Characterizing the Hydrogen Chain: Efficiency, Costs, and Applications across Different Sectors

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Master Dissertation

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Abstract

The global energy panorama is presently undergoing a significant transformation driven by the imperative of addressing climate change and guaranteeing sustainable energy access. The burning of coal, oil, and natural gas remains a primary contributor to greenhouse gas emissions, exacerbating global environmental challenges and climate crises. In the journey towards a cleaner and more resilient energy future, hydrogen has emerged as a compelling avenue. This versatile energy carrier presents the potential to tackle energy security concerns, reduce carbon emissions, and facilitate the shift to low-carbon economies.

This thesis seeks to explore the potential of integrating hydrogen gas into the Portuguese energy system, with the objective of assessing its capacity for cost-effective decarbonization and enhanced energy conversion efficiency. Additionally, the thesis aims to depict the hydrogen value chain, emphasizing key conversion pathways spanning from production to end-use applications.

The development of the hydrogen value chain encompassed an extensive examination of potential conversion pathways. This spanned from the production, transmission, distribution, and storage of hydrogen, extending to its potential end-use applications. This investigation also incorporated hydrogen-based fuels within the spectrum. Furthermore, comprehensive techno-economic data pertaining to each conceivable technology was compiled.

The incorporation of hydrogen gas conversion sequences within the Reference Energy System (REF) was facilitated by employing the OSeMOSYS framework. The end-uses were disaggregated into various technologies in the model to provide a more comprehensive understanding of the system. This enabled the simulation of five distinct scenarios, facilitating subsequent comparative analysis.

The findings have highlighted a persistent challenge in achieving emissions reduction without incurring substantial investments in new technologies. It became evident that the pursuit of greenhouse gas (GHG) emissions reduction often entails a significant increase in total costs, even when integrating new vectors in the system, such as hydrogen.

Keywords: Decarbonization, energy modeling, energy transition, energy systems, hydrogen, hydrogen economy, OSeMOSYS, techno-economic analysis.

Resumo

O panorama energético mundial está atualmente a sofrer uma transformação significativa, impulsionada pelo objetivo de enfrentar as alterações climáticas e garantir um acesso sustentável à energia. A queima de carvão, petróleo e gás natural continua a ser um dos principais contribuintes para as emissões de gases com efeito de estufa, exacerbando os desafios ambientais globais e as crises climáticas. No caminho para um futuro energético mais limpo e mais resiliente, o hidrogénio surgiu como uma via atrativa. Este vetor energético tão versátil apresenta o potencial para resolver os problemas de segurança energética, reduzir as emissões de carbono e facilitar a transição para uma economia com baixo teor de carbono.

Esta tese procura explorar o potencial de integração do hidrogénio gasoso no sistema energético português, com o objetivo de avaliar a sua capacidade de descarbonização e de aumentar a eficiência da conversão energética. Adicionalmente, a tese pretende descrever a cadeia de valor do hidrogénio, enfatizando as principais vias de conversão que vão desde a produção até às aplicações de utilização final.

O desenvolvimento da cadeia de valor do hidrogénio englobou uma análise exaustiva das potenciais vias de conversão. Estas abrangeram desde a produção, transmissão, distribuição e armazenamento de hidrogénio, até às suas potenciais aplicações finais. Esta investigação também incluiu no seu espetro os combustíveis à base de hidrogénio. Além disso, foram compilados dados técnico-económicos abrangentes relativos a cada tecnologia concebível.

A incorporação de cadeias de conversão de hidrogénio gasoso no Sistema Energético de Referência (REF) foi facilitada pela utilização da estrutura OSeMOSYS. Os usos finais foram desagregados em várias tecnologias no modelo para proporcionar uma compreensão mais abrangente do sistema. Isto permitiu a simulação de cinco cenários distintos, facilitando a análise comparativa subsequente.

Os resultados evidenciaram um desafio persistente na obtenção de uma redução das emissões sem incorrer em investimentos substanciais em novas tecnologias. Assim, tornou-se evidente que a busca da redução das emissões de gases com efeito de estufa (GEE) implica frequentemente um aumento significativo dos custos totais, mesmo quando se integram novos vetores no sistema, como o hidrogénio.

Palavras-chave: Análise técnico-económica, descarbonização, economia do hidrogénio, hidrogénio, modelação energética, *OSeMOSYS*, sistemas energéticos, transição energética.

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“No human is limited.”

Eliud Kipchoge

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Chapter 1

Introduction

1.1 Background on hydrogen economy

Although renewable energy sources are gaining traction, many energy systems worldwide still depend on fossil fuels like coal, oil, and natural gas. Using these fuels in power generation, transportation, and industrial processes leads to a significant increase in greenhouse gas emissions, exacerbating the challenges of air pollution and climate change.

The persistent reliance on fossil fuels is a major health and environmental concern. Despite the global commitment to mitigating climate change, current policies have not effectively limited energy-related emissions. This has led to a steady increase in emissions, driven by the growing demand for energy [1].

Hydrogen has gained significant attention in recent years as a potential solution to address the challenges of energy security, climate change, and the transition towards a low-carbon future [2]. Hydrogen is a versatile and clean energy carrier that can be produced from various sources, including natural gas, coal, and water, using methods like steam methane reforming, gasification, and electrolysis. Its potential applications span multiple sectors, such as power generation, transportation, heating, and industrial processes, as presented in Figure 1.1 [3].

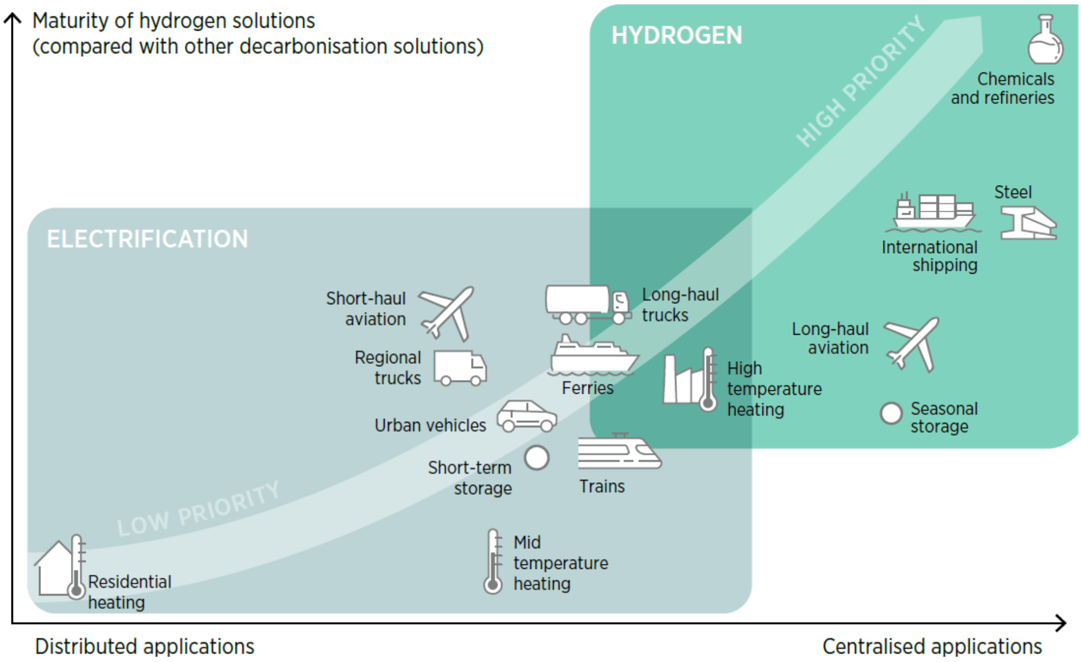

Figure 1.1: Priority settings for hydrogen applications across the energy system [4].

Countries and industries have recognized the potential of hydrogen for the decarbonization of economies, leading to increased research and development efforts. The focus of these efforts has been the enhancement of the efficiency and cost-effectiveness of hydrogen production, storage, and utilization. Hydrogen may be a crucial contributor to the reduction of emissions in hard-to-decarbonize sectors and the decarbonization of energy systems where heating systems are heavily dependent on natural gas. Additionally, hydrogen can help achieve a broader range of policy objectives related to energy independence, and play a major role in the continued growth of renewable electricity by adding storage capacity to power systems [4].

Although the hydrogen economy offers a promising path toward a sustainable and decarbonized future, it faces several challenges, including that the majority of hydrogen is currently produced from coal and natural gas, uncertainty around policies and existing technologies, the complexity of the value chain, and infrastructure needs. Furthermore, the lack of regulations and standards, coupled with slow hydrogen acceptance, are impediments to its widespread adoption [3].

To fully realize the potential of hydrogen as a clean energy source, governments can play a crucial role in facilitating its development. One way to support the growth of low-carbon hydrogen is for governments to increase their efforts in providing funding, incentives, and regulatory frameworks that promote both research and development and the deployment of hydrogen technologies. Additionally, establishing international collaborations can help to encourage the global adoption of low-carbon hydrogen, which could have significant positive impacts on the environment and energy security [3] [5]. Figure 1.2 displays the initial measures taken for international cooperation in the H_2 trade sector, specifically involving bilateral export and import agreements that were established by March 2022.

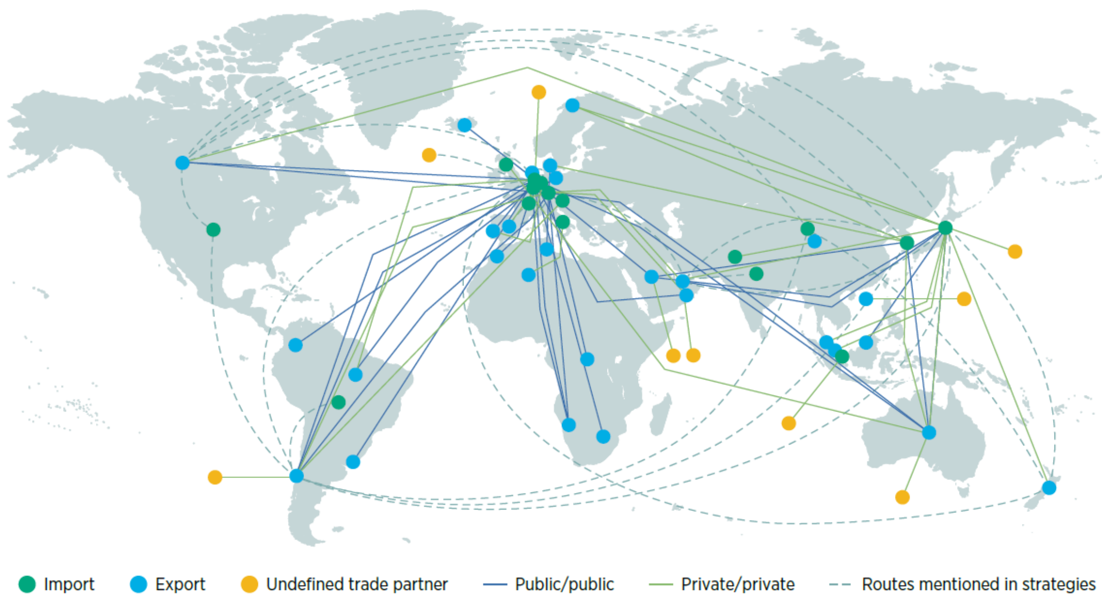

Figure 1.2: Bilateral trade announcements for global hydrogen trade until March 2022 [4].

