, pellets, or fines) into iron by a reducing gas or elemental carbon produced from NG or coal. The ore is heated to temperatures below its melting point. Because the material is 90% to 95% metallized, it can be used as a charge in BF, BOF, and EAF processes [115]. Steelmakers can dilute lower grade ores and lower cost ferrous scrap with DRI to achieve acceptable levels of contamination in the mix. The amount of coke would also be lowered.

Both processes consume large amounts of energy in order to process the materials at high temperatures. If this energy comes from fossil fuels, these furnaces are responsible for significant contribution to CO_2 emissions. As mentioned, the emission footprint of the two major steelmaking processes differ substantially. The values for net energy consumption and specific CO_2 emissions per tonne of crude steel for the three main manufacturing routes (agglomeration and coke production, ironmaking and steelmaking and casting) are summarized in Table 2.13. Indirect emissions are caused by the generation of electricity and imported heat [116].

Table 2.13: Conventional technologies in steel manufacturing plants [113]

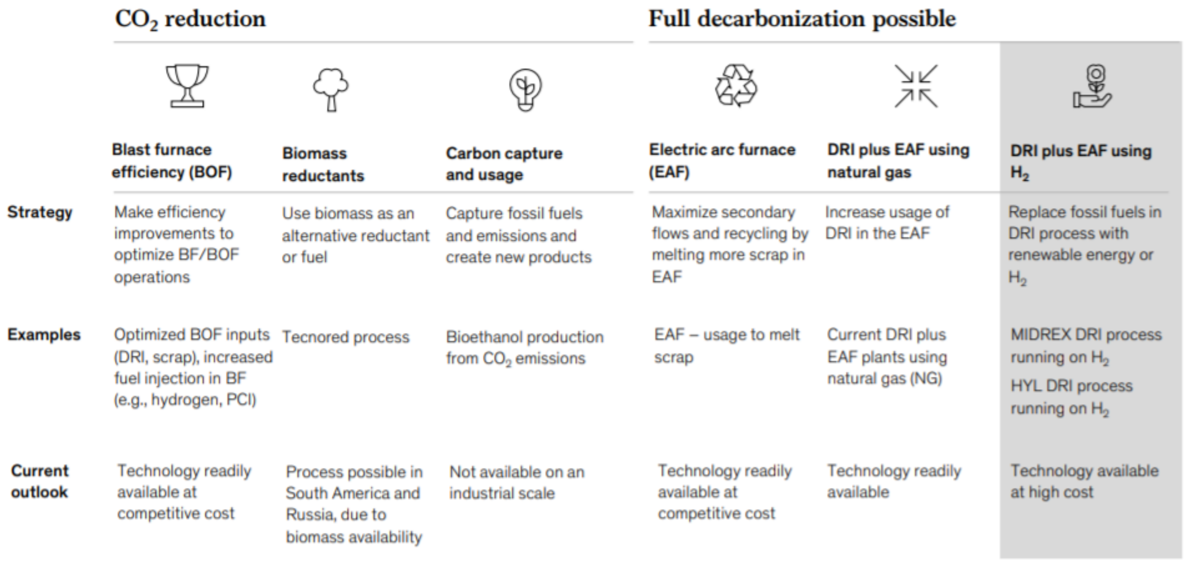
Production route	Energy consumption (GJ/t)	Direct emissions (tCO_2/t)	Indirect emissions (tCO_2/t)
BF-BOF	21-23	1.2	1.0
NG-DRI-EAF	17-22	1.0	0.4
Scrap-EAF	2.1-5.2	0.04	0.3

The competitiveness of the BF-BOF process, also referred to as the primary production route, vs the EAF process varies by region, with factors like scrap supply and fuel costs having a big impact, as shown in the following Table 2.14. EAF steelmaking has a bigger share in places where scrap and/or NG are readily available at reasonable prices, such as North America, Middle East and North Africa. In Europe, the scenario is quite different, with BF-BOF process being predominant. Without demand reduction, because this conventional method accounts for 60% of European steel production [117], substantial emission reduction is only possible through the implementation of new breakthrough technologies.

Table 2.14: Global steelmaking in 2019 (Sources: worldsteel, BHP estimates)

	Crude Steel (Mt)	Global Share (%)	BF-BOF Share (%)	EAF Share (%)	DRI in EAF (%)
China	996	53.3	90	10	1
EU	158	8.5	59	41	6
North America	119	6.4	32	68	14
India	111	6.0	44	56	57
Japan	99	5.3	75	25	0
Korea	71	3.8	68	38	2
Africa and ME	60	3.2	10	90	87

There are a few options to decarbonize the process, as shown in Figure 2.19 [117], including increasing the efficiency of current production methods, recycling steel, CCS (designed to reduce carbon usage by recycling CO gas to the BF for use as reductant rather than exporting it as a combustion fuel) and $\mathrm{H_2}$. $\mathrm{H_2}$ can be used in steel production in two ways: both as an auxiliary RA and fuel in the BF-BOF route ($\mathrm{H_2}$-BF) or as the sole RA in the DRI process.



	CO_2 reduction			Full decarbonization possible		
	Blast furnace efficiency (BOF)	**Biomass reductants**	**Carbon capture and usage**	**Electric arc furnace (EAF)**	**DRI plus EAF using natural gas**	**DRI plus EAF using H_2**
Strategy	Make efficiency improvements to optimize BF/BOF operations	Use biomass as an alternative reductant or fuel	Capture fossil fuels and emissions and create new products	Maximize secondary flows and recycling by melting more scrap in EAF	Increase usage of DRI in the EAF	Replace fossil fuels in DRI process with renewable energy or H_2
Examples	Optimized BOF inputs (DRI, scrap), increased fuel injection in BF (e.g., hydrogen, PCI)	Tecnored process	Bioethanol production from CO_2 emissions	EAF – usage to melt scrap	Current DRI plus EAF plants using natural gas (NG)	MIDREX DRI process running on H_2 HYL DRI process running on H_2
Current outlook	Technology readily available at competitive cost	Process possible in South America and Russia, due to biomass availability	Not available on an industrial scale	Technology readily available at competitive cost	Technology readily available	Technology available at high cost

Figure 2.19: Steel production possible decarbonization strategies [117]

$\mathrm{H_2}$-BF has the potential to cut emissions in both the coke plant and the BF because it uses less coal and only produces water, instead of $\mathrm{CO_2}$, after interacting with iron ore. $\mathrm{H_2}$ injected provides a source of heat and acts as a RA to partially replace PCI into the BF. According to Yilmaz et al., green $\mathrm{H_2}$ injection into the BF–BOF route can only lower emissions by up to 21%, merely reducing $\mathrm{CO_2}$ emissions rather than completely eliminating them.

In the $\mathrm{H_2}$-DRI production step, the process replaces fossil fuels with $\mathrm{H_2}$ produced with renewable electricity. Using H_2 as a RA leads to the formation of H_2O rather than CO_2 as a by-product. With 100% renewable H_2 production, this route can be virtually free of CO_2 emission. However, zero emission electricity is not sufficient for producing zero emission steel. CO_2 emissions are still embedded in, for example, the extraction and generation of iron ore and limestone, in lime calcination and through the addition of carbon as an essential component of steel. It's a tested production technology that allows for nearly emission-free steel manufacture with several publications, such as [118] [119] [120], mentioning this technology as a strong candidate to decarbonize steelmaking. However, similar to scrap, there is not enough high quality iron ore suitable for efficient DRI-EAF production and that supply falls far short of global needs.

The H_2-DRI-EAF strategy has been investigated by several research groups, but only now it is starting to get implemented in an industrial setting, being studied by leading steelmakers such as ArcelorMittal, China BaoWu and ThyssenKrupp Steel and as part of Japan's National COURSE50 (CO_2 Ultimate Reduction in Steelmaking Process by Innovative Technology for Cool Earth 50) program. Steel manufacturer SSAB, mining company LKAB, and energy company Vattenfall [121] are also developing and testing this steelmaking processes in a pilot plant implemented in Sweden, aiming to develop an entire fossil-free value chain for primary steel - the Hydrogen Breakthrough Ironmaking Technology (HYBRIT) (see Figure A.4) [121], where the potential for reduced emissions is significant. In the HYBRIT pilot plant, H_2 produced by electrolyzing water is used to make DRI, also called sponge iron. The DRI is then used as virgin material together with recycled scrap for steelmaking.

Lastly, as mentioned in Section 2.1.2, oxy-fuel combustion technology has been widely regarded as a viable way to improve the performance of fossil fuel combustion processes while lowering pollution emissions, particularly in high temperature intensive industry furnaces. The Oxygen Blast Furnace (OBF) is an oxy-fuel BF. It injects highly O_2-enriched or even full O_2. In theory, the process is similar to the traditional BF, except that a portion of the top gas is recycled back into the furnace, allowing the carbon in the top gas to be reused as a RA. Substituting traditional blast air with near-100% O_2 enriches the BF top-gas in CO_2, allowing for more efficient CO_2 extraction (produces primarily CO_2 and H_2 in the combustion gases, resulting in almost complete CO_2 capture). Secondly, by removing CO_2 from the top gas, a CO-rich gas stream may be pumped back into the BF, allowing more carbon from coke and PCI to be used for reduction and lowering the BF's overall carbon consumption. Overall, the OBF process is an emerging ironmaking process aiming to achieve very low CO_2 emissions, energy and fuel consumption.

Because an extensive amount of H_2 is required to be used as a RA, prolonged electrolysis of alkaline aqueous solution is required; this will be accompanied by a large amount of O_2 that can be integrated in an OBF, apart from being useful for industry and health purposes. Several options will be investigated in this work in order to provide different perspectives for the usage of these components in the steel industry's decarbonization and possible ways to achieve competitiveness with the current methods.

Chapter 3

Implementation

In this section, different study cases will be developed for the application in the paper and pulp industry (2.3) and for the metallurgical sector (2.4). The production of the chemicals will be onsite at the place of consumption in order to minimize transportation and infrastructure costs. The methodology used for the modelling of the study cases is based on different alternatives considered for the $\mathrm{H_2}$ and $\mathrm{O_2}$ production, conversion, utilization, and prices. Therefore, the bibliographic research of annual consumption's, efficiencies of the processes, energy requirements and economic values is the key first step in order to assess the feasibility of the different options. The goal of this study was to look at the technical potential and constraints of incorporating renewable fuel into the above listed sectors, as well as to determine the economic feasibility of the models that were chosen. The techno-economic implications were investigated by looking at the mass and energy balances.

Once the values are known/deducted and the most logical pathways are described, a mathematical tool is developed, that will be further explained in this section, in order to determine economic indicators in function of the previously stated values. Technical parameters (mass, energy intensity, efficiency, and so on) were obtained from relevant literature. For a comprehensive techno-economic analysis, potential future pricing, cost, and income data are studied and incorporated into technical models. These models were made using Microsoft Excel to screen the large quantities of data and determine the variables which offer high potential. These theoretical simulations describe potential development trajectories towards climate-neutral efforts.

3.1 Definition of Assessment Model

3.1.1 Economic Characteristics and Assumptions

To find out the profitability of the case studies, some economic indicators were used to understand the potential of each case. Assumptions were required to be taken in certain circumstances such as this kind of innovative study, where it is challenging to forecast some factors like the degradation of the equipment and its maintenance in the long term.

The determination of the levelized cost of $\mathrm{H_2}$ (**LCOH**) is key in order to know the approximate cost of $\mathrm{H_2}$ production and have an insight of in which markets $\mathrm{H_2}$ could be competitive. The determination of this value, is performed following the equation:

$$LCOH = \frac{\sum_{t=1}^{n} \frac{I_t+M_t+F_t}{(1+r)^t}}{\sum_{t=1}^{n} \frac{E_t}{(1+r)^t}} \tag{3.1}$$

$\mathrm{I_t}$ stands for the expenditures in year t, $\mathrm{M_t}$ accounts for the OPEX in year t, $\mathrm{F_t}$ represents the expenses related with electricity costs, while the total $\mathrm{H_2}$ generation in year t is denoted by $\mathrm{E_t}$. r is the discount rate. Only the $\mathrm{H_2}$ infrastructure is considered in the calculations for LCOH determination.

The net present value (**NPV**) of the project is analysed in order to determine if it makes sense financially, this means the profitability of the project. The Equation used for calculating the NPVs is as follows:

$$NPV = \sum_{t=1}^{n} \frac{CF_t}{(1+r)^t} - Investment \tag{3.2}$$

In order to improve the project's economical values, $\mathrm{O_2}$ revenues are taken into account in the NPV calculation.

The payback period (**PBP)** is calculated to see the amount of time it takes to recover the cost of an investment. The desirability of an investment is directly related to its payback period - shorter paybacks mean more attractive investments. The Equation used for calculating the NPVs is as follows:

$$PBP = \sum_{t=1}^{n} \frac{Investment}{CF_t} \tag{3.3}$$

The Internal rate of return (**IRR**) is seen as the minimum rentability that an investor lending institution aims to obtain from a project, as it is the rate for which the NPV equals zero. This is the rate at which the capital invested equals the present value of net income and is calculated as it follows:

$$0 = \sum_{t=1}^{n} \frac{CF_t}{(1+IRR)^t} - Investment \tag{3.4}$$

With $\mathrm{CF_t}$ meaning the cash flow in year t. The expenses are subtracted from the revenue (Revenue - Expenses = Cash flow) in order to obtain the net income for every period t. The discount rate for the project is considered 7%, which is a common value for renewable energy projects [122]. No financial costs (WACC) due to credit interests or equity raising are considered in the analysis. Income tax is typically around 20% in Portugal, which also corresponds to the average value for the EU countries (20.71% in 2021) [123]. However, in the context of this work, a tax of only 10% is assumed since there is great political will to develop these innovative projects that will need support to get off the ground.

CAPEX: Only the initial investment is considered (electrolyzer) since no other acquisitions are expected to be accomplished (transmission systems, cables, compressors, storage, etc.). There is no requirement for storage if an electrolyzer operates as an online unit and produces $\mathrm{H_2}$ or $\mathrm{O_2}$ directly for use in the combustion processes. This simplifies and secures the process while also lowering the investment cost.

AEL is the most developed water electrolysis technology, as previously seen in Section 2.1.1, and it is also the most used commercially available technology for an industrial-scale electrolysis process, therefore being the chosen method for this study. The estimated plant lifetime (20-30 years), stack lifetime ($<$ 90000 hours of operation), operational time (around 8400 hours per year) are the main parameters to have into account [124]. As mentioned in the state of art of electrolysis process, 33.30 kWh of input power is required for to produce 1 kg of H_2, when considering an 100% efficiency. However, typical commercial AEL electrolyzer system efficiencies are between 63%–70% (Table 3.1) [36]. This means that a standardized electrical consumption in relation to the H_2 production is approximately 47 kWh/kgH_2, the value assumed for modulation of the study cases. For each kg of H_2 produced, 8 kg of O_2 are produced as by-product.