1.2 Importance of hydrogen as an energy carrier

The established hydrogen value chain is not sustainable or green, as the majority of hydrogen is generated from non-renewable sources such as coal and natural gas, and its primary usage is in oil refining and the production of ammonia. Additionally, roughly one-third of the global supply of hydrogen is considered a by-product, meaning it is generated in facilities that are not primarily designed for hydrogen production. Compared to other fuels (as shown in Table 1.1), hydrogen is an appealing chemical energy carrier, thanks to its high energy density and the relatively low impact of the hydrogen combustion by-products, which produce mainly water with no emissions of greenhouse gases, sulfur oxides, primary particulates, or ground-level ozone. Hydrogen's versatility as an energy carrier enables it to store and transport energy from renewable sources like wind and solar power, making it an ideal option for balancing variable renewable power generation and enhancing the energy system's resilience [3].

Table 1.1: Physical properties of hydrogen and the comparison with other fuels [3]

Property	Hydrogen	Comparison
Density (gaseous)	0,089 kg/m^3 (0°C, 1 bar)	1/10 of natural gas
Density (liquid)	70,79 kg/m^3 (-253°C, 1 bar)	1/6 of natural gas
Boiling Point	-252,76°C (1 bar)	90°C below LNG
Energy per unit of mass (LHV)	120,1 MJ/kg	3x that of gasoline
Energy density (ambient cond., LHV)	0,01 MJ/L	1/3 of natural gas
Specific energy (liquefied, LHV)	8,5 MJ/L	1/3 of natural gas
Flame velocity	346 cm/s	8x methane
Ignition range	4-77% in air by volume	6x wider than methane
Auto-ignition temperature	585°C	220°C for gasoline
Ignition energy	0,02 MJ	1/10 of methane

The use of hydrogen as an option for hard-to-decarbonize sectors such as transportation, is predicated on shifting the production of hydrogen from predominantly fossil to renewable sources and nuclear power and possibly retrofitting some of the fossil fuel plants with CCUS (Carbon Capture, Utilization, and Storage) technology. As an alternative for the transportation sector, hydrogen or hydrogen-based fuels from renewable sources can replace fossil fuels in internal combustion engines and fuel cell vehicles. Furthermore, hydrogen has the potential to reduce greenhouse gas emissions in energy-intensive industries like steel and cement production by replacing conventional fuels and feedstocks [2].

1.3 Motivation for the thesis

Energy modeling plays a pivotal role across all sectors of society as it serves as a fundamental tool for fostering sustainable progress within nations. It encompasses the comprehensive analysis and management of energy resources, including the assessment of their quality, availability, and environmental impacts. By capturing the intricate details of various technologies and energy sources, energy modeling facilitates informed decision-making and enables the development of sustainable energy systems [6].

An open-source energy optimization model offers a unique opportunity for stakeholders and various sectors of society, including students and policymakers, to actively contribute to the growth and development of the model. By allowing users to add more accurate data and updated information, this collaborative approach fosters the shared goal of decarbonizing the energy system, which results in a more robust and accurate model.

At present, there is a notable absence of an open-source energy optimization model that incorporates hydrogen conversion chains specifically tailored to the Portuguese energy system. Consequently, the lack of such a model hinders the ability of various end-users to simulate different scenarios related to the introduction of hydrogen within the energy landscape. This research endeavor aims to serve as the initial stride towards constructing a more comprehensive and intricate energy system model for Portugal, encompassing the entire energy value chain from primary sources to final utilization. By bridging this gap, the intention is to facilitate a more accurate representation of the Portuguese energy system.

1.4 General and specific objectives

The primary goal of this dissertation is to create a flexible model that expands the current Portuguese Reference Energy System (RES). The RES represents energy usage at the final energy level and aims to encompass all conversion chains from primary sources to end-use applications. Specifically, this research focuses on hydrogen conversion chains and aims to simulate various scenarios for introducing hydrogen as an energy carrier to facilitate the decarbonization of energy systems.

To comprehensively explore the hydrogen conversion chains, it is essential to identify all potential technologies and pathways from primary sources to final applications. Therefore, conducting an extensive literature review is of utmost importance to uncover various conversion chains and potential applications across different sectors. Furthermore, it is crucial to assess techno-economic factors such as efficiency, and costs (CAPEX and OPEX), and examine the climate mitigation potential of different scenarios involving hydrogen integration.

This thesis was developed with specific objectives in mind. Initially, the goal encompassed the establishment of the hydrogen value chain to gain a comprehensive understanding of potential conversion sequences. Furthermore, the objective was to develop an energy model that incorporates a range of hydrogen conversion pathways, with a specific limitation on utilizing gaseous hydrogen and pipelines as the mode of transportation. This involved implementing these chains into the existing OSeMOSYS model, which represents the Portuguese energy system. Secondly, the thesis focused on simulating different scenarios to analyze the potential impact of hydrogen penetration across all sectors of the energy system.

1.5 Outline of the thesis structure

The thesis is organized into the following 8 chapters:

1. Introduction: This chapter provides an overview of hydrogen in the world economy, highlighting its significance as an energy carrier. It also presents the research's motivation and objectives.

2. Hydrogen Value Chain: This chapter conducts a comprehensive literature review to explore the hydrogen conversion chains, covering everything from primary sources to hydrogen production, transmission, distribution, storage, and end-use applications.

3. Energy Modelling: This chapter explores the domain of energy models, examining their core elements and delving into specific models. It offers an in-depth examination of the particular model utilized in the study, specifically OSeMOSYS.

4. Methodology: This chapter outlines the methodology utilized in the thesis. It begins by detailing the development of the hydrogen value chain, involving an extensive literature review covering hydrogen production, transmission, distribution, storage, and end-use applications. Subsequently, it delves into the compilation of techno-economic data pertaining to the identified technologies within the hydrogen value chain. Moving on to the creation of the energy model, the process commences with the reference energy model that served as the foundational framework for this study. It then proceeds to the disaggregation of end-use sectors, categorizing them into distinct segments and technologies. The chapter further elucidates how the hydrogen conversion chains and end-use technologies were integrated into the model, providing an overview of the process and the requisite parameters. Upon completion of the model, the chapter describes five scenarios, outlining the chosen emissions reduction goals and the extent to which hydrogen is employed in end-use applications. Additionally, it presents data pertaining to sector-specific demand characterization.

5. Results and Discussion: This chapter presents the findings of the research, focusing on the hydrogen value chain built and the possibilities of hydrogen integration within the Portuguese energy context. It includes a complete analysis and discussion of the results obtained.

6. Conclusions: This chapter summarizes the main findings of the research and underscores their significance in driving the transition to a hydrogen-based economy.

7. Future Work: This chapter proposes areas of improvement for further research.

8. Appendixes: This section showcases all additional data that was not included in the main document to avoid excessive lengthening.

Chapter 2

Hydrogen Value Chain

This chapter provides a comprehensive overview of fuels, technologies, and potential applications for hydrogen, which play a crucial role in establishing a robust and interconnected hydrogen value chain.

2.1 Hydrogen production methods

The focus of this literature review is on examining the various methods for hydrogen production, such as steam methane reforming (SMR), gasification, and several types of electrolysis (including alkaline, proton exchange membrane, and solid oxide electrolysis). Each technique has its own set of benefits and challenges, such as efficiency, cost, lifetime, and environmental impact. Additionally, the literature review emphasizes the current research and development initiatives aimed at enhancing these methods and devising new production technologies.

2.1.1 Hydrogen from water

2.1.1.1 Water Electrolysis

Water electrolysis is a technique used to separate hydrogen and oxygen in water through an electrochemical process that requires the input of electrical and thermal energy [7]. The process is typically carried out in a cell that contains two electrodes separated by an electrolyte. There are three primary technological alternatives for water electrolysis: alkaline electrolysis (AE), proton exchange membrane (PEM) electrolysis, and solid oxide electrolysis cells (SOECs). These techniques are distinguished by the type of electrolyte utilized, the operating pressure, and the temperature of the reaction [5]. Further details on these distinctions are provided in Table 2.1.

Table 2.1: Basic characterization of different types of electrolyzers [3] [5]

	AE	**PEM**	**SOEC**
Operating Temperature	70-90°C	50-80°C	700-850°C
Operating Pressure	1-30 bar	70 bar	1 bar
Electrolyte	Potassium hydroxide (KOH) 5-7 mol/L	PFSA membranes	Yttria-stabilized Zirconia (YSZ)

Alkaline electrolyzers are considered the most established and commercially viable technology among the three types mentioned previously, which are suitable for large-scale hydrogen production [8]. They are simple to manufacture due to their straightforward stack and system design. These electrolyzers can operate within a range of 10% of their minimum load up to their maximum design capacity. Unlike other electrolysis technologies, alkaline electrolyzers do not require precious materials, resulting in relatively low capital costs [3]. They are also highly reliable and have a potential lifetime of up to 30 years [5].

PEM electrolyzers use pure water as an electrolyte solution, making them highly susceptible to water impurities and vulnerable to calcination. However, they are advantageous in densely populated urban areas due to their small and compact size. PEM electrolyzers are capable of producing highly compressed hydrogen for decentralized production and storage at refueling stations. They operate within a wide range, from 0% to a maximum of 160% of their design capacity, allowing for flexible operation and overloading when possible [3]. Despite these advantages, membranes and noble metal-based electrodes have high investment costs, making the total cost of PEM electrolyzers higher than that of alkaline electrolyzers. For them to be wider used in the production of hydrogen, the production capacities need to increase [8]. Furthermore, the reliability and lifespan of PEM electrolyzers are uncertain, and research and development in this area are ongoing [5].

Of the three technologies mentioned, solid oxide electrolysis cells (SOECs) are the least mature [7]. They employ ceramics as an electrolyte, resulting in reduced material costs. SOECs operate at higher temperatures, resulting in higher electrical efficiencies [7] [8]. However, they rely on heat due to steam usage, and the high temperatures can compromise the materials involved, leading to a decrease in lifespan. One significant advantage of SOECs is their reversibility, allowing for the conversion of hydrogen back into electricity [3] [5].

In the past ten years, the installation of electrolyzers has increased, with a particular emphasis on PEM technology. This growth is a positive sign, as electrolysis-based hydrogen production is a process that can support the decarbonization of energy systems.

2.1.2 Hydrogen from coal

2.1.2.1 Coal gasification

Coal gasification is a well-established technology, that accounts for 30% of the total hydrogen production in the world [9]. It has been utilized for a long time to generate syngas, which consist primarily of carbon monoxide and hydrogen, along with other gases such as methane and carbon dioxide. One significant drawback of coal gasification is the high levels of CO_2 emissions, which are twice as much as those generated by natural gas. However, the implementation of carbon capture, utilization, and storage (CCUS) technology can prevent the release of CO_2 and other harmful gases into the atmosphere, enabling the production of low-carbon electricity. Nonetheless, using this technology does come with some drawbacks, such as a low hydrogen-to-carbon ratio when compared to other technologies, as well as the likelihood of impurities in the feedstock, such as sulfur, nitrogen, and minerals. The process can also be quite complex and expensive, requiring significant amounts of energy and water [3].

2.1.3 Hydrogen from natural gas

Below are presented some details on the main technologies used to produce hydrogen from natural gas, including steam methane reforming, autothermal reforming, and methane pyrolysis.

2.1.3.1 Steam Methane Reforming

Steam methane reforming (SMR) is currently the most widely used and established technology for the large-scale production of hydrogen from natural gas. It has been in use for several years and accounts for 48% of global hydrogen production [10]. This method is cost-effective and utilizes natural gas and water as fuel and feedstock [11]. However, it also generates significant greenhouse gas emissions, making it the highest contributor among natural gas reforming technologies. Moreover, it has negative impacts such as fossil fuel depletion and water consumption. To tackle these issues, integrating carbon capture utilization and storage (CCUS) technology shows promise. By implementing CCUS, emissions can be reduced by up to 50% to 92%, and captured carbon dioxide can be utilized in other applications [3] [10] [12].

2.1.3.2 Autothermal reforming

Autothermal reforming is a technology utilized for producing hydrogen from natural gas, which bears a resemblance to steam methane reforming. The key distinction lies in the fact that it generates its own heat within the reformer. By employing oxygen and steam, methane is partially oxidized inside reforming tubes, resulting in higher reforming temperatures and enhanced methane conversion compared to SMR. This technology provides a notable advantage in terms of carbon dioxide capture within the reactor, as it improves the capture rate when compared to SMR. Consequently, the costs associated with carbon dioxide capture are reduced. However, the production costs are higher than steam methane reforming due to the elevated purity requirement for oxygen [3] [10] [12].

2.1.3.3 Methane Pyrolysis

Methane pyrolysis offers an alternative approach to obtaining hydrogen from natural gas. This method involves directly splitting methane, the primary component of natural gas, into hydrogen and carbon. Unlike other techniques, it does not rely on steam, oxygen, or air, thereby eliminating the production of harmful byproducts like carbon monoxide and dioxide [10] [13]. Moreover, the hydrogen produced through this process is inherently pure, eliminating the need for additional purification steps. However, effectively managing the carbon generated during the process remains a challenge. Although the technology is still in the developmental stage, its potential for large-scale production is limited due to insufficient investment. Additionally, the cost and complexity of the pyrolysis process depend on factors such as the desired level of conversion and purity required for different applications [3] [11].

2.1.4 Hydrogen from biomass

When it comes to producing hydrogen from biomass, there are two primary technologies used: biomass gasification and biomass steam reforming, presented below.

2.1.4.1 Biomass gasification

Biomass gasification is a technology that shares similarities with coal gasification. It involves converting biomass into syngas, which consists of hydrogen, methane, carbon monoxide, nitrogen, and carbon dioxide. This syngas can then be further processed to obtain hydrogen and other desired components. The oxidizing agent used in the process can be air, oxygen, or steam [3] [14]. One notable advantage of biomass gasification is its high energy conversion efficiency and its potential to achieve negative carbon emissions, particularly when renewable biomass is used. This makes it a promising option for green hydrogen production [15].

However, biomass gasification is a complex process, and achieving low-emission hydrogen production from biomass requires substantial effort. The feasibility of large-scale biomass gasification plants largely depends on the availability of cost-effective biomass [3]. Despite the challenges, biomass gasification is considered a promising alternative to the natural gas reforming technologies mentioned earlier [16].

2.1.4.2 Biomass steam reforming

Biomass steam reforming is a technology used to produce hydrogen from syngas generated through biomass gasification. By reacting the syngas with steam at high temperatures, the carbon-to-hydrogen mass ratio is reduced, leading to a higher concentration of hydrogen in the final product. If biomass is sourced sustainably, it is possible to achieve negative carbon dioxide emissions during the process, which can then be captured and stored. However, the broad implementation of biomass steam reforming faces challenges due to the availability and high costs of biomass feedstocks [14].

2.1.5 Other technologies

In addition to the aforementioned technologies, there are numerous other methods for hydrogen production that are either currently available or predicted to be used in the future. However, in order to avoid an excessively lengthy analysis of existing and future technologies, the study will focus on describing the most significant and widely used ones that hold the greatest potential. Examples of these technologies include microbial electrolysis [17], dark fermentation [18], and photoelectrochemical (PEC) water splitting [19], among others.

It is important to note that the technologies mentioned above are still in less mature stages of development and deployment. Further advancements and innovations are expected to enhance their efficiency, cost-effectiveness, and widespread adoption in the future.

2.2 Hydrogen-based fuels

Hydrogen-based fuels can be generated by subjecting hydrogen to various chemical reactions, resulting in the production of different fuel options. These fuels include ammonia, synthetic methane, synthetic diesel (kerosene), and synthetic methanol.

The utilization of these hydrogen-based fuels offers potential solutions to the challenges posed by hydrogen's low energy density. Furthermore, they can be conveniently transported, stored, and distributed using the current infrastructure, possibly lowering costs to the final users [3].

2.2.1 Ammonia

Ammonia consists of hydrogen and nitrogen, making it a carbon-free compound that does not contribute to greenhouse gas emissions. It can be produced from various sources, including fossil fuels, but it can also be synthesized through 100% renewable processes [3] [20]. The most commonly used method for ammonia production is the Haber-Bosch process [21]. Compared to hydrogen, ammonia offers the advantages of lower storage pressure and volume, leading to significant reductions in storage and transportation costs. Additionally, since there is already existing infrastructure for ammonia and well-established production chains, it presents itself as an optimal candidate for replacing fossil fuels with relatively low investments [20]. However, the main challenge associated with ammonia lies in its toxicity, which demands careful handling and additional training for operators, and the high energy requirements for the reconversion back to hydrogen [3] [22].

2.2.2 Synthetic methane

Methanation is an exothermic catalytic process that produces synthetic methane (CH_4), and one of its main advantages is the ability to utilize excess carbon monoxide (CO) and carbon dioxide (CO_2) [3] [22] [23] [24]. When coupled with low-carbon hydrogen (H_2) and CO_2 inputs, methanation has the potential to fully decarbonize the gas [24]. Synthetic methane produced through methanation can be used in existing natural gas grids for specific applications such as residential and industrial use. To enable the widespread adoption of synthetic methane, investments in methanation plants would be required [25]. Additionally, efforts should be made to improve the efficiency of the methanation process to enhance its viability and economic competitiveness. These investments and improvements are crucial for successfully integrating synthetic methane into the existing gas infrastructure and achieving decarbonization goals [22] [23].

2.2.3 Synthetic diesel

Synthetic diesel, also known as kerosene, is derived from the combination of hydrogen and carbon monoxide. Alternatively, it can be produced from carbon dioxide, which needs to be converted to carbon monoxide first [3] [26] [27]. The production method for kerosene is called Fischer-Tropsch (FT) synthesis, which comprises three stages: syngas generation, FT synthesis, and refining of the synthesized crude to obtain the final product [26]. By incorporating renewable electricity and green hydrogen into the FT process, synthetic diesel can be rendered environmentally friendly, thereby reducing emissions associated with its production [27]. However, a notable drawback of FT synthesis is its sluggishness and the requirement for relatively high costs [3] [25].

2.2.4 Synthetic methanol

Synthetic methanol can be generated through hydrogenation technology by combining carbon dioxide and hydrogen, or by using carbon monoxide (derived from carbon dioxide) and hydrogen [25] [28] [29]. Synthetic methanol, which is the simplest form of alcohol, boasts a higher energy density compared to hydrogen and is easily transportable. It possesses water solubility and biodegradability [3] [28]. Methanol holds immense potential and offers various future prospects as a low-carbon fuel, energy carrier, or blending component for fuels [29]. Consequently, ensuring a green production process for synthetic methanol necessitates careful consideration of the hydrogen source. Utilizing hydrogen derived from renewable energy sources can effectively meet this objective [28].

2.3 Hydrogen and its derivatives transport and storage methods

The literature review extensively explores the various methods utilized for the transportation and storage of hydrogen. It carefully examines the strengths and weaknesses of each approach, considering factors such as efficiency, cost, safety, and environmental impact. By presenting a comprehensive summary of the most recent research and technological advancements in this domain, along with the key considerations influencing the choice of appropriate transport and storage techniques for diverse applications, the review strives to provide valuable perspectives on this significant field.

For hydrogen to be transported, it needs to be in one of three forms: pure hydrogen that is either pressurized or in liquid form, or in the form of hydrogen carriers like ammonia and liquid organic hydrogen carriers (LOHC). Therefore, hydrogen must undergo compression, liquefaction, or chemical reactions to be converted into different types of energy carriers [30].

The transport of hydrogen across the value chain can be accomplished through four primary methods: via rail, ships, trucks, or pipelines [3]. One of the persisting challenges with hydrogen is its low energy density, which can result in high costs when transported over long distances [3] [31]. To address the high costs associated with transporting hydrogen over long distances, various options are available, including liquefaction, compression, or incorporating hydrogen into larger molecules in different forms, as mentioned earlier [3] [30].

2.3.1 Transmission

When it comes to transmitting hydrogen or hydrogen-based carriers, as previously mentioned, there are four primary methods, transmission pipelines, trucks, rail, and ships. Regarding pipelines, there are three potential options: retrofitting and repurposing the existing natural gas pipelines to the use of hydrogen, blending hydrogen into existing natural gas grids, or establishing new infrastructure with dedicated pipeline and shipping networks. Each approach has its own set of advantages, disadvantages, and associated costs [3] [22] [30].

The global presence of natural gas grids offers a significant advantage in terms of retrofitting and repurposing existing pipelines for hydrogen transmission. Nonetheless, retrofitting and repurposing natural gas pipelines will necessitate substantial reconfiguration and adaptation. Extensive research is required, for onshore and offshore pipelines, to achieve success in this endeavor. If successful, this will enable increased hydrogen circulation and result in a significant reduction in overall costs [30] [31]. Several critical aspects require assessment before utilizing existing natural gas grids for hydrogen transmission. These considerations arise from differences between natural gas and hydrogen properties. Notably, natural gas boasts three times the calorific heating value of hydrogen, resulting in hydrogen's higher flow velocity, which can be up to three times greater than that of methane. This phenomenon allows the same pipeline to transport three times the volume of hydrogen within a given timeframe at the same pressure, with only a slightly reduced energy transportation capacity. Another concern pertains to the integrity of steel pipes and fittings, which may exacerbate crack propagation and reduce operational lifetimes by up to 50 percent. Additionally, adapting the compressors initially designed for natural gas is imperative to enable the transition to hydrogen [32].