Table 3.1: Electrolyzer proprieties assumed for the base case scenarios [124]

	Current State	Unit
Stack Lifetime	84000	h
Efficiency	70	%
Input Power	47	kWh/kgH_2
CAPEX	900	€/kW

The project's lifetime was considered 10 years due to the annual operational days these industries have and the operational and stack lifetime the electrolyzer presents.

OPEX: Only the expenses associated to normal and predicable activities are included as OPEX in the calculations, these include: equipment maintenance, electricity cost and other recurring expenses. This value is assumed 3% of the electrolyzer CAPEX according to the values currently practiced [47]. Electricity accounts for the largest share in the OPEX costs breakdown [50], so the value used will have major influence on the prospects of the study. The value considered will be a fixed price over the project's 10 years that consists of the average of the values practiced over the last 5 years reviewed in Table 2.10. Other possible operational costs, apart from the electrolyzer purchase, related to the scenarios further described, are specified within the scenario's description.

Regarding O_2, it is assumed that it is sold to an industrial gas provider, which would provide the storage cylinders. Therefore, additional costs due to O_2 needed infrastructure will be non-existent, because O_2 can be liquefied at 50 bar with compression, heat exchange and expansion, in cycle. In the case of H_2, it is mostly directly consumed in the process onsite. When excess gas is produced, it is assumed that it is sold to be injected into the NG distribution system, with no additional costs taken into account.

The methodology used to calculate the revenues coming from the gases sales/purchases considers fixed prices for O_2 and H_2 along the lifetime of the project. For the current study it is assumed, on a first attempt, that the produced O_2 in excess is not sold with medical purposes but to industrial ones. Given the market's volatility and uncertainty, the value considered for NG is the average of the prices practiced over the last 5 years reviewed in Table 2.9. These values will be increased and manipulated, as later explained in Section 3.4.

Table 3.2: Economical values related to the gases and fuels production/consumption [3] [53] [99] [125]

Gases	Prices	Unit
Industrial O_2	0.100 - 0.400	€/kg
Medical O_2	0.850 - 2.500	€/kg
NG	27.864	€/MWh
CO_2 emissions	60	€/tCO_2

3.1.2 Fuel Properties

When comparing the LHV of H_2 to the LHV of NG, it is shown, in Table 3.3, that 1 kg of H_2, in combustion, emits around 2.6 more energy than 1 kg of NG, something to be taken into account when replacing NG as a fuel with H_2. As previously mentioned, the values used for the development of this study are the ones corresponding to the LHV.

Table 3.3: Basic Properties of H_2 and CH_4 [126] [127] [128]

Gas Properties	H_2	CH_4	Unit
Molecular Weight	2.016	16.040	g/mol
Gas Density	0.0808	0.6430	kg/m^3
LHV	120.0	50.0	MJ/kg
HHV	142.0	55.5	MJ/kg
Energy Content LHV	33.3	13,9	kWh/kg
Energy Content HHV	39.4	15.4	kWh/kg
Adiabatic Flame Temperature	2380	2226	K

Table 3.4 shows the CO_2 emission factors of the most important energy carriers and gases that are used in the processes of the industrial sectors in analysis. These theoretical values can be later adjusted for the possible scenarios, depending on the information available.

Table 3.4: CO_2 emission factors of fuels and feedstocks [129]

Energy Carrier/Gases	CO_2 Emission Factor	Unit
NG	56.0	kgCO_2/GJ
Coke	105.0	kgCO_2/GJ
Coal	94.2	kgCO_2/GJ

3.2 Paper and Pulp

Due to the vast amount of information that could be acquired online, the group Altri was used as the starting point for this sub-sector study, beginning with a particular situation and progressing to a generic case. A total of 1.185 million ADt (air dry) of pulp is produced every year and 91% of the electricity used in the process is already green [104]. Moreover, through Greenvolt, Altri increasingly contributes to the electricity production from RES. This green energy, is fully and directly injected into the grid which helps to make the energy mix of the national grid less carbon intensive and more diversified. They inject in the national grid around 973 GWh, annually, of which 733 GWh come from the five Greenvolt's thermoelectric biomass power plants [104]. This means that there is an energy surplus of around 240 GWh that is excess electricity produced at the mills. Consequently, this electricity instead of being sold could potentially be coupled with H_2 production. Another alternative would be to use green electricity from the biomass plants or, instead, buy the excess need for the H_2 production from the grid.

The company produced 444 kton of CO_2 with 31% of the total corresponding to fuels (direct emissions), 5% to electricity and the other 63% to other emissions associated with the value chain (transportation, purchase of services, etc) [104]. These last two percentages account for the indirect emissions. Altri's direct emissions refer, mostly, to stationary NG equipment's, therefore being the only ones taken into account for the calculations.

For the course of this work some assumptions had to be made with estimates. Considering the percentages of pulp produced at each industrial facility, the remaining local consumption of electricity, CO_2 emissions, gases and fuels were deducted from Altri's overall figures with percentages. The prices of NG, CO_2 emissions and O_2 were estimated based on Table 3.2 and the value of the O_2 consumption was assumed based on literature review from Kuparinen et al. (see Section 3.2). The distribution is presented in the following Table 3.5 and Table 3.6 presents information about the energy consumption.

Table 3.5: Altri's gases consumption values in 2020 [104]

	Pulp kton	Emissions ton	NG ton	O_2 ton	Emissions €	NG €	O_2 €
CELBI	800	79008.40	18571.19	16000.00	11250018	6985589	3200000
Caima	125	12345.06	2901.75	2500.00	1757815	1091498	500000
Celtejo	260	46170.54	10852.54	9350.00	6574229	4082204	1870000
Altri	1185	137524.00	32325.48	27850.00	19582063	12159293	5570000

The same principle was taken into account to particularize the electricity production per plant, now considering the electric power installed capacity (see Figure 2.18), instead of the pulp annual production. Table 3.7 shows the distribution of the values. Table 3.8 shows the average price at which the company sells the energy produced to the national grid.

In order to produce 1 ton of pulp, 22 m^3 of water are needed [104], therefore auxiliary equipment costs

Table 3.6: Altri's energy values in 2020 [104]

Energy Consumed	16 945 375	GJ
Electricity	2 423 597	GJ
Steam	14 521 778	GJ
Electricity Sold	3 504 614	GJ

Table 3.7: Greenvolt annual electricity production through biomass [104]

Power Plant	Installed Capacity (MW)	RE Annual Production (GWh)
CELBI I	35.00	264,21
CELBI II	27.90	210,61
Caima	12.80	96,63
Celtejo	12.80	96,63
Mortágua	8.60	64,92
Total	97.10	733.00

Table 3.8: Altri's energy sales in the first trimester of 2021 [130]

Energy sales	179.200	GWh
Energy sales	21.142	M€
Energy price	0.1179	€/kWh

are reduced due to the availability of water treatment equipment used to return water to the environment and by the already existing usage of $\mathrm{O_2}$ in the process [104]. For this study, the cogeneration process and its implications on the steam release for the process with the new implemented green fuel will not be taken into consideration, assuming the same amounts of consumption/production. Only the increase in final water consumption will be taken into account.

It is possible to extract correlations from this particular data and apply it to general situations of other pulp production processes that use similar technology, processes, and fuels. For comparison purposes, the data presented in Table 3.9 have been standardized per tonne of air dried pulp produced (ADt).

Table 3.9: Standardized data for the pulp and paper industry

$\mathrm{CO_2}$ Emissions ($\mathrm{kg_{CO_2}/ADt}$)	NG ($\mathrm{kg_{NG}/ADt}$)	$\mathrm{O_2}$ ($\mathrm{kg_{O_2}/ADt}$)	Electricity Consumed (GJ/ADt)	Water ($\mathrm{m^3/ADt}$)
98.76	23.21	20.00	0.17	22.00

Definition of Assessment Model

Because of its geographical location and the fact that it is the group's largest pulp producer, CELBI was utilized as a model for the construction of this research case. With 350 operating days per year, CELBI's mill produces 800 000 ADt of eucalyptus pulp, which is equivalent to 2285.72 ADt/d. According to the assumptions (see Section 3.2), the amount of $\mathrm{O_2}$ required for delignification and bleaching is 45.72 t/d. The heat demand of lime klin is met by 53.00 t/d of NG. Around 1.11 GWh/d of electricity are consumed, 393.95 MWh/d is excess produced electricity and, therefore, sold to the grid by the mill. Around 1.36 GWh/d of RE are produced at the local biomass plants. These values lead to a release of around 225.74 $\mathrm{tCO_2}$/d.

Three cases of different configuration are studied in aiming to find out how electrolysis integration would affect the main mill mass and energy balances. The scenario without electrolysis is represented by the base case in Figure 3.1.

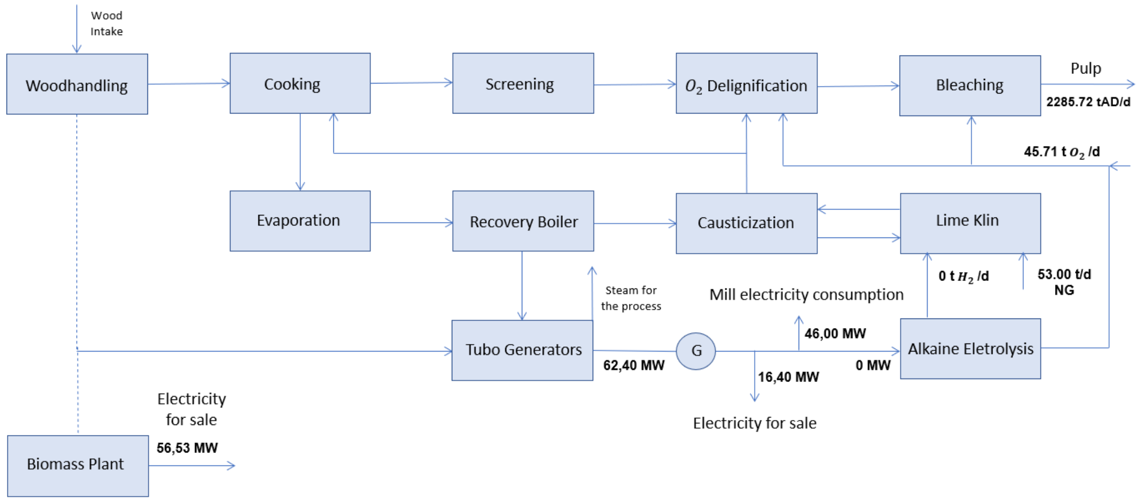


Figure 3.1: Main process flows in the Base Case – No electrolysis

The technological viability of utilizing the energy produced by both the cogeneration system and bio-electricity is examined in the following situations. In the medium run, this would be the optimum scenario, while renewables do not completely dominate the national grid. However, not knowing the cost of producing this electricity due to the lack of information, because the selling price of the energy produced (Table 3.8) exceeds the purchasing price, buying electricity from the grid seems to be the most cost-effective option for the development of the models, from the gathered data. Taking into consideration that this specific facility is located in the central region of the country which, as discussed in Section 2.1.3, has a strong incidence of wind power and that the biomass plants which generate and inject electricity into the grid are located just near the pulp production site, for the development of this work it will be assumed that the electricity purchased from the grid is renewable. It is assumed that a renewable energy guarantee is owned, emitted by the Origin Guarantee Issuing Entity (EEGO).

In the economic evaluation, all electricity is acquired from the national grid, retaining the value of sales that create profit relative to the value at which electricity is purchased. Nonetheless, the scenarios demonstrate how the excess electricity and the electricity produced through biomass at the plant would fluctuate to provide the understanding that these industries already produce excess electricity that does not significantly exceed the electrolyzer's electricity needs.

Pathway A: the electrolysis process is scaled to meet the O_2 demand for the different purposes of its application. H_2 is combusted in the lime kiln to replace as much fossil fuel as possible. Figure 3.2 summarizes this process:

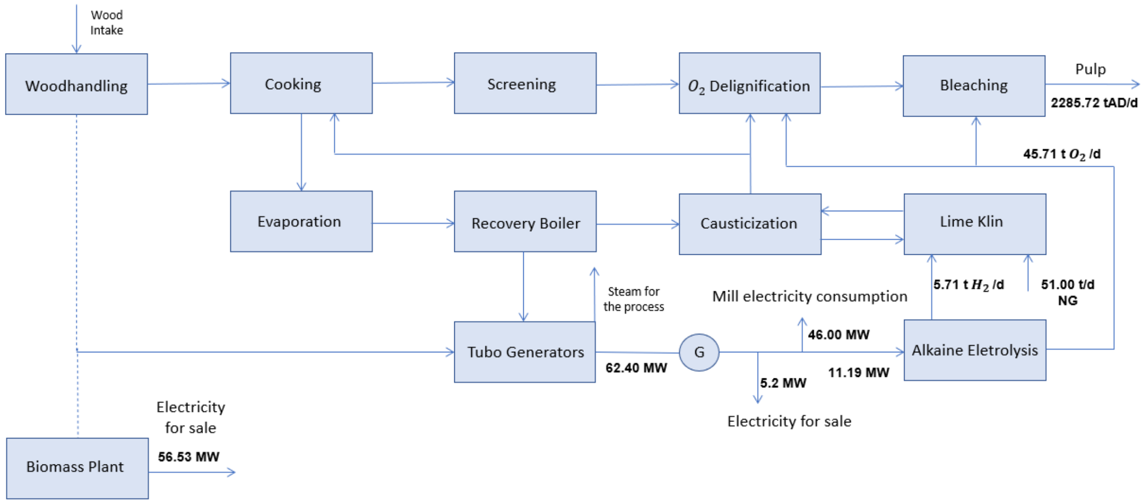


Figure 3.2: Main process flows in the Scenario A – Scaled to meet the O_2 demand

To cover the O_2 demand, the required electrolysis power is 11.19 MW. In the case where the own electricity produced is consumed, this would mean that auxiliary systems would consume 68% of the excess electricity produced at the mill. H_2 production covers 30% of the fuel demand of the lime kiln with the production of 5.71 t/d of H_2, therefore decreasing the consumption of NG to 51.00 t/d.