Blending hydrogen into existing natural gas grids is considered one of the most favorable options for the initial transition from natural gas to hydrogen. This approach offers the advantage of minimizing the need for significant upfront investments in new infrastructure, thanks to the widespread presence of natural gas grids worldwide. Implementing such a system has the potential to drive substantial growth in global hydrogen usage, leading to a reduction in carbon emissions associated with natural gas. However, there are several challenges that need to be addressed when using natural gas grids for hydrogen transportation. One challenge is the higher burning rate of hydrogen compared to methane, which increases the risk of flames spreading invisibly. Moreover, there are limitations related to the materials used in the pipelines, which may impose restrictions on the maximum capacity for hydrogen blending. The varying volume of blended hydrogen may also have adverse effects on equipment operation, as it is typically designed to handle specific gas mixtures within narrow ranges. Currently, blending specifications typically range from 2% to 8%, but there is belief that it could potentially be increased to 20%. Although, there are still uncertainties regarding the long-term impacts on infrastructure. Additionally, higher operational costs are expected due to the adjustments required for handling hydrogen within the existing natural gas infrastructure [3] [30] [31].

Long-distance transmission using dedicated hydrogen pipelines encounters notable challenges due to the substantial capital costs involved and the requirement for securing rights of way. Moreover, the low density of hydrogen necessitates the transportation of large volumes, resulting in additional cost escalations. However, the transportation of ammonia through pipelines presents a feasible and comparatively simpler alternative, offering significantly reduced expenses compared to utilizing pure hydrogen grids. Nevertheless, it is important to consider the costs associated with the reconversion of ammonia back into hydrogen [3] [30] [31] [33].

The use of trucks for hydrogen transmission is a well-established option, offering versatility in transporting hydrogen in different forms, including gas, liquid, or through energy carriers like ammonia or LOHC. However, for longer distances, trucks may not be the most cost-effective solution and could encounter challenges with boil-off. Liquid hydrogen transportation via trucks becomes more feasible for extended distances. Additionally, there are limitations on the quantities that can be transported by trucks. Nonetheless, trucks hold a significant advantage in their ability to deliver hydrogen to multiple locations before requiring connection to a pipeline [3] [22] [30].

Trains are an alternative option for hydrogen transmission, although they are still in the intermediate stage of development and not utilized in the final use form. Trains offer the advantage of facilitating longer transportation distances and handling larger quantities of hydrogen compared to trucks, all at reduced costs. However, it is worth noting that trains have limited flexibility when it comes to route selection [22].

Shipping offers a potential method for transporting hydrogen over long distances, although it is not practical to ship pure hydrogen. Instead, options such as liquid hydrogen (for shorter distances), ammonia, LOHC, and synthetic hydrocarbon fuels can be employed. Among these alternatives, LOHC is considered the preferable choice, despite the challenges associated with conversion and reconversion processes back to hydrogen. However, establishing the necessary shipping infrastructure, including storage tanks, liquefaction and regasification plants, as well as conversion and reconversion facilities, would require significant capital investment, especially in terminal areas. As hydrogen trade between countries continues to grow, these costs could potentially be offset by the substantial quantities of hydrogen being traded [3] [30] [31].

2.3.2 Distribution

The local distribution of hydrogen, ammonia, or LOHC depends on various factors, including volume, distance, and the specific requirements of end-users. Distribution can be achieved through either trucks or pipelines. Liquid hydrogen tanker trucks are the preferred method for truck transportation due to their comparatively lower transport costs and high demand, which helps offset the expenses involved in the liquefaction process. Similarly, trucks can be used for transporting ammonia or LOHC. Dedicated hydrogen pipelines, as mentioned earlier, entail significant capital costs for long-distance transmission, and even for local distribution, the costs remain substantial. Establishing a gas distribution network involves a complex system comprising pressure-reducing stations, metering stations, valve stations, main lines, service lines, injection stations, and blending stations for decarbonized gases. This complexity poses a challenge for the widespread use of hydrogen in heating buildings, where the pipeline costs at such a scale become even more substantial. While the distribution of ammonia is relatively less expensive, its viability is contingent upon demand. On the other hand, transporting LOHC through pipelines for transmission may not be feasible [3] [22] [30].

Ultimately, decisions regarding the use of these various options for hydrogen distribution and transmission will depend on factors such as the scale of production, demand, distance, and associated costs.

2.3.3 Storage

Ensuring flexibility and security of energy supply is essential in any energy system, especially during periods of low energy production and high demand. As the world strives towards decarbonization objectives, the utilization of renewable energy sources becomes crucial. To address the challenge of matching energy supply with demand, energy storage solutions play a significant role, and hydrogen emerges as a promising candidate [3] [30] [34].

Hydrogen offers diverse easy and safe storage methods, including high-pressure storage as hydrogen gas, low-temperature storage as liquefied hydrogen, and alternative hydrogen-based energy carriers such as ammonia and LOHC [3] [30] [33]. Compressed gas hydrogen, being the oldest and most established technology, requires either low temperature or high pressure for storage due to its low density. It offers the advantage of fast filling and release. On the other hand, liquid hydrogen storage also operates at low temperatures but may face issues with boil-off. Nevertheless, it boasts high liquid density and storage efficiency compared to other options. Ammonia necessitates a significant amount of energy for storage, while LOHC demonstrates promising potential in liquid-state hydrogen storage, reducing energy losses and enabling extended storage times. The primary challenge with LOHC lies in the high temperature required for its production. These alternative carriers facilitate safer and more convenient transportation and storage of hydrogen [34].

The selection of appropriate storage types depends on several factors such as required storage volume, discharge rate, injectability, discharge duration, response time, energy intensity, cost per unit stored, safety, location, and time to market. In general, these storage options can be broadly categorized into two groups: geological storage and storage tanks [3] [30] [35]. In addition, there is a third type of hydrogen storage known as solid-state hydrogen storage, which is currently undergoing investigation and development to enhance its potential [34].

Geological storage offers various underground options for hydrogen storage, such as salt caverns, depleted natural gas or oil reservoirs, and aquifers. This method is widely considered the most suitable choice for large-scale and long-term storage [30] [36]. These geological formations, already used for natural gas storage, can be readily adapted for hydrogen storage. The advantages of utilizing geological storage for hydrogen include significant economies of scale, high efficiencies, and cost-effectiveness in terms of operations and land usage [3].

However, for short-term and smaller-scale storage needs, storage tanks present a more suitable solution due to geographic considerations, minimum pressure requirements, and their smaller sizes. There are two main types of storage tanks for hydrogen: compressed or liquefied hydrogen and ammonia. Both compressed and liquefied hydrogen tanks offer excellent discharge rates and efficiencies, reaching approximately 99%. In contrast, ammonia tanks would be smaller in size due to their higher energy density. Nevertheless, the process of converting and reconverting ammonia into pure hydrogen incurs energy losses and requires specific equipment. [3] [34].

2.4 End uses of hydrogen and its derivatives in different sectors

The literature review investigates the diverse end-user applications of hydrogen in different sectors, such as heating systems in buildings, transportation for passengers and freight, and process heat in industries. Hydrogen can be utilized in various forms, including hydrogen boilers, fuel cells, hybrid systems, hydrogen fuel cell vehicles, internal combustion engines fueled by hydrogen, high-temperature fuel cells, and hydrogen combustion in boilers and furnaces. The review explores the current state of research and development, as well as the efficiency, costs, and environmental impacts associated with these applications.

2.4.1 Industrial uses

Industrial applications account for the majority of the hydrogen demand, representing around 74% of the global demand. The primary end-uses of hydrogen in the industry include the chemical sector, oil refining, iron and steel production, and high-temperature heat. Unfortunately, nearly all of the hydrogen utilized by these industries comes from fossil fuels, such as coal, oil, or natural gas, leading to the associated carbon emissions [3] [31].

2.4.1.1 Oil refining

Approximately 33% of the global demand for hydrogen is attributed to oil refining [22]. The main objective of oil refining is to convert crude oil into various end products, including transportation fuels and petrochemical feedstocks. Within this context, hydrogen plays a crucial role in two primary processes: hydrotreatment and hydrocracking [3] [31] [37] [38].

Hydrotreatment is employed to enhance the hydrogen content of products, thereby eliminating impurities, primarily sulfur, and saturating olefinic aromatic bonds in the presence of a catalyst. Hydrocracking, on the other hand, is utilized to convert heavy residual oils into higher-value oil products while removing polluting elements. Roughly two-thirds of the hydrogen used in these processes is produced in specialized fossil fuel plants situated near the refinery, obtained through merchant supply, while the remaining portion is derived as by-products within the refinery itself. Some of this hydrogen is consumed and burned as fuel in specific waste gas mixtures [3] [22] [39].

As oil product sulfur content regulations are projected to become more stringent, it is expected that demand for hydrogen will increase, which could lead to growth in the use of hydrogen in cleaner production methods [3] [31].

2.4.1.2 Chemical sector

The chemical sector currently represents 38% of the global hydrogen demand, primarily driven by the production of ammonia and methanol. It also plays a role in manufacturing other chemicals such as ethylene, propylene, benzene, toluene, and mixed xylenes. Hydrogen serves as a crucial feedstock in these processes, creating a substantial need for its production in large quantities [3] [22] [40].

At present, natural gas and coal are the primary sources of hydrogen due to their cost-effectiveness and the generation of carbon, which is an essential component for ammonia and methanol production. Methane reforming and coal gasification are the primary technologies employed for hydrogen production in this sector, with methane reforming being more commonly utilized [3] [41].

However, the production of methanol and ammonia using hydrogen as a feedstock results in significant carbon dioxide (CO_2) emissions. Therefore, it is vital to explore cleaner methods of hydrogen production, even if they entail increased costs. Policy measures can play a crucial role in driving demand for low-carbon hydrogen in the chemical sector, potentially leading to increased investments in cleaner hydrogen supply. This would help reduce emissions and encourage efficiency measures that could lower the overall demand for hydrogen in the future [3] [41] [42].

2.4.1.3 Iron and steel production

Presently, the demand for hydrogen in the iron and steel production sector accounts for approximately 3% of the total hydrogen demand. However, in the future, hydrogen is expected to play a crucial role in this industry as a means to reduce emissions and save costs. The integration of low-emission hydrogen into existing processes that rely on natural gas and coal can help decrease carbon intensity [3] [40].

In the iron and steel sector, hydrogen is often produced as a by-product and is commonly mixed with other gases. This hydrogen can be utilized within the industry itself or distributed to other sectors for consumption [3] [43].

Two primary technologies are used in steel production: blast furnace-basic oxygen furnace (BF-BOF) and direct reduction of iron-electric arc furnace (DRI-EAF). The BF-BOF method, which represents about 90% of steel production, generates hydrogen as a by-product of coal, along with other gases. On the other hand, the DRI-EAF method accounts for approximately 7% of global primary steel production and utilizes a mixture of hydrogen and carbon monoxide as a reduction agent. Natural gas is typically the primary source of hydrogen for these processes [3] [22] [41] [43].

The demand for hydrogen in the steel industry is projected to increase, offering an opportunity to address associated emissions. By providing cleaner hydrogen or incorporating carbon capture, utilization, and storage (CCUS) technologies when utilizing hydrogen derived from fossil fuels, it is possible to mitigate emissions related to the steel sector [22] [31] [43].

2.4.1.4 Industrial heat

Approximately 40% of emissions in industrial applications result from fuel combustion for heating purposes, with a significant portion attributed to electricity generation processes. Heat plays a vital role in numerous industrial operations such as melting, gasifying, drying, and chemical reactions. As medium to high-temperature heat is predominantly required for these processes, hydrogen can play a crucial role in decarbonizing the heating sector [3] [41].

Currently, the applicability of hydrogen in industrial high-temperature applications may be limited. Fossil fuels have traditionally been the primary source of heat, although electricity, biomass, and waste are also utilized to a lesser extent. To address the imperative of reducing carbon emissions, there is significant potential in transitioning to sustainable bioenergy, hydrogen, hydrogen-based fuels, and hydrogen-methane blends for combustion [3] [41].

Hydrogen burners, which involve a mixture of hydrogen and oxygen, can be one of the solutions to reduce emissions of carbon monoxide (CO) and carbon dioxide (CO_2). One significant drawback of hydrogen burners is their elevated nitrogen oxide (NO_X) emissions, which remain considerably higher when compared to those of natural gas burners. Existing industrial burners could potentially be converted to operate with hydrogen instead of natural gas [41] [44]. However, the current cost of hydrogen remains higher than that of fossil fuels, posing a challenge to its widespread adoption in industrial settings [3].

2.4.2 Transport sector

The transport sector holds significant promise for adopting hydrogen as a fuel source, contingent on the improved competitiveness of production and utilization costs. Nearly all modes of transportation, as detailed in the subsequent sections, possess the capacity to function using hydrogen or hydrogen-based fuels [3].

2.4.2.1 Road transport

The road transport sector currently heavily relies on fossil fuels, leading to significant CO_2 emissions released into the environment. To achieve independence from fossil fuels, electrification is considered the preferable solution. Hydrogen can be used as a fuel for road transport through two options: fuel-cell powered vehicles (FCEVs) or internal combustion engine vehicles (ICEs). This applies to cars, buses, trucks, and other goods vehicles [3] [30].

In small vehicles, hydrogen fuel cell electric forklifts have already gained commercial viability. These forklifts use compressed hydrogen gas stored in tanks and convert it into electricity through a fuel cell, powering an electric engine. Hydrogen bikes are still in the development and demonstration phase. They rely on compressed hydrogen gas cylinders, and the fuel cell converts hydrogen into electricity to power an electric motor. However, bikes still require human muscular energy for motion, and further development and testing are needed for wider adoption [22].

Hydrogen-powered scooters, using fuel cells, are already available for deployment, providing emission-free and low-noise mobility solutions for intra-city travel [22]. Cars are a significant application for hydrogen, primarily through fuel-cell power or internal combustion engines, similar to hydrogen scooters. However, electric vehicles (BEVs) are expected to experience more significant growth due to higher overall efficiency compared to fuel-cell vehicles. By 2050, fuel-cell electric vehicles (FCEVs) are estimated to represent about 4% of the market share [3] [30] [45].

Fuel cell electric buses offer a promising solution for long-range transportation, as they don't require frequent recharging, allowing for extended mileage and operational flexibility. They additionally ensure zero emissions of greenhouse gases (GHGs) and produce less noise pollution, making them a viable contender for cost-competitiveness against the existing options of electric and diesel buses. [3] [22].

In the realm of heavy-duty and long-distance commercial vehicles, hydrogen is seen as an alternative fuel [41]. Initially, biomethane may play a transitional role, but the focus will shift towards electricity and hydrogen. Some trucks can be equipped with hydrogen tanks and use a combination of proton exchange membrane (PEM) fuel cells, lithium-ion batteries, and electric motors for efficient energy conversion and storage, resulting in reduced emissions and increased range [3] [22] [30].

The widespread adoption and cost-effectiveness of hydrogen-based transportation options hinge on global implementation and supportive policies. To facilitate this, it is crucial to establish hydrogen refueling stations that ensure a steady supply and support the growing demand for hydrogen. A well-coordinated expansion of both vehicle and refueling station networks is essential to promote the broader use of hydrogen-based transportation, leading to significant reductions in greenhouse gas emissions and fostering a more sustainable and environmentally friendly transport sector. By investing in infrastructure and implementing supportive policies, we can accelerate the transition to a cleaner and greener transportation system, benefiting both the environment and society as a whole [3] [31].

2.4.2.2 Maritime transport

Maritime transportation is renowned for its high energy efficiency in terms of energy per tonne-kilometer [30]. However, the extensive use of oil-based products and international shipping routes results in the sector contributing significantly to global CO_2 emissions [3].

To decarbonize the maritime sector and reduce emissions, hydrogen in the form of hydrogen-based fuels, such as ammonia, e-methanol, e-methane, and various biofuels, emerges as a promising option [30] [41]. Integrating hydrogen-based fuels in ships not only lowers emissions but also fosters the utilization of hydrogen in ports, thereby improving air quality and creating synergies with forklifts, trucks, and cargo movement. Nevertheless, this transition necessitates the development of supporting infrastructure, including storage facilities, bunker vessels, and pipelines or trucks for hydrogen transportation to ports [3].

For shorter voyages, fuel cells could potentially be employed in ferries, but for long-distance ships, fuel cell systems, and hydrogen storage have a lesser impact on costs compared to fuel expenses. To facilitate widespread adoption and achieve cost reductions, larger facilities and broader deployment of infrastructure become essential [3] [30] [45].

In the future, ship designs may require adaptation to accommodate shorter trips with more frequent refueling or reduced cargo volumes, taking into account the increased volume requirements of hydrogen or ammonia as compared to oil-based fuels. Hydrogen occupies five times more volume, while ammonia requires three times more volume. To harness the potential of hydrogen-based fuels and achieve significant emissions reductions in the maritime sector, proactive measures and infrastructure investments will be essential. These investments will play a crucial role in promoting a more sustainable and environmentally friendly shipping industry. By anticipating the volume challenges and strategically planning for refueling and cargo considerations, we can pave the way for a successful transition to hydrogen-based fuels and contribute to a cleaner and greener future for the maritime industry [3] [22] [30].

2.4.2.3 Aviation

The aviation sector significantly contributes to annual CO_2 emissions, and while efforts are being made to improve efficiency and reduce fuel consumption, the adoption of alternative fuels remains crucial to achieve substantial emission reductions. In this regard, hydrogen-based fuels present a promising solution [3] [41].

Currently, pure hydrogen presents challenges due to its low energy density and the need for cryogenic storage, which would necessitate significant changes in aircraft design and airport infrastructure. Ongoing research aims to explore the feasibility of using hydrogen in different types of flights, including short (use of fuel cells), medium, and long-haul journeys. However, the most viable near-term alternative lies in hydrogen-based fuels that do not require modifications to aircraft design or airport refueling infrastructure. Nevertheless, their main drawback is the cost, which could be four to six times higher than conventional fuels. Since fuel constitutes a significant portion of aircraft operating costs, the use of hydrogen-based fuels would lead to substantial increases in operational expenses. As a result, the primary approach is to blend hydrogen-based fuels with conventional jet fuels at a certain percentage to strike a balance between emission reduction and cost efficiency [3] [22] [41] [45].

2.4.2.4 Rail

Rail transport has seen significant electrification, especially in countries where electrification is well-established or still in progress for heavily utilized rail lines, to replace large amounts of diesel trains. Furthermore, some companies in specific countries are exploring the development of fuel-cell trains, indicating a growing interest in utilizing fuel-cell technology as an alternative power source for rail transportation. While there are associated costs, hydrogen fuel cell technology proves most competitive for services requiring long-distance movement of large trains with low-frequency network utilization [3] [22] [31] [41].

In the rail sector, hydrogen can be applied not only to trains but also in conjunction with forklifts, trucks, and other equipment at railyards. This integration brings about cost reductions and enhances the flexibility of hydrogen usage across various applications within the rail industry. This growing interest in hydrogen as a power source for rail transport holds promising potential for improving the sector's environmental impact and fostering more sustainable and efficient rail operations [3].

2.4.3 Buildings sector

The global buildings sector currently accounts for approximately 30% of the total final energy use each year, heavily relying on fossil fuels, especially natural gas, for heating purposes. The remaining energy demand is fulfilled by conventional electric equipment powered by electricity. Fully replacing fossil fuels with low-carbon alternatives in this sector is challenging due to the substantial heat requirements of buildings [3] [31].

Considering the diverse nature of buildings in terms of type, location, ownership, customer preferences, equipment costs, energy prices, and convenience, it is expected that a variety of energy sources and technologies will coexist in the future. This coexistence will provide flexibility to the overall energy network. Various options involving hydrogen are being explored to supply heat to buildings. These options include blending hydrogen with natural gas through existing gas grids, employing methanation processes, utilizing 100% hydrogen gas in hydrogen boilers, and adopting fuel cells and cogeneration systems. Each of these approaches offers potential solutions to reduce carbon emissions in the building sector while providing alternative and sustainable sources of heat. By embracing these diverse approaches, the buildings sector can make significant strides towards a more environmentally friendly and energy-efficient future [3] [31] [46].

2.4.3.1 Blending hydrogen

Blending hydrogen into existing natural gas grids is considered a cost-effective option due to the already established infrastructure, requiring minimal adjustments [3] [31] [47]. To ensure minimal impact on end-use equipment, hydrogen is typically blended at low percentages, around 3% to 5%. However, for higher shares of hydrogen, comprehensive efficiency, and performance tests are necessary, along with upgrades to the existing systems. This is particularly important as some infrastructure and equipment might be outdated and unsuitable for handling higher concentrations of hydrogen [3] [22].

Several challenges arise when blending higher percentages of hydrogen into natural gas. Firstly, hydrogen's lower energy density in gas form reduces the overall energy transported through the grid. Secondly, there is a higher risk of flame spreading due to hydrogen's high flame velocity. Additionally, the variability in hydrogen volumes can pose operational risks for certain end-use equipment. The safe maximum share of hydrogen that can be blended into the natural gas grid is limited by the capabilities of the equipment to handle it [3] [22].

To achieve higher hydrogen shares, such as 20%, in residential and industrial applications, hydrogen-based fuels like synthetic methane can be considered. This approach allows for the injection of synthetic methane into the gas grid without the need to replace or upgrade major applications. However, it is essential to note that this method would significantly increase gas prices compared to using pure hydrogen blends due to the higher cost per unit of delivered energy. Careful consideration and evaluation of these options are crucial in effectively transitioning towards a more hydrogen-inclusive energy system while addressing the associated challenges and economic implications [3] [22] [47].

2.4.3.2 100% hydrogen

The use of 100% hydrogen in the context of heating buildings presents a promising opportunity, particularly for large commercial buildings, building complexes, and district energy networks [3] [45]. Hydrogen boilers or fuel cells can be employed to provide the required heating in such settings. To meet energy storage requirements and ensure a stable energy supply for buildings, fuel cells (low-temperature and high-temperature), co-generation technologies, or hybrid systems can be utilized, especially in district energy networks. These implementations contribute to improving the balance and flexibility of the power grid by minimizing large seasonal peaks [3] [22] [41] [45] [48].

Additionally, combining district energy options with large-scale heat pumps can significantly enhance the overall efficiency of heat production for buildings. However, the choice of technology and system will ultimately depend on cost considerations, as some customers prioritize upfront purchase prices over lifetime costs. Different building types may be better suited for hydrogen applications, and the potential market for hydrogen-based heating solutions is considerable [3] [31].