Pathway B: the electrolysis process is scaled to meet the lime kiln fuel demand. The generated O_2 is firstly used to different purposes of its application and then sold to industrial facilities. Figure 3.3 summarizes this process.

To cover the total fuel demand, the required electrolysis power is 38.69 MW. In the case where the own electricity produced is consumed, this would mean that auxiliary systems would consume 100% of the excess electricity produced at the mill, therefore being necessary to use 39% of the electricity produced at the biomass power plant. H_2 production covers 100% of the fuel demand of the lime kiln. As a by product, 148.57 tO_2/d are produced, the 102.86 tO_2/d overproduced are sold to industrial facilities.

Because it is expected that H_2 will be gradually injected, given the fact that the implications for the combustion of the furnaces/burners are still unknown, the change on H_2 percentages was also explored and the results are sown in Table 3.10. This study will be crucial to understand what will pay off in the future in comparison to the present.

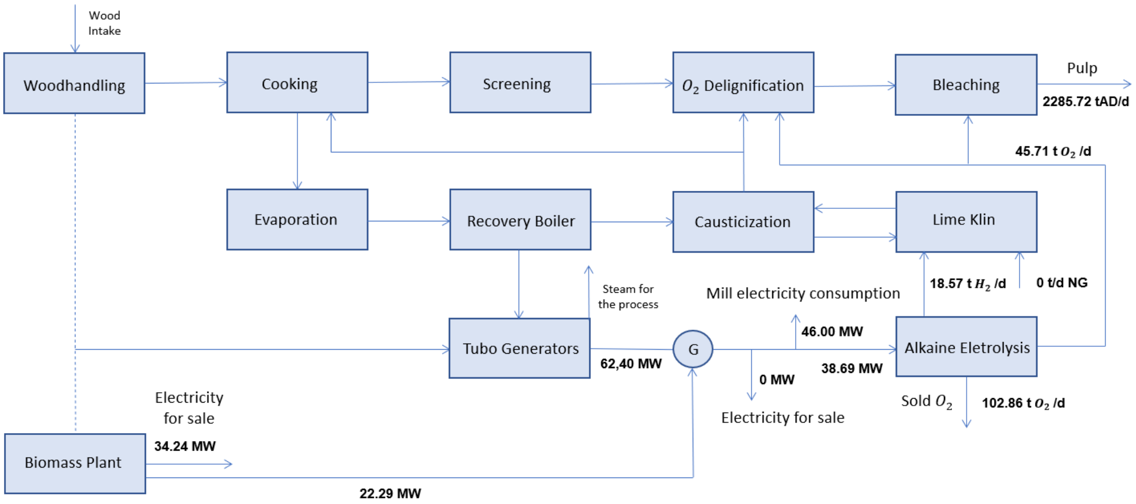


Figure 3.3: Main process flows in the Scenario B – Scaled to meet the fuel demand

Table 3.10: H_2 increment injection share

	20%	40%	60%	80%	100%	Unit
Electrolysis power consumption	5.82	14.55	21.82	29.09	38.69	MW
H_2 production	2.97	7.43	11.14	14.85	18.57	t/d
O_2 production	23.47	59.42	89.14	118.86	148.57	t/d
NG requirement	44.57	31.84	21.22	10.61	0	t/d
Excess electricity for sale	10.58	1.85	0	0	0	MW
Biomass electricity for sale	56.53	56.53	51.11	43.84	34.24	MW
Water flows increase	0.05	0.13	0.20	0.27	0.33	%
CO_2 reduction	19	41	61	81	100	%

In Section 2.1.2, it was explained that in lime kilns and black liquor boilers is possible to explore the potential of burning NG with O_2 enhanced combustion (oxy combustion). Therefore, in the presented bellow scenario, the decarbonization measure is not to replace the fossil fuel itself, but to decrease its consumption by injecting 100% highly-pure O_2 instead of air. According to Figure 2.9, for the implementation case, and considering eventual heat losses and inefficiencies, a 25% decrease in the NG consumption is projected, as temperatures at the lime kiln usually are in the range of 950 ℃ [131], especially because in oxy combustion there is no injection of nitrogen in the furnaces that dilute the gases heat transfers, increasing the overall combustion efficiency.

When NG (CH_4) burns, it combines with O_2 gas to form CO_2 and H_2O. This reaction's equation is:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \tag{3.5}$$

In order to burn 1kg of CH_4, approximately 4kg of O_2 are needed.

For Pathway C, it is desired to investigate markets other than the sale of O_2, as these localized plants may have strong potential to incorporate other markets, such as the sale of H_2 for different purposes.

The achievable H_2 storage densities are limited by the storage pressures: at 100 bar and 20 ℃, the density of H_2 gas is approximately 7.8 kg/m^3 [132]. Because of the low H_2 density, large storage specific volumes are required, resulting in high investment costs [133]. As a result, intermediate storage is not taken into account, and it is believed that this component is injected directly into the distribution network at the pressure it leaves the electrolyzer.

Pathway C: the electrolysis process is scaled to meet the O_2 demand for both the different purposes of its application and for boosting the combustion at the lime kiln with the O_2 enhanced combustion. The H_2 produced is sold for the calculated LCOH. Figure 3.4 summarizes this process:

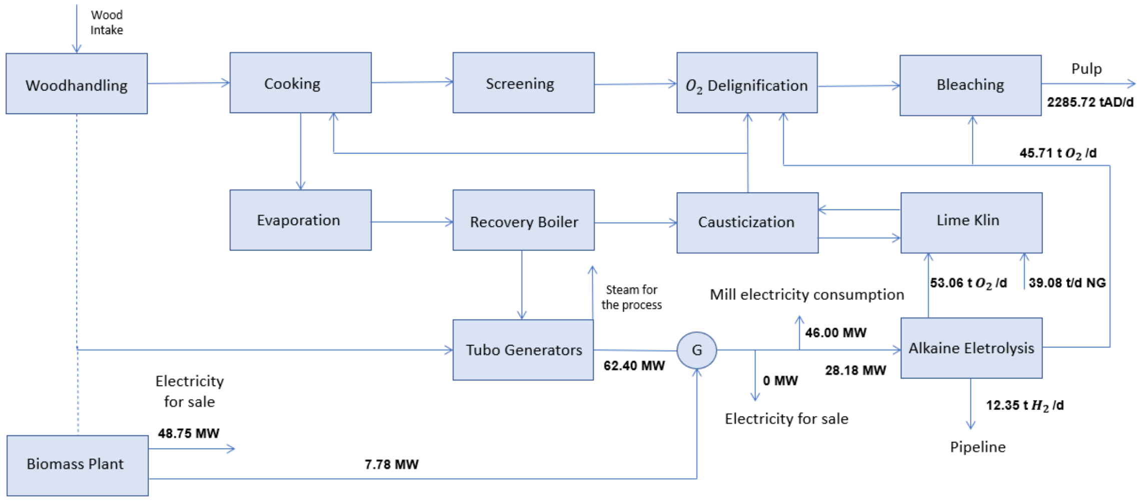


Figure 3.4: Main process flows in the Scenario C – Scaled to meet the O_2 demand with O_2 enhanced combustion

To cover the total O_2 needs, the required electrolysis power is 24.18 MW. In the case where the own electricity produced is consumed, this would mean that auxiliary systems would consume 100% of the excess electricity produced at the mill, therefore being necessary to use 14.5% of the electricity produced at the biomass power plant. To burn the NG in an oxy-fuel combustion, 53.06 tO_2/d are needed to be injected, consequently decreasing by 25% the fuel demand of the lime kiln, and reducing the CO_2 emissions. As a by-product, 12.35 tH_2/d are injected into the NG distribution pipelines.

General Assumptions

For the study case, the following assumptions have been made: the mill works 350 operating days per year; O_2 and H_2 produced have been considered pure; Labour costs are assumed to be the same; Feed water quality has been considered to meet the requirements for water quality with the type of electrolyzer; The feed water for electrolysis is assumed to come from the existing mill water treatment plant, and is not taken into account in the feasibility model; In the sample delignification process, the researched O_2 charge is 16 kg/ADt, which corresponds to a typical charge according to [58]. In addition, oxidized white liquor is utilized at a rate of 2 kg/ADt. During bleaching 2 kg/ADt is assumed [58]. A total of 20kg/ADt; The value of realised emissions is adjusted to 4.25 kg$_{CO_2}$/kg$_{NG}$ given the data; It is currently unknown what burner adjustments are required to burn $\mathrm{H_2}$, as a result, it is assumed in this study that the NG burners support all the injected $\mathrm{H_2}$ without major investments.

Table 3.11 summarizes the values to be taken into consideration for the technical assessment in each of the following scenarios.

Table 3.11: Main process variables for the case scenarios for the pulp and paper study case

	Base Case	A	B	C	Unit
Electrolysis power consumption	0	11.19	38.69	24.18	MW
$\mathrm{H_2}$ production	0	5.71	18.57	12.35	t/d
$\mathrm{O_2}$ production	0	45.71	148.57	98.77	t/d
NG requirement	53.00	51.00	0	39.75	t/d
Excess electricity for sale	16.40	5.20	0	0	MW
Biomass electricity for sale	56.53	56.53	34.24	48.75	MW
Water flows increase	-	0.10	0.33	0.22	%
$\mathrm{CO_2}$ reduction	-	33	100	25	%

For the economical assessment, it is assumed that the increase in the water need is insignificant as it represents for all case scenarios less than 1% increase.

3.3 Steel

A reference integrated steel plant assumed to produce crude steel, not based on a specific plant, was utilized as a model for the construction of this research case. The goal is to give a general picture of an European integrated steelmaking. As reference case, the most established route for steelmaking, the integrated route (BF-BOF), is selected.

The evaluation is based on an average yearly production in Portugal of 30000 ton of hot metal with an annual operation of 350 days. In this section, careful look at cost estimates and emission reduction will be taken, for system-wide improvements to understand the competitiveness of an OBF, a $\mathrm{H_2}$-BF and a $\mathrm{H_2}$-DRI-EAF process (which concepts were previously explained in Section 3.3), with a conventional BF and BF-BOF plant, as well as optimization possibilities and solutions. Section 2.4 provided a description of the above mentioned processes and it is therefore necessary to understand the inputs and outputs of these new technologies in order to create a techno-economic comparison. Given the need for these processes to utilize approximate pure $\mathrm{O_2}$ and $\mathrm{H_2}$, which may result through electrolysis, an integration of an electrolyzer with the conditions of Table 3.1 will be explored.

Resource costs (coke, ore, lime, scrap, alloys), have fluctuating market prices, as these resources are internationally traded commodities. The cost estimates for these materials are considered fixed given the lack of substantial information regarding future prices and trends. In Table 3.12 the costs are presented, based on market prices from 2015-2018, reviewed by Vogl et al. Some of these values were adjusted to more recent market prices, however no big breakthroughs happened. The cost of ion ore is determined by its purity. The iron ore used in the DRI process is predicted to be slightly more expensive, but for the purposes of this study, the purity and thus pricing will be considered the same.

Table 3.12: Resources market prices [134]

Iron Ore (€/t)	Scrap (€/t)	Lime (€/t)	Alloy (€/t)	Coke (New) (€/t)	Coal (€/t)	PCI (€/t)
120	180	100	1777	300	200	177

H_2-**BF**

The technical feasibility of injecting H_2 as a RA into a BF is now discussed.Yilmaz et al. did a systematic analysis of the influence of both mass rate and temperature of the injected H_2 on energy demand, coke rate and adiabatic flame temperature. With no auxiliary RA, a coke rate of 498.1 kg/t was examined as the initial condition. It was then shown that, with a small injection rate of 10 kgH_2/t, for example, significant reduction in the coke rate is observed compared with an operation using only coke (from 498.1 to 461.7 kg/t). Further reduction is achieved at higher injection rates. However, since H_2 possesses a very high specific heat capacity, the adiabatic temperature drops. Consequently, there is a reduction of the hot blast rate and, simultaneous, O_2 enrichment is necessary meaning that when the injection rate is raised, a higher O_2 content is required. Thus, even more coke is burnt in order to maintain the thermal state of the furnace, indicating that with increasing injection rates, higher temperatures yield better outcomes. As a result, H_2 serves as both a reducing agent and a heat source. Table 3.13 shows the correlations achieved, utilized as a reference, expressed for one tonne of hot metal (t_{HM}).

Table 3.13: Comparison of process parameters with H_2 injection vs PCI (base case) [118]

	H_2	PCI	Unit
RA	27.5	120.0	kg/t_{HM}
Coke	389.8	373.9	kg/t_{HM}
Replacement ratio	3.93	1.03	kg_{coke}/kg_{RA}
AFT	2150.0	2150.0	℃
CO_2 emissions	1063.2	1352.3	kg/t_{HM}
O_2 content	21.1	22.7	%

The electrolysis process is scaled to meet the H_2 demand as a RA with the rate presented in the above Table 3.13. This requirement results in an electrolyzer dimension of 4.62 MW (all electricity is acquired from the national grid and is considered to already be renewable, with a PPA - Power purchase agreement) that produces 220 kgO_2/t_{HM}.

For the development of the economical assessment, the O_2 market is explored, given the fact that a typical BF consumes 100 kgO_2/t_{HM} [135], which leads to an over production of 120 kgO_2/t_{HM}. However, as mentioned, O_2 enrichment is necessary to maintain the thermal state of the furnace, adding 10 % of the O_2 produced to the BF for enrichment, and the remainder is sold.

From the economic point of view, the most important results from technical modelling of H_2-BF process are: decrease in PCI consumption, increase in coke consumption, increase in electricity consumption and the decreased CO_2 emissions. No initial investment is needed, apart from the electrolyzer to produce the needed H_2 and O_2.

H_2-DRI-EAF

The technical feasibility of utilizing H_2 as a RA to make DRI, to latter use in a EAF (electric furnace) for steelmaking, is discussed further bellow. Overall, because H_2 molecules are significantly smaller than CO molecules, H_2 molecules can penetrate much deeper into the iron oxide crystal structure, resulting in a higher degree of metallization [113] [136]. According to literature review, Table 3.14 summarizes the important values and correlations to take into consideration when obtaining the required resources and the specific energy consumption (SEC) for the production of one tonne of steel (ts).