For these hydrogen-based heating solutions to flourish, close coordination among policymakers, industry stakeholders, and investors is crucial. Additionally, support from consumers and the equipment service sector plays a pivotal role in ensuring the successful adoption of hydrogen technologies in the buildings sector. Together, through this collaborative effort, we can make significant strides towards achieving low-carbon objectives and realizing the full potential of hydrogen as a clean and sustainable energy source for heating buildings [3] [31] [45].

2.4.4 Power generation and electricity storage

At present, hydrogen's presence in power generation and electricity storage is limited, making up less than 0.2% of total electricity generation [31]. However, there are several promising applications for hydrogen and hydrogen-based fuels that can actively contribute to this sector. These applications include co-firing ammonia in coal power plants, supporting flexible power generation through gas turbines, combined cycle gas turbines (CCGTs), and fuel cells, as well as enabling large-scale and long-term energy storage to address fluctuations in electricity demand caused by seasonal variations and variable renewable power generation, as previously mentioned in subsection 2.3.3 [3] [41] [45].

2.4.4.1 Co-firing ammonia

Coal-fired power plants are widely utilized worldwide for electricity generation, but there is a promising approach to decrease coal consumption and carbon emissions at a low cost. This involves co-firing hydrogen-based fuel, particularly ammonia [3] [22] [49]. The advantage of this method lies in its feasibility to blend ammonia, up to 20% in a coal power plant, without significant modifications to the existing infrastructure. This offers a clear advantage for implementation [3] [22].

Apart from the potential reduction in CO_2 emissions associated with coal combustion, the use of ammonia can also lead to lower NOx emissions [50], but some treatment may be required. However, the effectiveness of CO_2 reduction hinges on the availability of low-carbon ammonia. To achieve cost-effectiveness, it is essential to ensure a reliable supply of low-cost ammonia derived from low-carbon hydrogen sources [3] [22].

2.4.4.2 Flexible power generation

Multiple viable options exist to enhance power generation flexibility through the utilization of hydrogen and hydrogen-based fuels. One such option is employing hydrogen as a fuel in gas turbines and combined cycle gas turbines (CCGTs) [45] [51]. Currently, these turbines can handle up to 3-5% hydrogen, but it is anticipated that in the future, standard turbines will be able to run on 100% hydrogen. Additionally, ammonia can be utilized as a fuel in gas turbines, though it poses challenges related to controlling NO_x emissions and maintaining flame stability. An alternative approach involves converting ammonia back to hydrogen, which can then be used in gas turbines. However, this process may lead to a decrease in overall efficiency [3] [22] [31].

Another avenue for enhancing power generation flexibility is through the use of fuel cells, which offer similar efficiencies to CCGTs. The choice between fuel cells and CCGTs depends on the associated costs, and the most suitable option should be determined through a comprehensive evaluation of the economic factors involved. Balancing power generation can be achieved effectively through the thoughtful consideration and integration of these various options [3] [22] [31] [45] [51].

2.5 Efficiency and costs in the hydrogen chain

In the literature review, an in-depth analysis is conducted on the efficiency and cost-related aspects of the hydrogen value chain. This investigation focuses on evaluating the conversion efficiency at each stage of the value chain, as well as examining the capital expenditures (CAPEX) and operational expenditures (OPEX) associated with hydrogen production, transportation, storage, and its applications in various sectors. The review aims to consolidate the available information on efficiency and costs, offering a comprehensive overview of the current state of the hydrogen economy. It also highlights the key factors that impact the competitiveness of hydrogen in different sectors. To gather data, the JRC-EU-TIMES model (References [52] and [53]), the IEA database (References [54] and [55]), and other relevant articles from the literature were utilized as primary sources. To avoid overwhelming the main chapter, the collected data is systematically organized into tables and presented in the Annexes (Chapter A).

Chapter 3

Energy Modeling

In this chapter, we will delve into the realm of energy models and their structural aspects. Our primary focus will be on the specific model employed in this project, OSeMOSYS, and its comprehensive exploration of hydrogen's definition and implications within the energy context.

3.1 Energy System Models

Energy plays a vital role in all aspects of societal activities across nations. Therefore, it is imperative to exercise prudent control over energy demand since the future of the world depends on the choices we make today. Optimal management of energy resources has emerged as the top priority for energy planners and policymakers, recognizing the critical need to handle these resources efficiently. To achieve sustainable development, an integrated approach to energy management is indispensable for any country. This approach encompasses the comprehensive exploration of all available options, with a particular emphasis on harnessing renewable energy sources. Key aspects of this integrated energy management approach include maximizing the effective utilization of energy resources, ensuring a reliable supply, implementing efficient resource management practices, promoting energy conservation, adopting combined heat and power systems, incorporating renewable energy systems, developing integrated energy systems, and establishing independent power delivery systems, among others [6].

To ensure a smooth transition of the energy system towards cleanliness, sustainability, and cost-effectiveness, it is crucial to consider the entirety of the energy network. This network encompasses all energy carriers, from primary sources to conversion and processing methods, as well as the end-use demands across various sectors, each with its distinct functions. To facilitate this comprehensive analysis of the energy system, energy system models come into play. These models serve as valuable tools for predicting and exploring future scenarios by making certain assumptions regarding economic behavior, resource requirements, technological advancements, and factors such as economic or population growth. Therefore, energy models present a simplified depiction of actual energy systems and genuine economies [56]. By conducting an overall energy system analysis that takes into account demand, supply, and balance, these models assist in unraveling the complexities of the energy landscape. Energy system models adopt different approaches and concepts, utilizing various mathematical formulations to address the inherent uncertainties associated with long-term projections [57].

When it comes to energy models, they can be categorized into two types: bottom-up models and top-down models. Bottom-up models provide extensive technological details, including technology costs, efficiencies, and environmental impacts. These models adopt a business economics approach to economically evaluate the technologies incorporated within the model. On the other hand, top-down models aim to forecast the overall economy at a national or regional level, taking into account the effects of energy and climate change policies in monetary terms. These models adopt an aggregated perspective on the energy sectors and the economy, simulating economic development, energy demand and supply, employment, and predicting energy price trends [56].

3.2 OSeMOSYS Energy System Model

OSeMOSYS, also known as the Open Source Energy Modeling System, is a bottom-up open-source framework for energy modeling. Its primary aim is to optimize a model for long-term energy planning. What sets OSeMOSYS apart is its user-friendly nature, as it doesn't demand extensive learning skills or a significant time commitment to fully comprehend its inner workings. Moreover, OSeMOSYS's appeal lies in its avoidance of proprietary software, commercial programming languages, and solvers, making it accessible without requiring a substantial financial investment. These attributes make it an attractive choice for students, business analysts, government specialists, and energy researchers alike [58] [59]. These qualities, combined with the enthusiasm of graduate students to learn and construct energy models, foster a collaborative effort aimed at constant improvement and optimization of energy systems. The ultimate objective is to decarbonize these systems and fulfill climate change agreements by reducing emissions and lowering global temperatures.

In summary, OSeMOSYS performs calculations to determine the energy supply mix, taking into account generation capacity and energy delivery, to meet the energy demands of various sectors on an annual basis and at each time step within a given scenario. It accomplishes this by considering a variety of technologies with different techno-economic information. The primary aim of OSeMOSYS is to minimize the total discounted costs associated with the energy system [60]. Additionally, constraints can be incorporated into the models used by OSeMOSYS. These constraints may involve factors such as efficiencies associated with end-users or specific technologies, interrelationships between different types of energy inputs or outputs, limitations on GHG emissions or the utilization of renewable generation, and restrictions on investment costs or energy and power capacity balances. By considering these constraints, OSeMOSYS provides a more comprehensive and realistic representation of the energy system being analyzed [59].

OSeMOSYS offers the flexibility for users to utilize it for specific analyses and provides convenient options for updating and modifying the framework. It is designed with a modular structure comprising various functional blocks. These blocks include a clear and concise plain English description of the model sets, parameters, variables, constraints, and objectives, along with the relationships between them. Additionally, there is an algebraic formulation of the model based on the plain English description. Furthermore, the framework includes the implementation of the model in a programming language and its practical application for conducting analyses [58].

The initial release of the OSeMOSYS code in 2008 featured a structure consisting of seven functional blocks: The objective function, which estimates the Net Present Cost (NPC) of the energy system based on predefined energy demands; Costs that are defined by specific equations that account for capital and O&M costs; Storage, which defines balances and limitations for stored energy within the system; Capacity adequacy, ensuring that the model simulates the required capacity to meet user-defined energy demands at each time step; Energy balance, assuring the yearly balance of energy production and consumption along the entire energy chain; Emissions, accounting user-defined restrictions or penalties related to emissions within a given time period and; Constraints, which enables users to define limits on the installed capacity or production of each technology. Up until now, numerous additional functionalities have been incorporated, including the modeling of smart grids and demand-side flexibility. The system now also supports the provision of reserve capacity, accounting for the cost of cyclic operation of fossil fuel power plants, and offers an enhanced representation of storage [59] [61].

In OSeMOSYS, to build energy system models, it is necessary to define sets, parameters, and variables. Sets define the physical structure of a model, providing the time domain, time split, spatial coverage, technologies, and energy vectors [60]. In this work, the sets utilized to construct the reference energy model and hydrogen conversion chains were TECHNOLOGY and FUEL. TECHNOLOGY represents the conversion of a commodity from one form to another, while FUEL represents all energy vectors, energy services, or proxies that enter or exit each technology.

The user-defined numerical inputs to the model are referred to as parameters [60]. These parameters play a crucial role in completely defining the characteristics of each technology employed and providing a comprehensive description of the energy system under development. Categorically, the parameters utilized in this study can be divided into distinct categories including Demands, Performance, Technology costs, and Emissions.

The parameters used are described below, as stated in [60].

For Demands:

- Specified Annual Demand - Total specified demand for the year, linked to a specific 'time of use' during the year;
- Specified Demand Profile - Annual fraction of energy-service or commodity demand that is required in each time slice. For each year, all the defined Specified Demand Profile input values should sum up to 1.

For Performance:

- Capacity to Activity Unit - Conversion factor relating the energy that would be produced when one unit of capacity is fully used in one year;
- Availability Factor - Maximum time a technology can run in the whole year, as a fraction of the year ranging from 0 to 1. It gives the possibility to account for planned outages;
- Operation Life - Useful lifetime of a technology, expressed in years;
- Input Activity Ratio - Rate of use of a commodity by a technology, as a ratio of the rate of activity;
- Output Activity Ratio - Rate of commodity output from a technology, as a ratio of the rate of activity.

For Technology costs:

- Capital Cost - Capital investment cost of a technology, per unit of capacity;
- Fixed Cost - Fixed O&M cost of a technology, per unit of capacity;
- Variable Cost - Cost of a technology for a given mode of operation (Variable O&M cost), per unit of activity.

To effectively map all value chains within the OSeMOSYS open-source framework, it is essential to have an open-source, accessible, and user-friendly interface. There are three main options available, each varying in difficulty. The first option is clicSAND (Simple And Nearly Done), which is a graphical user interface suitable for beginners. It employs an Excel spreadsheet capable of handling up to 200 technologies, 50 commodities, and 5 types of emissions. The second option, MoManI (Model Management Infrastructure), is designed for medium-skill-level users. It is a browser-based open-source interface that allows users to easily edit and update any part of the modeling process. The final option is otoole, which is a Python package providing a command-line interface. It generates input files through a set of Excel spreadsheets, which OSeMOSYS then process to generate output files. This interface is specifically tailored for advanced users [62]. In this study, the interface employed was otoole, as elaborated in Section 4.5.

3.3 OSeMOSYS vs other modeling tools

The selected framework for this study is OSeMOSYS, as mentioned earlier. This choice stems from its open-source characteristics, adaptability in constructing technological components, and the strong support provided by an active community. Additionally, the presence of an existing base model facilitated the development process. Nevertheless, there are alternative modeling tools available, such as EnergyPlan, or MARKAL/TIMES, each with its unique set of strengths and weaknesses.

EnergyPLAN is a user-friendly tool designed to support the formulation of national or regional energy planning strategies by simulating the entire energy system. Similar to OSeMOSYS, it operates as an optimization tool, fine-tuning the operation of energy systems. Several publications and simulations have already been conducted using EnergyPLAN, focusing on various countries' energy systems [63]. However, it's worth noting that its main drawbacks include its complexity and the steep learning curve required to effectively utilize it.

MARKAL/Times provides an integrated modeling framework and it finds the 'best' reference energy system for each time period, by selecting the set of options that minimises total discounted system cost or the total discounted surplus over the entire planning horizon. This is done within the limits of all imposed policies and physical constraints. As EnergyPLAN it has also some complexity and its learning curve requires more time [63].

OSeMOSYS stands out for its notable advantages compared to other tools. Its reduced complexity and open-source nature create an environment conducive to collaboration within its user community and support academic research. In contrast, when compared to the intricacies of MARKAL/TIMES, EnergyPLAN tends to offer a more accessible learning curve, making it an attractive option for users who are relatively new to energy system modeling.

3.4 Other models

Within the existing literature, numerous articles delve into the examination of hydrogen's impact on specific sectors, including transportation, industry, buildings, and comprehensive conversion chains. These prior studies or models provide valuable insights and serve as a reference for the present work, aiming to validate the obtained results. This subsection will showcase several of these studies, presenting their key findings and conclusions.

The first two studies analyzed were the article titled "How far away is hydrogen? Its role in the medium and long-term decarbonization of the European energy system" and the study "On the feasibility of direct hydrogen utilization in a fossil-free Europe"; both exploring the integration of hydrogen in the European energy system, shedding light on its potential and limitations [2] [64]. The study conducted by the European Commission utilizes the JRC-EU-TIMES model to assess the introduction of hydrogen under different scenarios. It emphasizes the importance of hydrogen in achieving long-term decarbonization goals, particularly in challenging sectors like transport and industry. By incorporating detailed hydrogen chains into the model, including production technologies, delivery pathways, and end-use applications, the study recognizes the positive impact of hydrogen on reducing overall CO_2 emissions. It also acknowledges the flexibility hydrogen provides in balancing energy demands [2]. The second study focuses on the feasibility of direct hydrogen utilization in a 100% renewable energy system in Europe, using the EnergyPLAN software. It examines whether hydrogen can offer economic and operational advantages compared to a system without hydrogen. The findings indicate that while hydrogen usage in small quantities has some benefits in the electricity sector, it increases system costs. For the transport sector, other alternatives such as liquid e-fuels and electrification are considered more favorable due to lower infrastructure costs and higher energy efficiency. In the industry and heating sectors, hydrogen shows potential for reducing biomass consumption, but electrification and e-methane are seen as more viable options [64]. By correlating these two perspectives, it becomes evident that hydrogen can indeed play a significant role in future energy systems. However, the studies suggest that its primary role may be as an e-fuel feedstock and energy carrier, rather than for direct utilization in certain hard-to-abate sectors. While hydrogen can contribute to decarbonization efforts, it is crucial to consider specific sector requirements, cost-effectiveness, and the integration of alternative technologies to achieve optimal results. Both studies emphasize the need for substantial investments in hydrogen infrastructure to support its cost-effectiveness and meet future demands [2] [64].

Following the comprehensive analysis of the aforementioned studies, the analysis covered three additional research papers that specifically investigate the utilization of hydrogen in distinct end-use sectors, including heat in buildings and road transportation. These studies also delve into the broader environmental impacts associated with hydrogen implementation.

The first one is titled "A review of four case studies assessing the potential for hydrogen penetration of the future energy system" and examines different scenarios exploring the utilization of hydrogen in the future energy system. The first case study focuses on global hydrogen use, considering factors such as CO_2 restrictions, costs, energy conversion, and usage across regions. It imposes limitations on hydrogen applications and emphasizes the need for infrastructure development. The second case study assesses the true impact of hydrogen utilization on climate change by analyzing the social cost of carbon emissions. The third case study investigates hydrogen's potential in US road transportation, estimating required demand, renewable power growth, and water usage, based on insights drawn from the Lawrence Livermore National Laboratory's (LLNL) national assessment of energy sources and end-uses. The fourth case study examines hydrogen's role in decarbonizing the UK's heating sector, considering fuel cells and hydrogen boilers. It employs the UK TIMES Model (UKTM), a tool also adopted by the UK government. The article draws several conclusions based on these case studies. It highlights the potential benefits of hydrogen in road transportation, including reduced energy rejection and CO_2 emissions. In the UK's heating sector, hydrogen emerges as a promising option for decarbonization. However, the article also acknowledges the challenges of cost competitiveness, emphasizing the need for dedicated infrastructure. Additionally, hydrogen consumption is projected to represent around 3% of total energy consumption in 2050 [65]. Another article, "Delivering net-zero carbon heat: Technoeconomic and whole-system comparisons of domestic electricity- and hydrogen-driven technologies in the UK", also focuses on the impact of hydrogen and electrification in the UK's buildings sector. The evaluated technologies are integrated into an existing model known as the Whole-electricity System Investment Model (WeSIM). This model aids in forecasting decarbonization trajectories for heating, simulating the most cost-effective routes for the transition, and determining viable and appropriate technology blends. The study assesses various technologies and concludes that, for most electricity and hydrogen prices, electric heat pumps offer the most reliable and cost-effective solution for decarbonizing residential heating. It suggests that electrification is a superior approach, while hydrogen boilers would require substantial price reductions to become viable [46]. Furthermore, the article titled “Market Penetration Analysis of Fuel Cell Vehicles in Japan Using the Energy System Model MARKAL” investigates the potential adoption of hydrogen in the transportation sector, particularly fuel cell vehicles. The study evaluates the impact of carbon taxes as an incentive and utilizes the MARKAL model to assess market penetration. The findings suggest that hydrogen fuel cell vehicles would require increased carbon taxes to become cost-competitive before 2050. Lower vehicle and hydrogen fuel costs or subsidies for hydrogen infrastructure are also identified as potential factors for earlier market penetration [66]. Correlating these three studies, it is evident that hydrogen’s potential and challenges are examined from different perspectives. The case studies highlight hydrogen’s role in various sectors, such as global energy systems, road transportation, and heating. They emphasize the need for infrastructure development, cost competitiveness, and policy incentives like carbon taxes to drive market penetration. The studies underscore the importance of considering factors such as regional variations, social costs, and technology comparisons when assessing hydrogen’s role in decarbonization efforts. Collectively, these insights contribute to a comprehensive understanding of hydrogen’s potential and limitations across different sectors and regions [65] [46] [66].

Chapter 4

Methodology

In this chapter, the methodology of the study is outlined. It commences by establishing the hydrogen value chain, encompassing current and future technologies and potential applications across end-use sectors. Subsequently, a techno-economic analysis is conducted to characterize the various technologies involved. Next, the model's starting point, known as the reference energy model, is presented, along with an explanation of its construction. The next step consists in integrating the hydrogen conversion chains into the OSeMOSYS model, followed by simulating multiple scenarios that consider diverse demands and varying restrictions on greenhouse gas emissions. The objective of these simulations is to identify the most economically efficient solutions.

4.1 Developing the hydrogen value chain

In order to gain a comprehensive understanding of the potential utilization of hydrogen within the Portuguese energy system, it is crucial first to establish its value chain. This involves examining the range of technologies, both current and future, that enable hydrogen production, transmission, distribution, and storage, as well as identifying potential applications in various sectors. Therefore, the initial phase of the study involved conducting a literature review to explore the different conversion chains, spanning from hydrogen production to its ultimate utilization.

The search primarily concentrated on reports from esteemed organizations such as the International Energy Agency (IEA), the International Renewable Energy Agency (IRENA), the World Energy Council (WEC), and articles from the literature. Some of the notable reports explored include "The Future of Hydrogen", "Global Hydrogen Review 2022", and "Green Hydrogen Cost Reduction: Scaling up Electrolysers to Meet the 1.5ºC Climate Goal", among others. The objective was to grasp the extensive scope of hydrogen as an energy carrier within energy systems and subsequently initiate the development of various conversion chains.

Initially, the focus of the investigation was directed towards the existing fuels employed in the current hydrogen production process. This preliminary phase aimed to understand the various types of fuels commonly utilized in hydrogen production. Furthermore, the research expanded to encompass an exploration of the diverse technologies employed for the conversion of these fuels into hydrogen. The research also prioritized the identification of the strengths, limitations, and environmental implications linked to each fuel type and technology concerning hydrogen production. The study aimed to evaluate the technological advancements, challenges, and potential breakthroughs associated with each method, thereby promoting a comprehensive understanding of hydrogen production technologies.

Following this, the research also placed significant emphasis on the development of hydrogen conversion chains, particularly with regard to hydrogen-based fuels. This phase involved identifying and evaluating the various types of hydrogen-based fuels and the associated technologies used in their production and utilization.

Subsequently, the study shifted its focus towards examining the methods of delivering hydrogen to the end consumers. The investigation categorized these delivery methods into distinct groups, including collection, transmission, distribution, and storage, among others. Within this phase, all existing and prospective technologies were thoroughly reviewed, considering their respective advantages and disadvantages. The primary objective was to establish efficient connections between hydrogen production sites and potential end users, taking into account the various technological options available.

Finally, the research proceeded to identify and characterize the sectors that either have the potential to utilize hydrogen or are already employing hydrogen-based fuels. The end-use sectors were primarily categorized into four main categories: industry, transport, buildings, and power/electricity generation. Furthermore, within each of these main sectors, a detailed disaggregation was conducted to comprehensively understand the range of applications for hydrogen or hydrogen-based fuels. This detailed analysis aimed to provide a comprehensive overview of how hydrogen is utilized within each sector and its potential impact in various applications.

The subsequent stage of this process involved comprehending the transfer of energy between various sources and the ultimate consumers, establishing the connections between different fuels and technologies. Subsequently, the focus shifted towards establishing diverse hydrogen conversion chains.

The figure provided in Figure 4.1 illustrates the sequential steps involved in the development of the hydrogen value chain.