Table 3.14: Literature review on DRI consumption values [134] [137] [138] [129]

	Iron Ore (kg/ts)	H_2 (kg/ts)	Scrap (kg/ts)	Electricity (GJ/ts)	NG (GJ/ts)	SEC (GJ/ts)
Vogl et al. (100% DRI)	1504	51	-	12.53	-	12.53
Vogl et al. (50% DRI)	738	25	536	-	-	-
Bhaskar et al.	-	-	-	12.50	5.60	19.96
Fischedick et al. and Weigel et al.	1500	-	352	13.10	-	13.10
Otto et al.	-	-	-	13.39	-	13.39

Vogl et al. studied a continuous operation on 100% DRI and equal shares of DRI and scrap, only considering the SEC for electricity. This study showed that the SEC would be of 12.53 GJ/t and 2.71 GJ/t for the extreme cases of 100% DRI and 100% scrap, respectively. Other researchers such as Fischedick et al. and Otto et al. also only considered the electricity consumption in their analysis. Instead, Bhaskar et al. also had into account the NG's demand.

In Fischedick et al.'s study, a technological comparison on the energy and raw material demand for one tonne of steel between both methodologies was explored. Therefore, it serves as a reference case for the study to be developed, with some adjustments based on other data acquired. These values were summarized in Table 3.15.

The electrolysis process is scaled to meet the H_2 demand as a RA. This requirement results in an electrolyzer dimension of 8.39 MW that produces 400 kgO_2/ts. When utilizing this steelmaking method, emissions decrease and the abatement potential is of 1575 kgCO_2/ts [121] [134].

For the development of the economical assessment, the O_2 market is explored. Because only H_2 will be needed for the process itself, all the produced O_2 is sold. From the economic point of view, the most

Table 3.15: Raw material and fuel consumption comparison for H_2-DRI-EAF and BF-BOF [113] [136]

	H_2-DRI-EAF	BF-BOF	Unit
Iron ore	1500	1800	kg/ts
Scrap	300	200	kg/ts
H_2 (RA)	50	0	kg/ts
Alloy	11	0	kg/ts
Lime	100	300	kg/ts
Electricity	12.5	0.2	GJ/ts
NG	0.85	5.60	GJ/ts
Coal	0	18.1	GJ/ts

important results from the technical modelling of this process are: decreased iron ore consumption, decreased coal consumption, increased electricity purchase and decreased CO_2 emissions.

OBF with CCS

For the modelling of this scenario, the study developed by Arasto et al. is used as a reference. The use of OBF (Oxygen Blast Furnace) with and without CCS in an integrated steel mill was examined in this work. The research is based on the current steel mill of Ruukki Metals Ltd., which is located in Raahe, Finland. The effects of using OBF on the site's energy and mass balances were investigated and correlations based on Table 3.16 are made for the development of the economical evaluation of the proposed implementations in Portuguese steel mills. Some studies go into great detail about the differences that lead to the disparity in these numbers, which can be consulted in [112] and [135]. However, only the most significant values are implemented for the study's purposes, and the overall values are bellow provided, expressed for one tonne of hot metal (t_{HM}).

Table 3.16: Raw material and fuel consumption comparison for BF and OBF [112] [135]

	BF	OBF	Unit
Coke	287	192	kg/t_{HM}
Pellets	1388	1388	kg/t_{HM}
Brinquettes	100	100	kg/t_{HM}
BOF slag	60	21	kg/t_{HM}
Lime	44	48	kg/t_{HM}
PCI	180	180	kg/t_{HM}
NG	0.85	5.04	GJ/t_{HM}
Coal	16.29	12.43	GJ/t_{HM}
Electricity	1.44	2.06	GJ/t_{HM}

According to Table 3.16, noticeable changes in coke output consumption is the most significant impact of the OBF on BF raw materials. Because there are only slight variations in other materials, these are not included in the modelling, as their consumption is not significantly modified. Changes in process gases streams also happen with the most significant being the increment of the mass flow of O_2 from 70 m^3/t_{HM} in the BF reference case to 220 m^3/t_{HM} in the OBF (100.03 kgO_2/t_{HM} to 314.38 kgO_2/t_{HM}). The avoided emissions when implemented a OBF with CCS is 975 kg/t of hot metal produced [135].

The electrolysis process is scaled to meet the OBF's O_2 demand. This requirement for pure O_2 results in an electrolyzer dimension of 6.60 MW that produces 39.30 kgH_2/t_{HM}. This H_2 is sold to be injected in the NG distribution pipelines at the LCOH price. In these conditions, additional 3600 t NG are still consumed and purchased annually.

From the economic point of view, the most important results from technical modelling of OBF process are: increased NG consumption, decreased coke consumption, increased electricity purchase, decreased CO_2 emissions.

General Assumptions

For the study case, the following assumptions have been made: the mill works 350 operating days per year; Only the major reactions of the process were addressed, and simplifications were made to keep the model basic, as it does not seek to go into detail of the chemical processes performed; All iron entering the electric furnace is considered to depart the process via the liquid steel product; Not all emissions from the integrated route are considered, only the most significant and direct ones; Labour costs are assumed to be the same; The coking plant remains as it is in the reference case; CO_2 is being separated from the recycle gas stream only for the operational requirements of the OBF, but there is no compression and transportation to permanent storage; No H_2 losses were considered; There is no electricity generation on the site; All electricity is acquired from the national grid and is considered to already be renewable (PPA - Power purchase agreement), not taking into consideration transmission/cables investments.

Table 3.17 summarizes the information regarding the electrolyzer specifications installed onsite:

Table 3.17: Main process variables for the case scenarios for the steel study case

	BF	H_2-BF	OBF	Unit	H_2-DRI-EAF	Unit
Electrolysis power consumption	0	4.62	6.60	MW	8.39	MW
H_2 production	0	27.50	39.30	kg/t_{HM}	50.00	kg/ts
O_2 consumption	100.00	110.00	314.18	kg/t_{HM}	0	kg/ts
O_2 production	0	220.00	314.18	kg/t_{HM}	400	kg/ts
Avoided CO_2 emissions	-	289	975	kg/t_{HM}	1575	kg/ts

3.4 Sensitive Analysis

The studied models are evaluated for specific industrial facilities, the physical and economic configuration of which were previously described. However, the goal of this study is not to provide the best solution for any individual situation, but to gain a set of insights that will assist decision makers. As a result, some of the variables that are identified to influence the final LCOH and NPV are investigated further by conducting a sensitivity analysis to determine their weight in the ultimate cost of H_2. These variables are:

Cost of electrolyzer systems: As introduced in Section 2.1.1, electrolyzer costs are in the range of 450-1260 €/kWe. However, costs are foreseen to be as low as 200 €/kWe in the long term (20% of current cost). This drop in the prices, mainly driven by a scale up of the H_2 supply chain are included in the sensitivity analysis due to the big influence of electrolysis costs in the total cost of the system.

Electrolyzer efficiency: No big breakthroughs are announced in the field of AEL electrolyzers. Even though new technological developments will gradually increase the performance of the electrolyzer systems, disregarding of the technology it is believed that the current efficiency of 70% will only increase to a maximum of 80% (maximum efficiency between SOEL, PEM and AEL). Therefore, as this value will not suffer significant change, it is believed that this characteristic improvement won't affect considerably the economical viability of the acquiring an electrolyzer, consequently not explored in this work.

LCOE: Along this thesis, it has been emphasized how impactful the electricity price is on the H_2 production costs. Therefore, the LCOE sensitivity analysis will study the cost variation from 20 to 200 €/MWh, according to the possible prices that are expected for renewables (offshore, onshore, solar, etc) to reach in the upcoming years without accounting for the transmission assets, reviewed in Section 2.1.3. Electricity prices are quite unstable at the current year of 2021, specially due to the emissions charge implemented when green electricity is not produced. Nevertheless, it is expected that these will gradually decrease and eventually reach prices as low as 20 €/MWh.

O_2 **cost**: A research will be done to determine the importance of selling the O_2 produced as a by-product, if the gases produced are sold according to the end-use and thus with different prices ranging from industrial to medical value. This final application for the O_2 will depend mostly on the possibility of selling O_2 to the health sector, since margins are much higher for the same product. It is supplied at the lowest price in the range specified earlier of 0.2 €/kgO_2 for a baseline case. Then, for a more optimistic case where it is sold for 0.3 €/kgO_2 and an even more extreme situation was explored, in which it was imagined that portion of the product was sold for industrial reasons and the other for medical uses, resulting in an average price of 0.6 €/kgO_2.

CO_2 **emissions cost**: The range of predicted growth over the next few years will be incorporated into a study of the pricing charged for CO_2 emissions. As introduced in Section 2.1.5, CO_2 prices are expected to significantly increase until 2050 and will be highly dependent on political regulations in every EU country. CO_2 prices in the range of 100 to 150 €/tCO_2 could be a reality in Europe until 2030 [24]. Therefore a price range of 60-300 €/tCO_2 will be implemented. Although price fluctuations increase is likely to be severe in the next years before flattening out, for the development of the models constant on emissions cost is assumed.

NG cost: As one of the strategies for reducing emissions is to raise the price of fossil fuels, a gradual increase in the price of NG will be undertaken. No reports or any kind of information about predictions for the increase of fossil fuels prices, mainly NG, were found. In the Table 2.9 and in the Figure 2.15, were reviewed the prices in the last 5 years and also how they have been increasing in 2021, respectively. Although prices have reached more recently (October 2021) values of 79.30 €/MWh, the base price considered corresponds to the average of the values of the last 5 years. The maximum value considered is 90 €/MWh (more than 3 times the current average).

In summary, the different variables studied in the sensitivity analysis are stated in Table 3.18:

Table 3.18: Variables included in the sensitivity analysis

	Minimum Value	Maximum Value	Unit
Electrolyzer CAPEX	200	900	€/kWe
Electrolyzer Efficiency	70	70	%
LCOE	20	200	€/MWh
O_2 cost	0.1	0.6	€/kg
CO_2 cost	60	300	€/t
NG cost	27.864	90.000	€/MWh

3.4.1 Definition of Scenarios

In attempt to predict how the future of H_2 would look, two alternative future scenarios are explored, that lead to different sets of model assumptions. Considering that the life of the project is 10 years, the first scenario is a more conservative look based on the technology advancements expected for 2030, with no big breakthroughs, predicted by the various sources surveyed, where electricity prices are lower, emissions are already at 110 €/tCO_2 and the initial investment in electrolyzers has decrease approximately 33%. Scenario 2 corresponds to more optimistic expectations, where the variables adopt values mentioned in the most optimistic cases of the above mentioned reports, where electricity prices dropped to 30 €/MWh, emissions are already at 200 €/tCO_2, NG price is approximately doubled than the value used for the reference case, and the initial investment in electrolyzers has decreased approximately 80%. All variables presented in Table 3.18 are explored and changed in order to see the effects it has on the economical assessment. Hence, the included values in the analysis are as shown in Table 3.19:

Table 3.19: Variables included in the sensitivity analysis of Scenario 1 and Scenario 2

	Baseline Case	Scenario 1	Scenario 2	Unit
Electrolyzer CAPEX	900	600	200	€/kWe
Electrolyzer Efficiency	70	70	70	%
LCOE	90	60	30	€/MWh
CO_2 cost	60	110	200	€/t
NG cost	27.864	36.000	58.896	€/MWh

Chapter 4

Results and Discussion

After defining the various scenarios and parameters utilized in the calculations, the essential results are displayed below.

4.1 Evaluation of Pathways

CAPEX

Regarding the initial expenditures, Figure 4.1 shows, as expected, very different values in terms of CAPEX for the possible pathways, Pulp and Paper and melting iron industries, ranging these between 10.07 M€ and 32.73 M€ for the pulp and paper applications and 4.15 M€ and 7.56 M€ for the steel study.

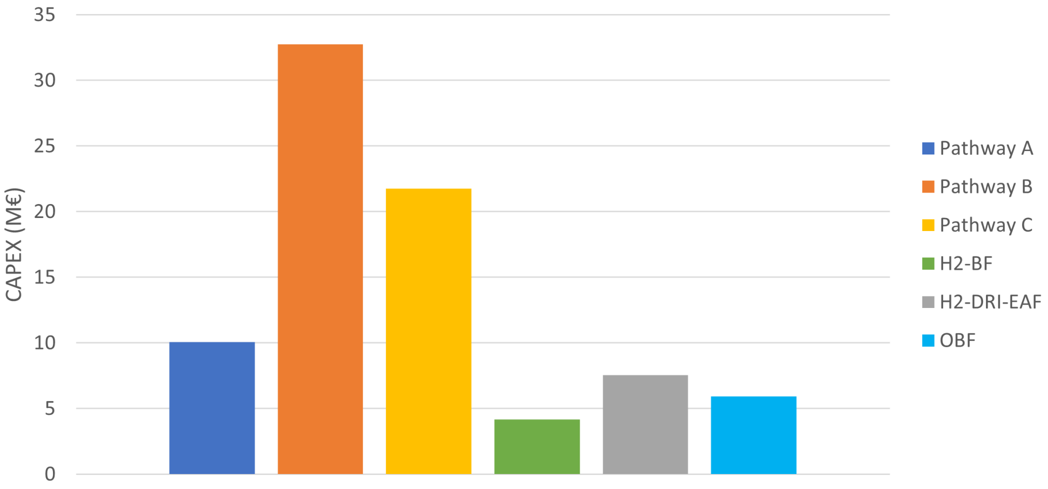


Figure 4.1: CAPEX Breakdown results. (Pathway A - Scaled to meet the O_2 demand; Pathway B - Scaled to meet the fuel demand; Pathway C - Scaled to meet the O_2 demand with O_2 enhanced combustion; H_2-BF - Scaled to meet H_2 demand as a RA; H_2-DRI-EAF - Scaled to meet H_2 demand as a RA in the DRI process; OBF - Scaled to meet O_2 demand for the oxy-combustion)

This results from the fact that in Pathway B the electrolyzer is dimensioned to meet a much larger amount of H_2, and consequently, O_2 production than the other applications, which increases the initial investment on the electrolyzer. The presence of a continuous demand of H_2 and distribution through pipelines to the final consumer erases the costs for storage which would significantly impact the initial investment of all pathways except Pathway A, that consumes both gases onsite. Other additional costs due to the compression of O_2 or H_2, would also impact all routes except Pathway A, but not as severely as storage issues. The possible routes for the steel industry and Pathway A are the cheapest due to the reduction in the size of the project components such as the electrolyzer.

OPEX

Figure 4.2, summarises the annual OPEX for every pathway, Pulp and Paper and melting iron industries. It can be observed how the OPEX varies between 13.65 M€ and 31.17 M€ for the pulp and paper applications and 3.61 M€ and 17.05 M€ for the steel industry.

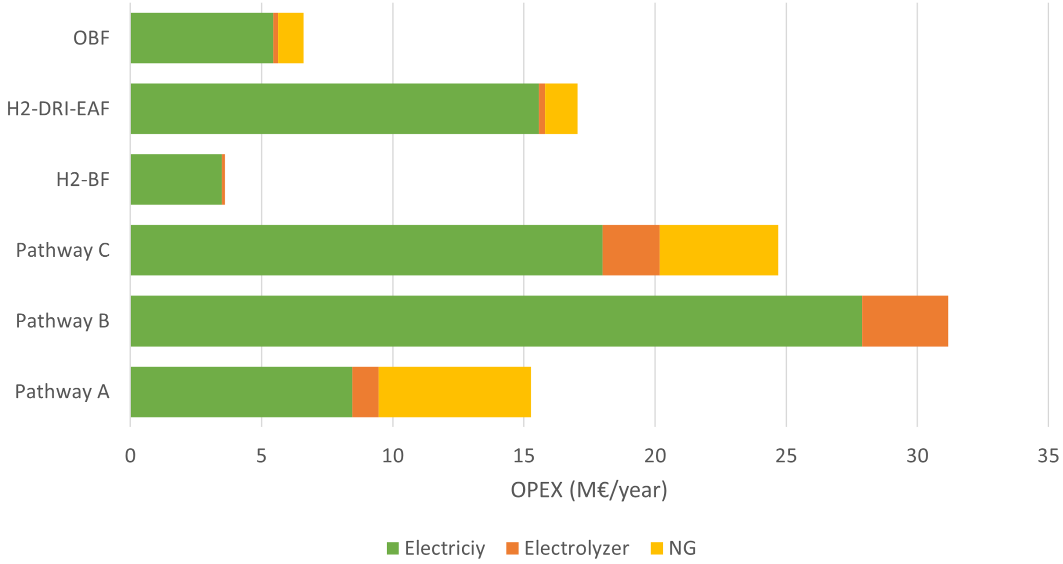


Figure 4.2: OPEX Breakdown results. (Pathway A - Scaled to meet the O_2 demand; Pathway B - Scaled to meet the fuel demand; Pathway C - Scaled to meet the O_2 demand with O_2 enhanced combustion; H_2-BF - Scaled to meet H_2 demand as a RA; H_2-DRI-EAF - Scaled to meet H_2 demand as a RA in the DRI process; OBF - Scaled to meet O_2 demand for the oxy-combustion)

The reason for Pathway B to have such high costs is mainly given to the fact that the quantity of H_2 that needs to be produced in order to burn in replacement of NG is higher, meaning that more electricity will be needed. Both Pathways A and C still require a considerable quantity of NG to be purchased (only about 25-30% of consumption is decreased), which raises the overall share of this component in the OPEX and lowers the percentage of electricity. Pathway A offers, again, the cheapest option due to a smaller system and much lesser electricity consumption.

H_2-DRI-EAF has the biggest annual expenses mainly due to the increased electricity consumption for the EAF system itself. It is worthwhile to note that although initial investments are similar for the possible routes of this industry, the OPEX varies significantly.

OPEX breakdown highlights two main factors as main contributors to operational expenses: electricity and NG related expenditures. Electricity is the necessary fuel to produce H_2 and O_2 and it accounts for up to 90-95% of the total annual expenditure in Pathway B, H_2-DRI-EAF and H_2-BF and around 62-82% for Pathway A, Pathway C and OBF due to the NG importance in the overall weight. OPEX of the electrolyzers represents a modest amount when compared to the CAPEX, which is especially interesting, since it points out the importance of considering the maintenance costs of this equipment rather than just their CAPEX, as these might have minimal maintenance compared to their initial investment. Another point to consider is that as electricity prices fall and NG prices increase, the percentages in the overall share of the OPEX will tend to balance out.

LCOH

Calculations for the determination of LCOH are performed considering only the H_2 infrastructure. However, in order to improve the economics of the project, O_2 sales are considered in the NPV calculation. For calculating the LCOH, an annual CAPEX was used, as if the total value were distributed evenly over the year. This value, for the current developments, would be of 4.88 €/kgH_2 on the production costs for all implementations. This was expected, given the stated conditions of only considering the infrastructure required to produce H_2, excluding the O_2 sales. Therefore, it is concluded that a project of these characteristics has certain fixed costs that are very high.

In Figure 4.11, the different contributions in the final price is represented and, once again, highlights electricity consumption, representing 87% of the total cost. However, it is important to state that the LCOH is not a fair comparison for these situations, because while Pathway A does not rely on any sales, the other scenarios do.

NPV

NPV is calculated for the previously determined LCOH and compared against the NPV of a project in which O_2 is sold at three different prices in order to emphasize the importance that the incorporation of O_2 can have in the economic results, without considering the infrastructure needed for this purpose. It is important to note that the value at which H_2 is sold in Pathway C and the OBF route is extremely important on the projects' viability. For the purposes of the study, it was assumed that it would be sold at the value of the calculated LCOH. Figures 4.3 and 4.4 show the NPV for the three different cases of each industrial sector.

At first glance the results show that only Pathway C presents a positive NPV wih a PBP of 4 years and an IRR of 27.63%, however when selling the produced O_2 at a price of 0.6 €/kgO_2, this would allow the NPV to become positive for Pathway B with a PBP of 7 years and an IRR of 9.00%. For this particular case, adding the O_2 to the sales is determinant to make the NPV turn into positive and therefore making the project viable under the assumptions presented.

Similar to what happened in the previous analysis, the OBF route appears to be the only profitable option to implement for the steel industry with a PBP of 3 years and an IRR of 46.00%. However, selling

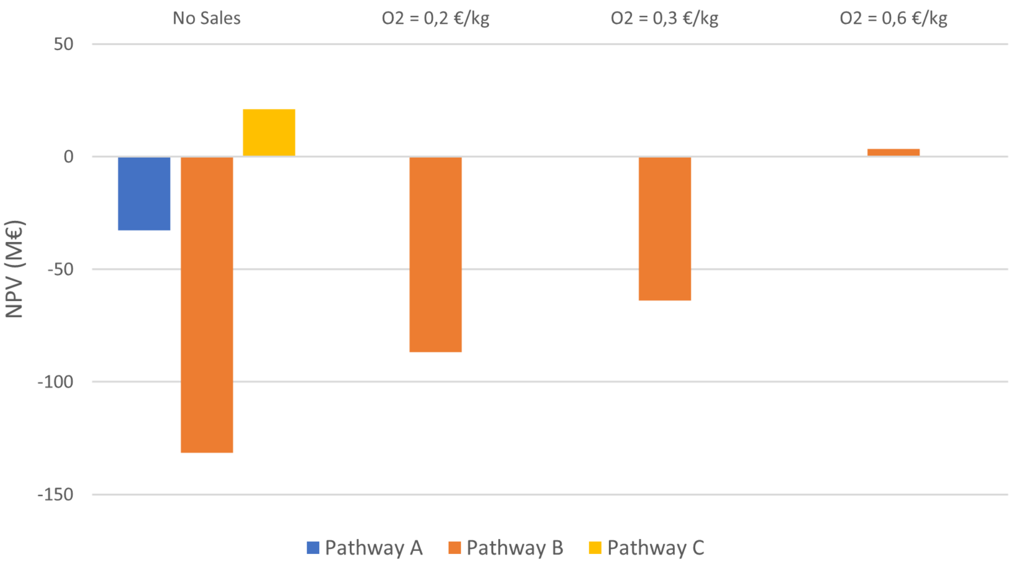


Figure 4.3: NPV - Puper and Pulp. (Pathway A - Scaled to meet the O_2 demand; Pathway B - Scaled to meet the fuel demand; Pathway C - Scaled to meet the O_2 demand with O_2 enhanced combustion)

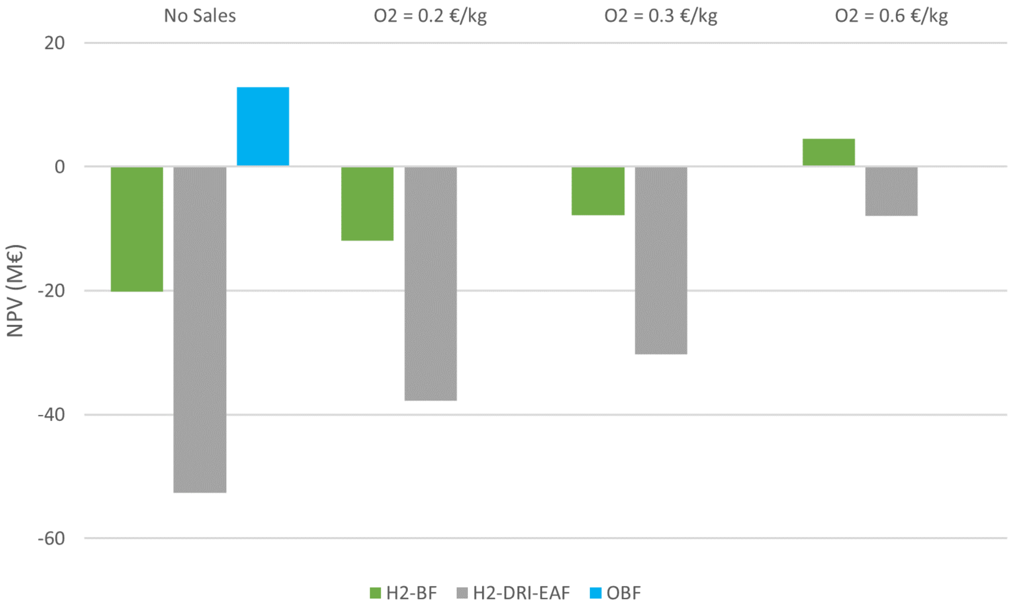


Figure 4.4: NPV - Steel (H_2-BF - Scaled to meet H_2 demand as a RA; H_2-DRI-EAF - Scaled to meet H_2 demand as a RA in the DRI process; OBF - Scaled to meet O_2 demand for the oxy-combustion)

O_2 at a price of 0.6 €/kgO_2, would allow the NPV to become positive for the H_2-BF with a PBP of 3 years and an IRR of 28.00%. Again, adding the O_2 to the sales is determinant to make the NPV turn into positive. However, it is unlikely that such a large quantity of O_2 could entirely be sold for that price, meaning that this would be a risky scenario for the current developments.

The feasibility of the case that aims to electrify the process and use H_2 to produce DRI is much more panning because, as notable in the the OPEX breakdown, costly additional electricity will have to be factored in. Even when the sub-product is sold at a higher price, this value remains negative, as opposed to the other scenarios considered, for which this price would make the projects competitive with the current methods.

4.2 Sensitive Analysis

Both LCOH and NPV are used as economic indicators to evaluate the project's performance. As a result, sensitive analyses will be conducted on the various variables that may influence the above mentioned indicators. The two industries produce similar results in some of the dependencies and parameters studied because the characteristics associated with $\mathrm{H_2}$ production are similar, regardless of the nature of the purpose for which it is used.

4.2.1 Sensitivity analysis for LCOH

For the LCOH, electrolyzer cost and the LCOE are the factors that may influence the most the final cost of $\mathrm{H_2}$, considering the variables in Equation 3.1.

Electrolyzer cost is the first tested variable in the sensitivity analysis, as presented in Figure 4.5 and then Figure 4.6 explores the influence of the LCOE.

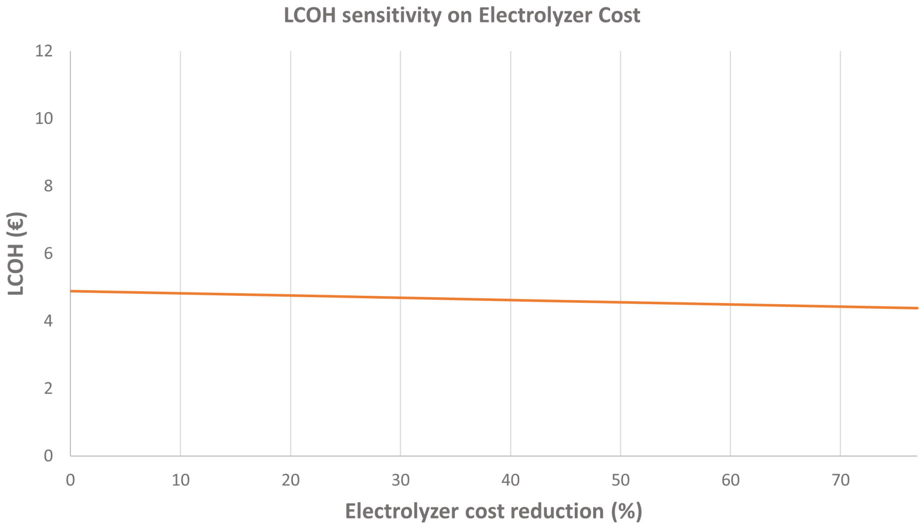


Figure 4.5: Influence of CAPEX variation

A reduction to the most optimistic value projected for the future price perspectives of 200 €/KWe is the limit of the reduction costs implemented from the initial value of the baseline case of 900 €/KWe. As expected due to the formula 3.1, this variation is linear and results in a cost reduction of around 10% of the LCOH when decreasing from 900 to 200 €/KWe. This states the importance of electrolyzers as one of the main contributors to $\mathrm{H_2}$ costs, however, it also evidences that electrolyzer cost reduction itself may not lead $\mathrm{H_2}$ to a point where it is cost competitive with many applications.

As mentioned during the development of this thesis, the LCOE is the largest contributor to LCOH,

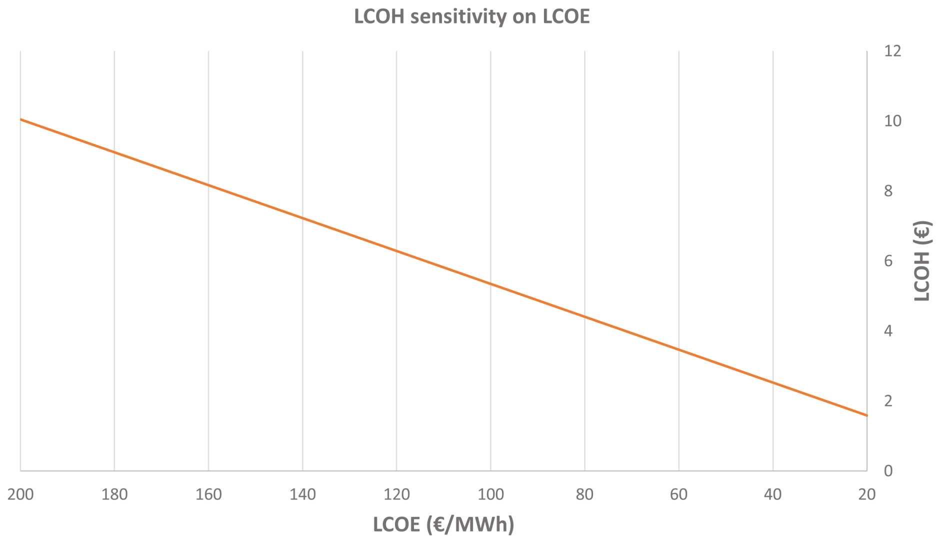


Figure 4.6: Influence of LCOE (€/MWh) variation

due to the high energy inputs required to produce H_2, therefore representing the main cost driver. This is clear to understand from the above presented graphs, where the lines in Figure 4.5 remain almost constant, as opposed to what happens in Figure 4.6, where they presents a steep decreasing slope. Variations between 200 to 20 €/MWh can represent cost reduction of 84%. In comparison, lowering the initial investment on the electrolyzer by 30% results in a 4% reduction in LCOH, while when lowering 30% of the LCOE, a 20% decrease in in the LCOH takes place.

4.2.2 Sensitivity analysis for NPV

Emission Price

When considering the NPV, as mentioned in Section 2.1.5, carbon pricing is expected to be the sector's most important climate change mitigation strategy, because this price may be imposed, whereas electricity prices are affected by various factors such as wind speed, sunshine hours, and so on. In Figure 4.7, the influence of the emissions' price is represented.

After analysing the results, it is possible to understand that Pathway B is the most sensitive (steeper slope of the line) to the increase of this value. This was expected, as Pathway B was designed to eliminate all CO_2 emissions related to the process, whereas A only eliminates 33% and C has a decrease on emissions of 25%. Pathway C is already profitable for the price of 60 €/tCO_2 considered in the beginning of the analysis.

The H_2-DRI-EAF is more sensitive (steeper slope of the line) to the increase of this value than the other two routes for the steelmaking and ironmaking processes. The greater the sensitivity to this parameter, the greater the potential for decarbonization. The OBF route is also already profitable for the price of 60 €/tCO_2.

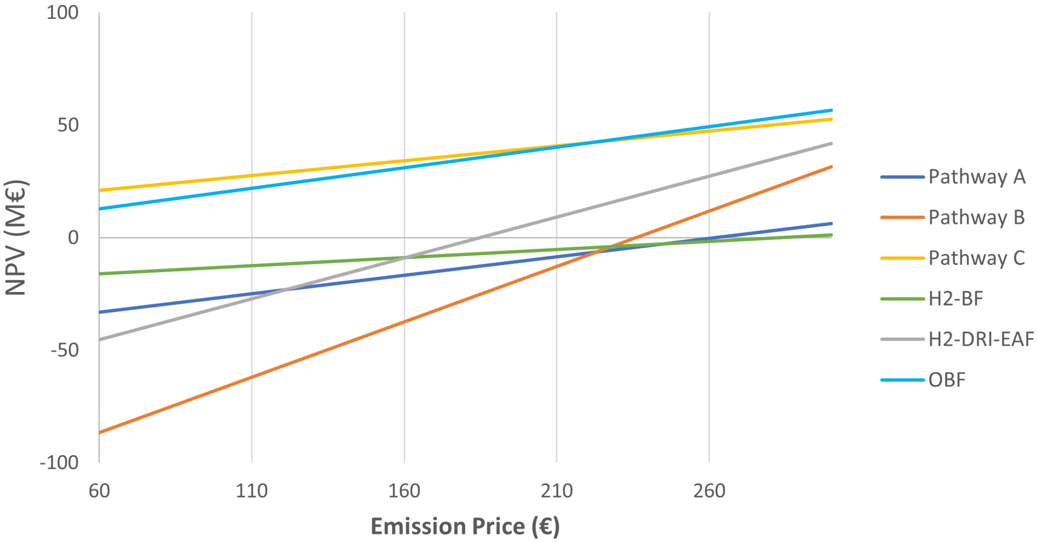


Figure 4.7: Price of emissions (€/tCO_2) influence on NPV. (Pathway A - Scaled to meet the O_2 demand; Pathway B - Scaled to meet the fuel demand; Pathway C - Scaled to meet the O_2 demand with O_2 enhanced combustion; H_2-BF - Scaled to meet H_2 demand as a RA; H_2-DRI-EAF - Scaled to meet H_2 demand as a RA in the DRI process; OBF - Scaled to meet O_2 demand for the oxy-combustion)

Table 4.1 summarizes the values for which the others routes would become competitive with the current methods when increasing the emissions price. Projects that are already competitive for current developments are not assessed, as this value is expected to increase rather than fall.

Table 4.1: Emission price necessary to turn the project profitable for the current developments

	No Sales	O_2 =0.2 €/kg	O_2 = 0.3 €/kg	O_2 = 0.6 €/kg	Unit
Pathway A	265	-	-	-	€/tCO_2
Pathway B	328	236	190	-	€/tCO_2
H_2-BF	433	281	205	-	€/tCO_2
H_2-DRI-EAF	239	189	163	87	€/tCO_2

This analysis demonstrates, once again, two important factors, one being the already emphasized importance of the O_2 sales, and secondly how important these penalty fees will be to trigger investments in green technologies, as this price is set to increase widely due to the strong impact they have in the potential investments becoming cost effective over time.

According to the trend lines, in a future when prices stabilize at higher values, forcing industries to participate in the transition, the higher the price, the more likely the routes with greater dedication to emitting less CO_2 will become the most viable option, as shown by the orange line versus the yellow and blue lines, and the grey versus the light blue and green lines with slower progressions. However, some of these values are quite high compared to the long-term expectations of the EU policy, meaning that this indicator alone, will not be sufficient to trigger competitiveness in response to the conventional production method.

LCOE

In Figure 4.8, the influence of the LCOE price on the NPV is represented.

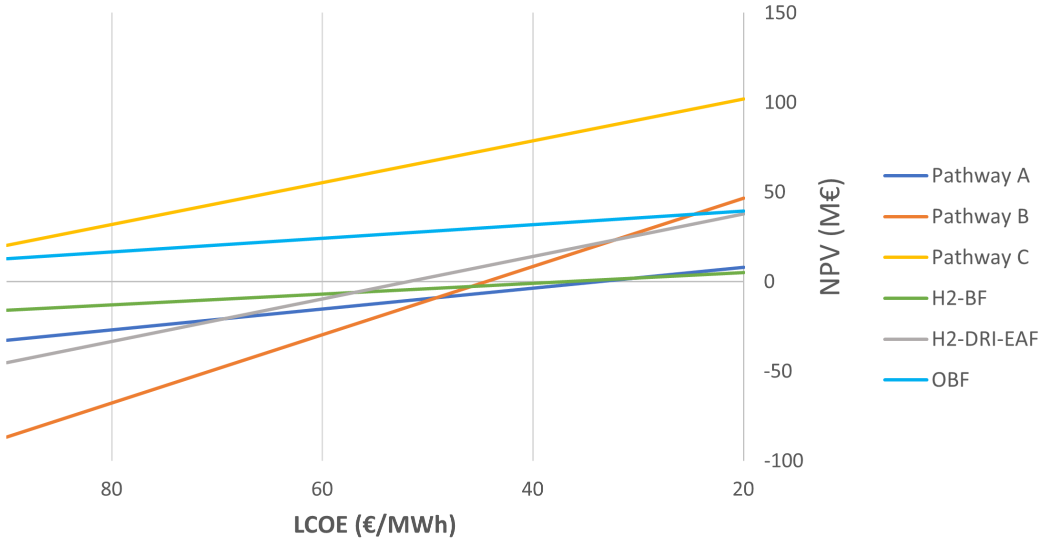


Figure 4.8: LCOE (€/kWh) influence on NPV. (Pathway A - Scaled to meet the O_2 demand; Pathway B - Scaled to meet the fuel demand; Pathway C - Scaled to meet the O_2 demand with O_2 enhanced combustion; H_2-BF - Scaled to meet H_2 demand as a RA; H_2-DRI-EAF - Scaled to meet H_2 demand as a RA in the DRI process; OBF - Scaled to meet O_2 demand for the oxy-combustion)

Pathway C would rapidly become non-profitable with a small increase of 19 €/MWh and the OBF route would follow the same path with an increase of 30 €/MWh (at an initial price of 90 €/MWh). Pathway B, has a much higher dependence on the price of electricity than the other paths, with the orange line presenting a much steeper slope than the others. In the case of the steel industry, as expected, H_2-DRI-EAF has a significantly stronger dependency than the other options analysed, because this pathway electrifies the entire production process rather than only using electricity to produce gases in the electrolyzer.

Table 4.2 summarizes the values for which the other routes would become competitive with the current methods when increasing the LCOE. Projects that are already competitive for current developments are assessed, as this value is unpredictable and could either increase or fall in the upcoming years.

Table 4.2: Electricity price necessary to turn the project profitable for the current developments

	No Sales	O_2 =0.2 €/kg	O_2 = 0.3 €/kg	O_2 = 0.6 €/kg	Unit
Pathway A	33	-	-	-	€/MWh
Pathway B	10	44	56	91	€/MWh
Pathway C	108	-	-	-	€/MWh
H_2-BF	6	40	57	112	€/MWh
H_2-DRI-EAF	41	54	61	82	€/MWh
OBF	120	-	-	-	€/MWh

This analysis demonstrates how a small change in the cost of electricity consumption can significantly alter the profitability of a project with these characteristics. Electricity prices fluctuate widely, which can be problematic when considering implementing a system that is heavily reliant on the value of this input.

It is crucial to note that, under the reasonable assumption that $\mathrm{O_2}$ may be supplied at a price of 0.2 €/kg, all options show values within the predicted range for a decrease in this price. This indicates that, once the increase of the penalty of the emission fee is also considered, these scenarios may become competitive sooner than anticipated.

Some of the conclusions to be reached in the scenarios' evaluation (Section 4.2) may be foreshadowed by the two above conducted analysis. Both Pathway A for the pulp and paper industry and the $\mathrm{H_2}$-BF route for the steel research, in fact, turn out to be the ones with the lowest initial investment, the lowest OPEX, and, while still non profitable, less harmful (NPV less negative) compared to Pathway B or the $\mathrm{H_2}$-DRI-EAF. However, they also depict the slowest progression to both the emissions price and the LCOE, therefore less sensitivity, for these indicators, predicted to the most important strategies to battle emissions in the future. This means that these paths may not show much potential for future improvements.

Natural Gas

In Figure 4.9, the influence of the NG price on the NPV is represented:

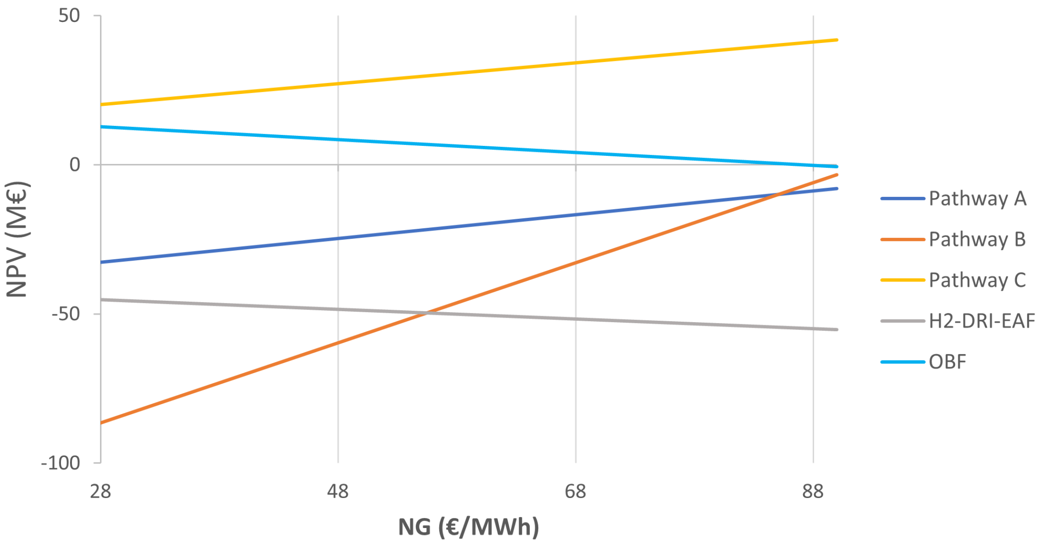


Figure 4.9: NG (€/GJ) influence on NPV. (Pathway A - Scaled to meet the $\mathrm{O_2}$ demand; Pathway B - Scaled to meet the fuel demand; Pathway C - Scaled to meet the $\mathrm{O_2}$ demand with $\mathrm{O_2}$ enhanced combustion; $\mathrm{H_2}$-BF - Scaled to meet $\mathrm{H_2}$ demand as a RA; $\mathrm{H_2}$-DRI-EAF - Scaled to meet $\mathrm{H_2}$ demand as a RA in the DRI process; OBF - Scaled to meet $\mathrm{O_2}$ demand for the oxy-combustion)

This study examines how NG prices may affect or benefit specific paths. This analysis demonstrates how an increase in this pricing might significantly boost investment for 100% green initiatives, especially considering the recent high prices reached. Pathway B, as expected, shows the largest sensitivity to this parameter due to the high fuel non-usage.

All the pathways that reduce this consumption (pulp and paper cases) present higher NPVs for higher price values, contrary to what happens for the routes that require higher consumption of this fuel (steel industry cases), for fixed emission rates. However, in these cases, despite an increase in NG consumption, there is a decrease in other more polluting resources/fuels consumption. Therefore, it is concluded that fossil fuel prices do not accurately indicate to markets the true social profitability of clean energy until they are adjusted by an appropriate carbon price.

4.2.3 Assessment of Scenarios

In the coming years, many companies will bet on a gradual implementation of H_2 injected and combusted with NG. This is due to the uncertain transition conditions in the burners, and these pilot studies should provide more information on what percentage of the already implemented methods can be supported for reuse, thereby reducing the initial investments. Figure 4.10 shows the viability of the projects in relation to the percentages of H_2 injected for ongoing and prospective developments.

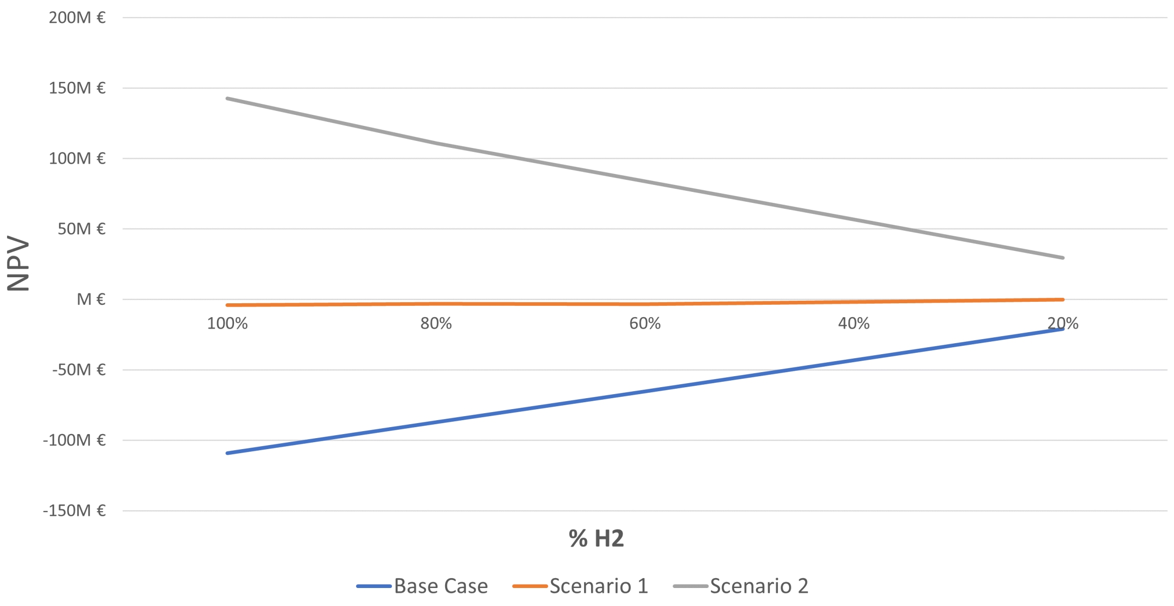


Figure 4.10: %H_2 influence for the different Scenarios

The straight lines show two distinct trends, until about 30% H_2, the O_2 produced is insufficient to meet the needs of the pulp production, so there is no income from selling the overproduction of this product. The other trend is from this value to 100%, where sales of O_2 are included.

As shown by the blue line, for the current developments, the least feasible option (although they are all non viable, because they all have negative NPVs) is when considering full NG replacement by 100% H_2. This demonstrates that, for the time being and probably for the scope of the next 10 years, radical substitutions are not justified because they represent higher consequences on the profitability of the project, with a tendency to decrease; the higher the percentage of H_2 injected, the less feasible the project presents.

For the developments of Scenario 1, considering a total substitution or only a 20% injection already has similar consequences, implying that electricity prices here have already fallen and those for emissions, CAPEX, and NG have risen sufficiently for these projects to have similar results, contrary to what happened in the Baseline case .

The same cannot be said for Scenario 2, the grey line shows that higher percentages represent better NPVs than small percentages, reversing the previously explained trend. This is due to all of the previously discussed factors, including the fact that the price of NG is expected to rise, that emissions are already at a very high price, and that the price of electricity has fallen to very low prices. Furthermore, the initial investment in an electrolyzer has also decreased, implying that it is no longer as expensive to aim for and invest in a larger production capacity. All percentages of injection are already justified in this scenario, generating profits that follow the trend seen in the previous discussed; the higher the percentage injected, the more profitable the project is.

For these Scenarios, as already detailed and explained in Section 3.18, four variables have been changed in order to better understand their combined effect in a future where the goal of reaching net zero targets boosts innovation and technological adoption, improving not only the costs as a result of scaling up, but also the performance as a result of technological advancement. Two of the four variables that changed have an effect on the LCOH. Figure 4.11 depicts the LCOH for both Scenarios 1 and 2.

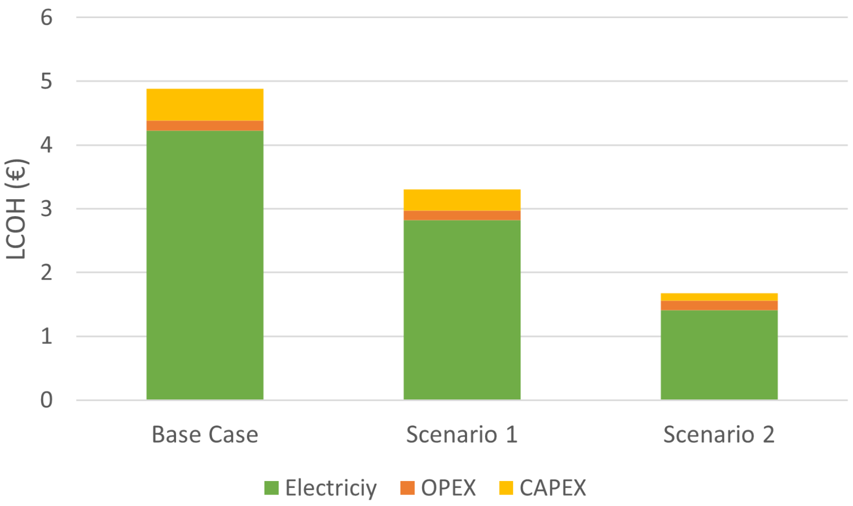


Figure 4.11: LCOH of future Scenarios

The weight of electricity is the same in all cases, being of 4.23 €/kgH_2 for the baseline case. This means that when the price of electricity, efficiency, and initial investment of the electrolyzer are taken into account, in conditions that aim to produce H_2 on-site for its own consumption, without relying on other initial investments, should be able to use the value of 4.88 €/kgH_2 as reference.

For **Scenario 1**, these new LCOH are significantly lower than the baseline case, this value has a decrease of around 30% compared to the baseline case for all pathways, reaching a value of 3.26 €/kgH_2, allowing for the introduction of H_2 into newer and larger markets. As explained in Section 2.1, blue H_2 is currently produced at a cost of around 2.50 €/kgH_2 in Europe. Therefore, achieving costs below this number, can help to decarbonize H_2 at a higher pace than expected, and this might happen for certain paths when considering the sales generated with the by-product.

For **Scenario 2**, the calculated LCOH are 70% lower than the baseline. The utmost possibility, according to this study, is to attain a price of 1.56 €/kgH_2, which is within the range of the expectations on price drop for 2050, mentioned at the start of this paper in Section 2.1.1. These low H_2 production costs allows to see where this technology can go in the medium term and long term for any application that aims to produce H_2 on-site for its own consumption, without relying on other initial investments related to compression and storage systems, reaching target costs and thus addressing more of these sectors sooner than than previously thought.

The influence of these these developments and cost reductions will have a significant impact on the projects' profitability, as shown in Figures 4.12 and 4.13.

Figure 4.12: NPVs of future Scenarios - Paper and Pulp. (Pathway A - Scaled to meet the O_2 demand; Pathway B - Scaled to meet the fuel demand; Pathway C - Scaled to meet the O_2 demand with O_2 enhanced combustion)

In fact, all projects in Scenario 2 are already competitive with the current methods. Pathway A and the H_2-BF route, as predicted, turn out to be the least profitable for the future scenario due to the previously stated reasons. In Figure 4.12, the NPV appears to be 0 for Scenario 1 in Pathway A, however this is due to scaling issues. In reality, the NPV of this approach is -0.3 M€.

It is also worth noting that, in this study, the OBF route wind up exhibiting less appealing values

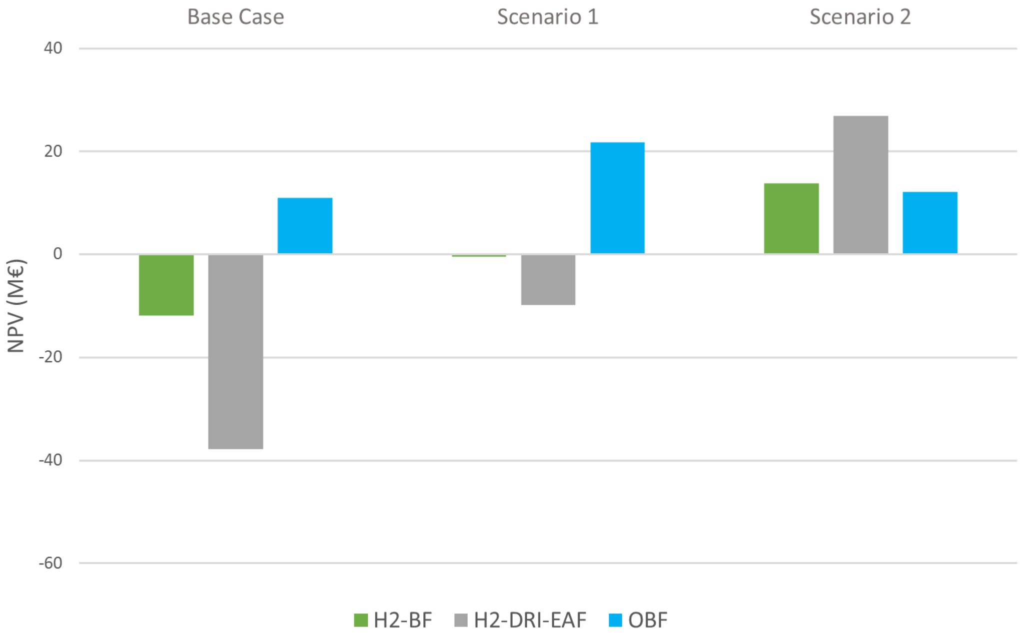


Figure 4.13: NPVs of future Scenarios - Steel (H_2-BF - Scaled to meet H_2 demand as a RA; H_2-DRI-EAF - Scaled to meet H_2 demand as a RA in the DRI process; OBF - Scaled to meet O_2 demand for the oxy-combustion)

than the baseline situation. This is because this approach still relies significantly on NG use and in the sales of the H_2 injected into the grid, which is now sold at a much lower price of 1.56 €/kgH_2 compared to 4.88 €/kgH_2 in the standard case. By that period, H_2 is already commercialized on a large scale, lowering its price, on which this model and Pathway C are heavily reliant. Pathway C, on the other hand, reduces NG consumption compared to the current practised methods, and thus this amount saved, by not consuming this fuel, compensates for the decrease in H_2 sales.

4.3 Limitations of the study

A large O_2 and H_2 production could require large volumes of storage and compression onsite, which was not considered to be an issue and incur additional costs.

When modelling, there is always a trade-off between recreating reality and keeping things simple enough to identify dependencies. Because of the scarcity of genuine data from the facilities, the models in this study are not exact replicas of individual plants. A simplified modelling technique was based on literature reviews and assumptions that, although thoroughly examined and seemingly representative, do not cover all inputs required for a clear understanding of the competitiveness's found.

It is assumed in this study that the lime kiln can support large amounts of injected H_2, however it is still uncertain if this is in fact true. Significant changes in the spark ignition, burn duration, burn capability, thermal efficiency and other technical properties of the NG engine, when injection the variable H_2 rates and O_2 enrichment, weren't considered an issue in this study. Otherwise, relevant investments costs would be added to the pathways, affecting all the analysis.

Before the fan can be cleaned, the kiln must cool down for 12 to 24 hours [106]. In addition, it takes 12-24 hours for the kiln to attain stable production after start-up. This equates to 3-4 days of lost production for each unexpected outage [106]. The frequency of unscheduled shutdowns varies between every 2-3 weeks to every 2-4 months. As a result, these periods may jeopardize the model developed, necessitating the adoption of an electrolyzer with a larger dimension and capacity than the ones anticipated.

An integrated steel mill is a complex operation, and the use of an OBF or replacement of the RA with $\mathrm{H_2}$, would involve substantial changes to the present steel mill's operations, that were not taken into account, such as the additional need for $\mathrm{H_2}$ storage.

Regarding the impacts of the recent NG shortages in the EU, since mid-August 2021, the price of energy on the Iberian market has been irrepressible, setting repeated highs due to a variety of causes, as seen in Section 2.2 in Figure 2.15. With the rising $\mathrm{CO_2}$ licensing costs, investors' willingness to put money into growing supplies of a fossil fuel they believe that will be essentially outdated in 30 years has been stifled. Meanwhile, prices are rising sharply, with the current value being at 79.30 €/MWh in October 2021 (which is around three times higher tan the value used in the calculations), and such outbreaks were not considered in this report due to the short time frame since the outbreak happened.

Even though it is expected that RE will be implemented on a large scale over the next 10 years, the recovery in infrastructure investment will still be reflected in the price, therefore these probably will not tend to fall dramatically until this return happens. The situation has been made worse by rising $\mathrm{CO_2}$ licensing costs and decreasing wind energy production due to a recent shortage of wind on the Iberian Peninsula. Another significant factor is the above mentioned rise in the price of NG, which is the fuel used in power plants and influences the final price of all energy supplied on the market. This has made electricity prices escalate in the Portuguese market and such outbreaks were also not covered in this work.

Chapter 5

Conclusions and Future Work

5.1 Conclusions

Integrating water electrolysis into a pulp mill process to produce $\mathrm{H_2}$ and $\mathrm{O_2}$ for use in the mill is a viable option for replacing NG. The daily amount of excess electricity generated at this particular pulp mill is sufficient to meet the mill's $\mathrm{O_2}$ demand while still selling the excess 5.20 MW to the national grid, eliminating the need for separate $\mathrm{O_2}$ production and purchase. 33% of the emitted $\mathrm{CO_2}$ would be avoided by utilizing the $\mathrm{H_2}$ produced together with NG. Furthermore, with the biomass plant near site, and some investments transmission/cables, the facility would be able to cover all the electricity demand for the production of $\mathrm{H_2}$ scaled to replace all NG consumed, while still injecting 34.24 MW into the national grid. However, the economic implications of these investments were not considered in the economical assessment.

For the current developments, and for the scope of the next years, radical substitutions of NG are not justified because they represent higher consequences on the profitability of the project, with a tendency to decrease; the higher the percentage of $\mathrm{H_2}$ injected, the less feasible the project presents. When implementing these injections, it is also necessary to understand the technical conditions and utility of existing equipment, which will be dictated in the upcoming years by pilot studies. However, if electricity prices reach 60 €/MWh, $\mathrm{CO_2}$ emission price reach 110 €/t$\mathrm{CO_2}$ and NG price rise to 36 €/MWh, these projects start to have similar results in terms of profitability, regardless of the percentage considered. Full NG replacement, represented by Pathway B in the present work, is expected to be the most cost-effective and environmentally friendly solution for the developments considered in Scenario 2.

The most promising road forward for present advancements looks to be implementing oxy-fuel combustion in both industries. This path remains the most viable alternative until the price ranges of Scenario 1, with superior NPV forecasts. However, with lower LCOH and higher NG prices expected in the coming years, both scenarios suffer significant penalties, reflecting a less favourable investment over a 10-year time horizon. Scenario 2 uses the achieved developments to turn the baseline case's worst investments, the most desirable in both industries. These are the ones that have the greatest potential for CO_2 emission reduction.

Based on the values seen in the LCOE sensitive, for the pulp and paper the necessary values to achieve competitiveness range between 33-44 €/MWh and for the steel industry, these values range from 40-54 €/MWh, both when considering the standard O_2 price of 0.2 €/kgO_2. Under the same conditions, when considering the emission penalties, these range from 236-265 €/tCO_2 for the pulp and paper and 189-281 €/tCO_2 for the steel applications. These values are rather high in comparison to EU's policy expectations for the upcoming years, implying that this measure alone will not be sufficient to trigger competitiveness in response to traditional methods.

When it comes to the steel industry, the outlook for H_2-DRI-EAF steelmaking appears to be technically promising for the future, assuming successful technology and process development and favourable market conditions in terms of relative electricity and carbon emissions prices, according to the assessment. This is supported by the fact that this approach is significantly more sensitive in both of these analysis. Because CO_2 emissions are negligible when compared to present production methods or even the other two scenarios of using H_2 as a RA or an OBF, H_2-DRI-EAF is a realistic alternative for fulfilling EU emissions targets for 2050. However, decarbonization of electricity production is a prerequisite for this.

The economic viability of these H_2-based projects is thus largely reliant on the availability of low-cost clean electricity and higher carbon-emissions costs and NG higher costs, with improvements in all areas required. However, it has been demonstrated that cost reductions in electrolyzers may not get H_2 to a position where it is cost competitive with many applications. Lowering the initial investment in the electrolyzer by 30% results in a 4% reduction in LCOH, whereas lowering the LCOE by 30% results in a 20% reduction in LCOH. These projects have the potential to attain an LCOH of 1.56 €/kgH_2.

This research showed that what appears to be a waste product, such as O_2, can considerably improve the project's economics and viability, improving the NPV by over 135 M€ (in the most optimistic case). If there is O_2 demand in the production value chain, some of this product can be used on-site; nevertheless, working with industrial gases providers will be crucial if this market is outside of these companies' scope.

5.2 Future Work

The producers considered in the development of this thesis have a distribution system that run from the factory to the end destination, either to a commercial port or directly to a consumer. Incorporating a fuel service station on-site could be an interesting solution for these stationary decentralized productions because these vehicles are expected to use H_2 fuel as a decarbonization measure rather than electric batteries. Today, there is still a scarcity of H_2 demand for transportation in Portugal, though this is expected to change in the future years as these heavy vehicles are expected to represent 40% to 68% of H_2 demand in transportation [100].

A typical fuel truck currently has a deposit that stores between 30-50 kgH_2 [140]. This means that the H_2 produced in Pathway C, if utilized for mobility purposes, would be able to fuel around 400 trucks/day. The first commercially available FC vehicles used an on board storage pressure of 700 bar [141], but compression and storage tanks capable of storing H_2 at this pressures are expensive due to the requirement for advanced vessel materials, such as carbon fibre [141]. As a result, such tanks or compressors were not considered viable for the purpose of this thesis. Nonetheless, it is possible that the future connection to the gas grid, with the ability to inject all of the produced H_2, or utilizing alternative energy carriers such as LOHC, could eliminate this problem and, with pipelines possibly incorporated, this scenario could become very interesting.

The use of H_2, along with H_2 storage, that, as mentioned in the limitations of this study, was not taken into consideration with the assumption that all the produced H_2 would immediately be incorporated in the process, could give the electricity system more flexibility in integrating intermittent RES, as well as providing new financial prospects for steel businesses by allowing them to participate in power reserve markets.

The cost and performance of the system should be compared between using grid electricity and employing specialised RES. Because of the excess energy generated by the cogeneration systems onsite and the biomass power plants, this comparison would be especially interesting for the pulp and paper industry. This option's technicality has been investigated, with the relevant values, fluxes, and variants reported in this paper. However, the economic implications should be further explored.

For all these reasons, although all H_2 is consumed onsite for most scenarios of both industrial sectors, the analysis performed for the LCOH is important to understand if the decrease of this value could represent a window of opportunity for these companies to produce more than they need and explore the potential of other markets, especially if electricity prices fall sharply and H_2 can be produced at very low prices.

For the particular geographical characteristics of the pulp and paper facility explored, it would be interesting to further investigate the potential O_2 market, as CELBI is located 16 minutes by road transport from a hospital, opening up the possibility of retaining high values in the sale of this sub-product for medical purposes.

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Appendix A

Figures

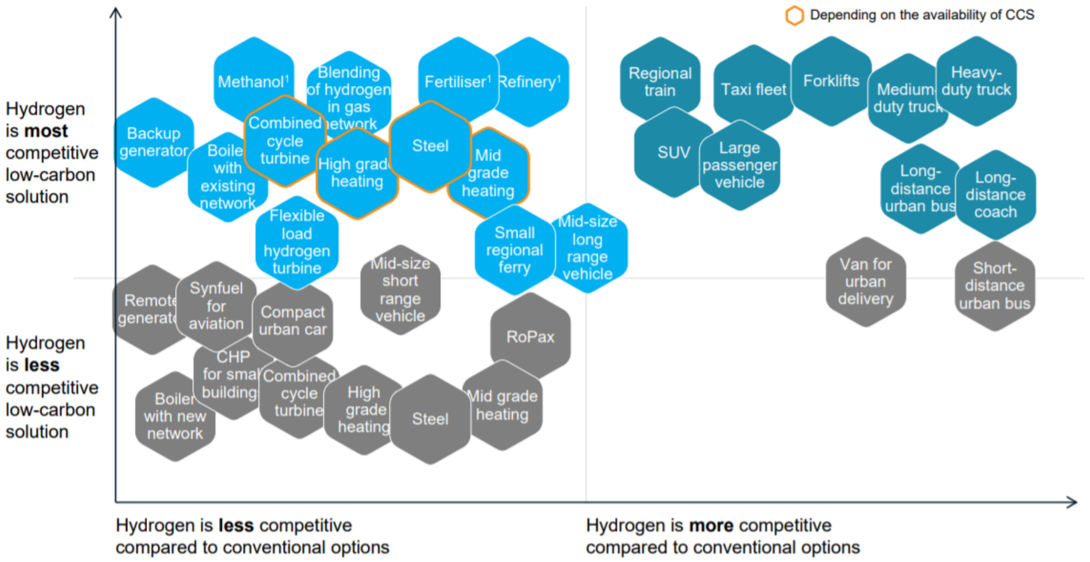
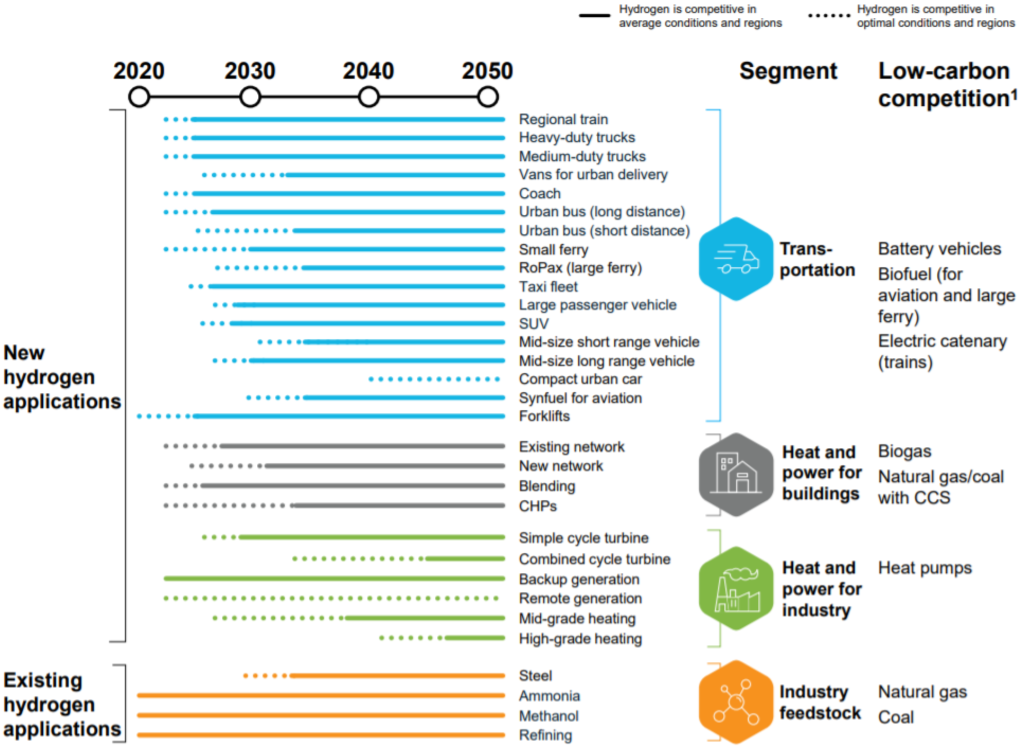


Figure A.1: Competitiveness of H_2 applications versus low-carbon and conventional alternatives [8]



1. In some cases hydrogen may be the only realistic alternative, e.g. for long-range heavy-duty transport and industrial zones without access to CCS

Figure A.2: Cost competitiveness trajectories of H_2 applications[8]

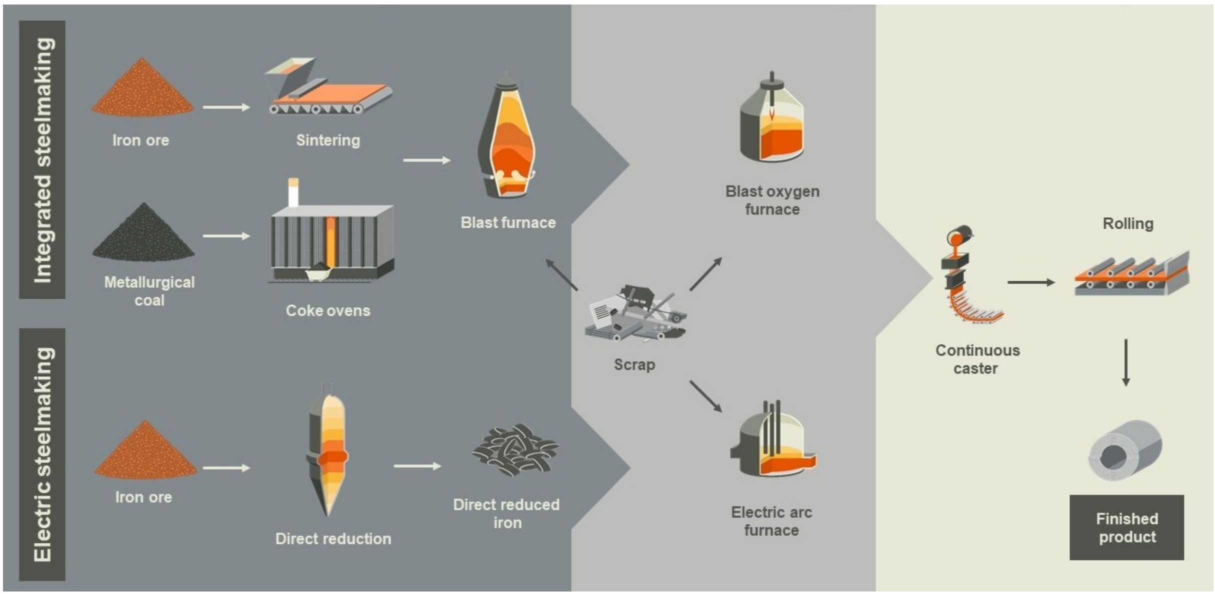
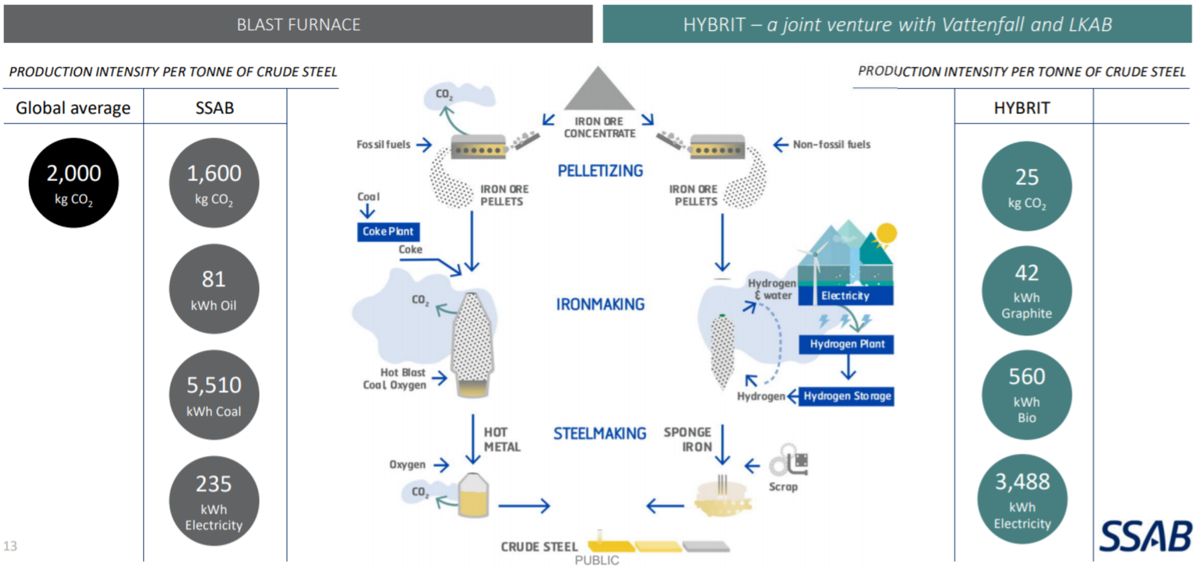


Figure A.3: Major steelmaking process routes [142]



BLAST FURNACE

HYBRIT – *a joint venture with Vattenfall and LKAB*

PRODUCTION INTENSITY PER TONNE OF CRUDE STEEL

Global average	SSAB
2,000 kg CO_2	1,600 kg CO_2
	81 kWh Oil
	5,510 kWh Coal
	235 kWh Electricity

PRODUCTION INTENSITY PER TONNE OF CRUDE STEEL

HYBRIT
25 kg CO_2
42 kWh Graphite
560 kWh Bio
3,488 kWh Electricity

Figure A.4: Traditional versus HYBRIT technology [121]