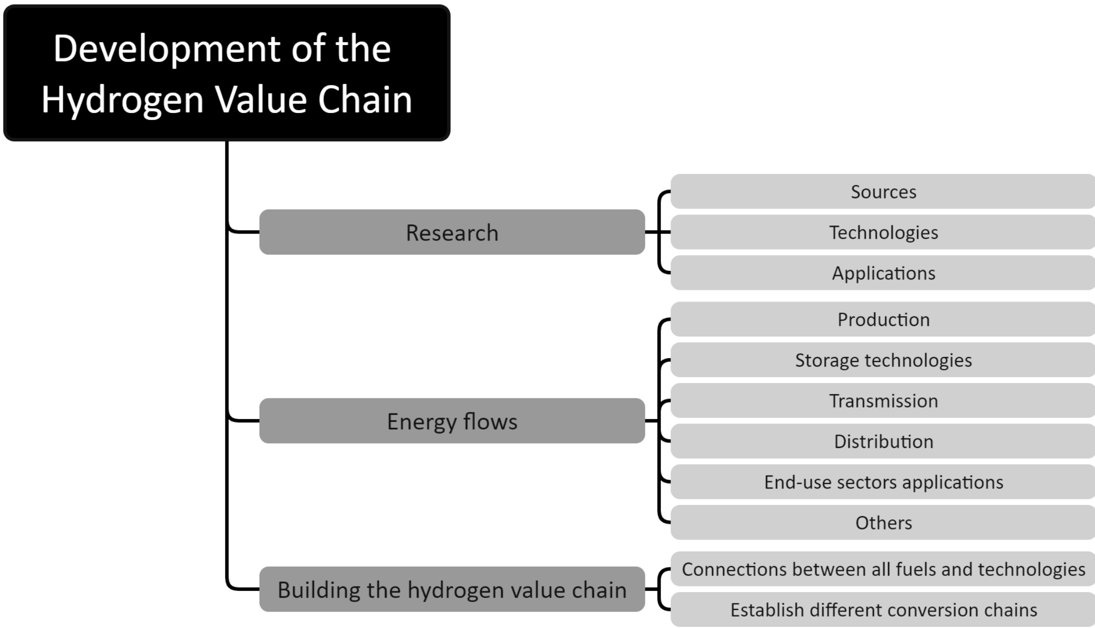

Figure 4.1: Development of the hydrogen value chain framework.

An example of the framework employed is depicted in Figure 4.2, highlighting its role in elucidating the intricate process involved in developing a smaller component within the broader hydrogen value chain.

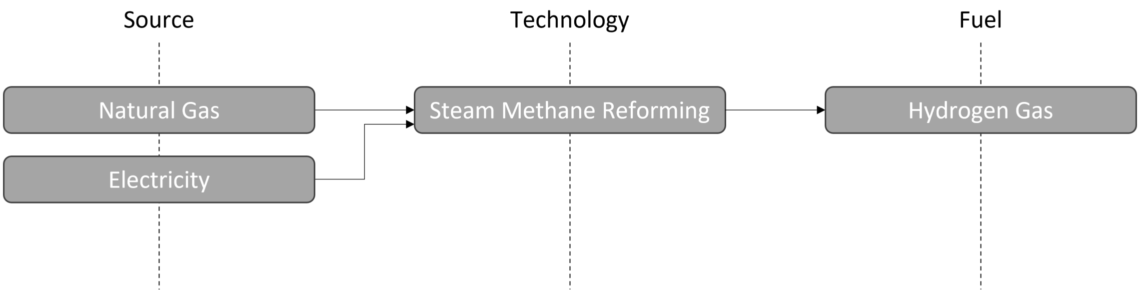

Figure 4.2: Example of developing a smaller component of the hydrogen value chain.

4.2 Techno-economic characterization of different technologies

To accurately represent the complete hydrogen conversion chain within the modeling software, OSeMOSYS, it is necessary to techno-economically characterize the various technologies involved in the conversion process. This involved conducting a comprehensive search for relevant techno-economic information from various sources.

To acquire this valuable techno-economic information, an extensive search was carried out across multiple databases and existing models, including the prominent JRC-EU-TIMES model. Additionally, reports from reputable organizations like the

International Energy Agency (IEA) and relevant articles in the literature were also consulted. These sources played a crucial role in identifying and presenting the required information, helping to establish a comprehensive understanding of the techno-economic aspects of the different technologies participating in the hydrogen conversion chains. By leveraging these diverse sources of information, the research aimed to ensure accurate and reliable characterization of the technologies within the hydrogen conversion chain.

The search primarily targeted the main techno-economic information related to different technologies, encompassing the following aspects:

- Investment costs (CAPEX);
- Fixed costs;
- Variable costs;
- Efficiency;
- Input of fuels;
- Output of hydrogen/hydrogen-based fuels;
- Availability factor;
- Lifetime.

While exploring various technologies, additional specific techno-economic information pertinent to each technology was also identified. This involved delving into the intricacies of individual technologies to uncover other relevant details.

4.3 Reference Energy Model

The modeling of the hydrogen conversion chains was built upon an existing national energy model that mapped the energy flows from primary sources to various end-use sectors, including agriculture and fisheries, residential buildings, services buildings, transport, and industry sectors. The model, known as the Reference Energy System (REF), has already been implemented using the OSeMOSYS framework, as illustrated in Figure 4.3. The REF model was initialized with data from the year 2015, serving as the foundation for the development of the hydrogen conversion chains model. Previously, the reference energy system (REF) has been utilized to simulate various scenarios for the Portuguese energy system, specifically addressing the requirements outlined in the RNC 2050 (National Roadmap for Carbon Neutrality 2050) scenarios. The model has already been populated with techno-economic data (data mentioned in the previous section 4.2), obtained primarily from the IEA (International Energy Agency) database.

While the existing model serves as a starting point, it should be noted that certain sources and future technologies are still yet to be incorporated throughout the energy system. These missing elements include potential energy sources and advanced technologies, both in terms of production and further along the chain. Additionally, there is a need for further disaggregation to adequately account for the diverse requirements of the final users. These gaps signify the ongoing development and refinement required to capture the full complexity of the hydrogen value chain and ensure a comprehensive representation within the model.

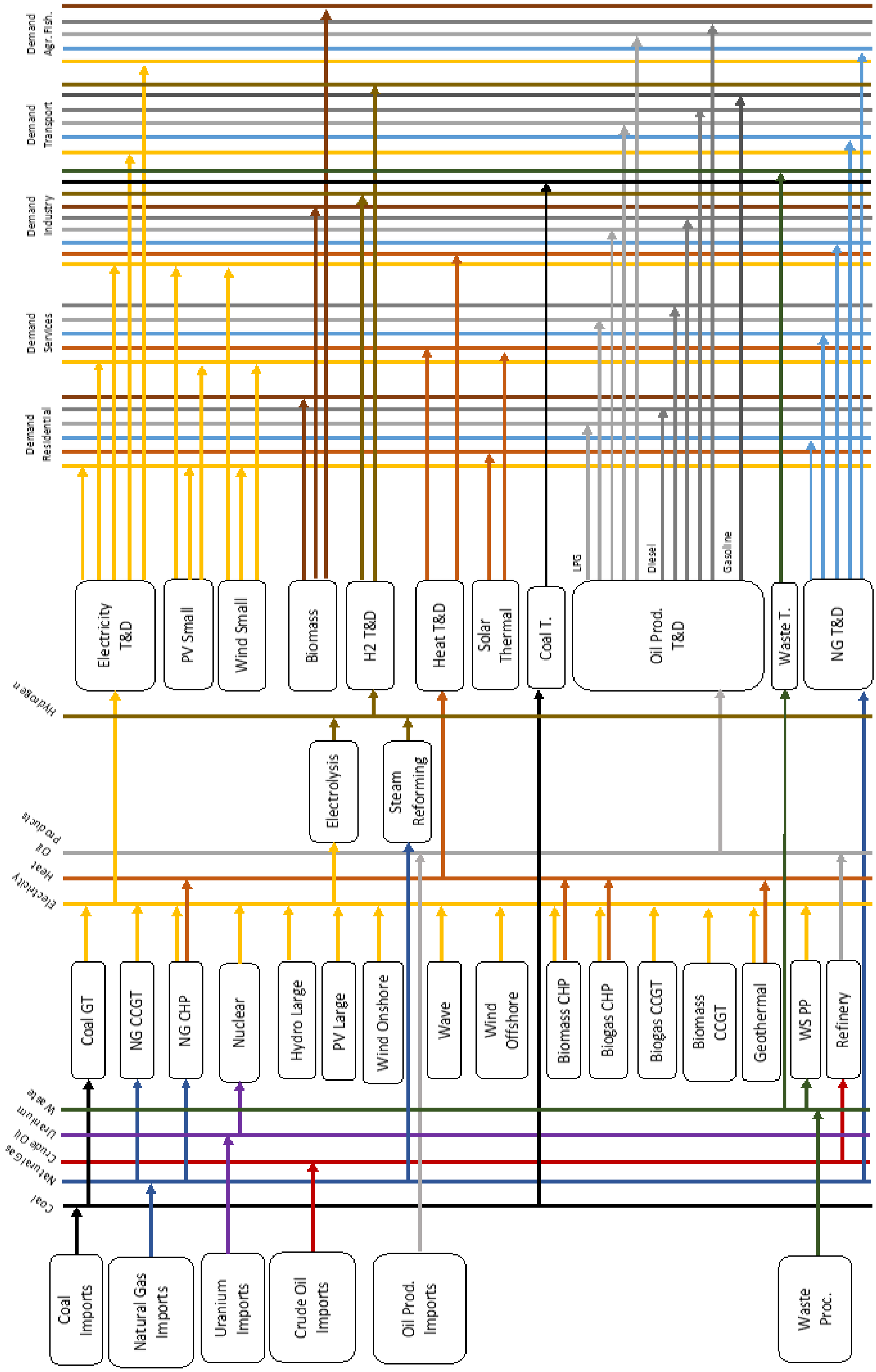

Figure 4.3: Reference Energy System (REF) for the Portuguese Energy System - The initial model used as a starting point.

4.4 Modeling of the end-use sectors

After comprehending the Reference Energy Model, the end-use sectors were initially presented without specific breakdowns, encompassing general sectors such as residential, services, industry, transport, and agriculture. However, recognizing the importance of a more detailed analysis, there arose a necessity to disaggregate the end-use sector. To achieve this, the sectors chosen for disaggregation were the industrial sector, the buildings sector (including both residential and commercial segments), the transport sector, and the agriculture + fisheries sector. In pursuit of the objective, this work will rely upon the knowledge and ideas garnered from other students' research (references [67] [68] [69]) and the JRC database ([52] [53]).

4.4.1 Industrial sector

The initial step in the process of disaggregating the industrial sector was encompassing all its sub-sectors into one comprehensive industrial sector. Furthermore, a clear distinction was made between energy used in production and energy consumed in chemical reactions. Subsequently, a thorough analysis was conducted across all sub-sectors, wherein all existing and potential future technologies were identified and taken into consideration. The analysis encompassed several sub-sectors, including process heat, steam, machine drive, refrigeration, HVAC, lighting, onsite transport and logistics, as well as other uses that accounted for less frequent processes. Within each of these sub-sectors, a comprehensive identification of relevant technologies was undertaken, along with the corresponding fuels associated with each technology. To illustrate the process of disaggregation, a simplified representation is depicted in Figure 4.4. The disaggregation process draws on two primary references, namely, the JRC database ([52] and [53]) and Gonçalo Oliveira's master thesis ([68]).

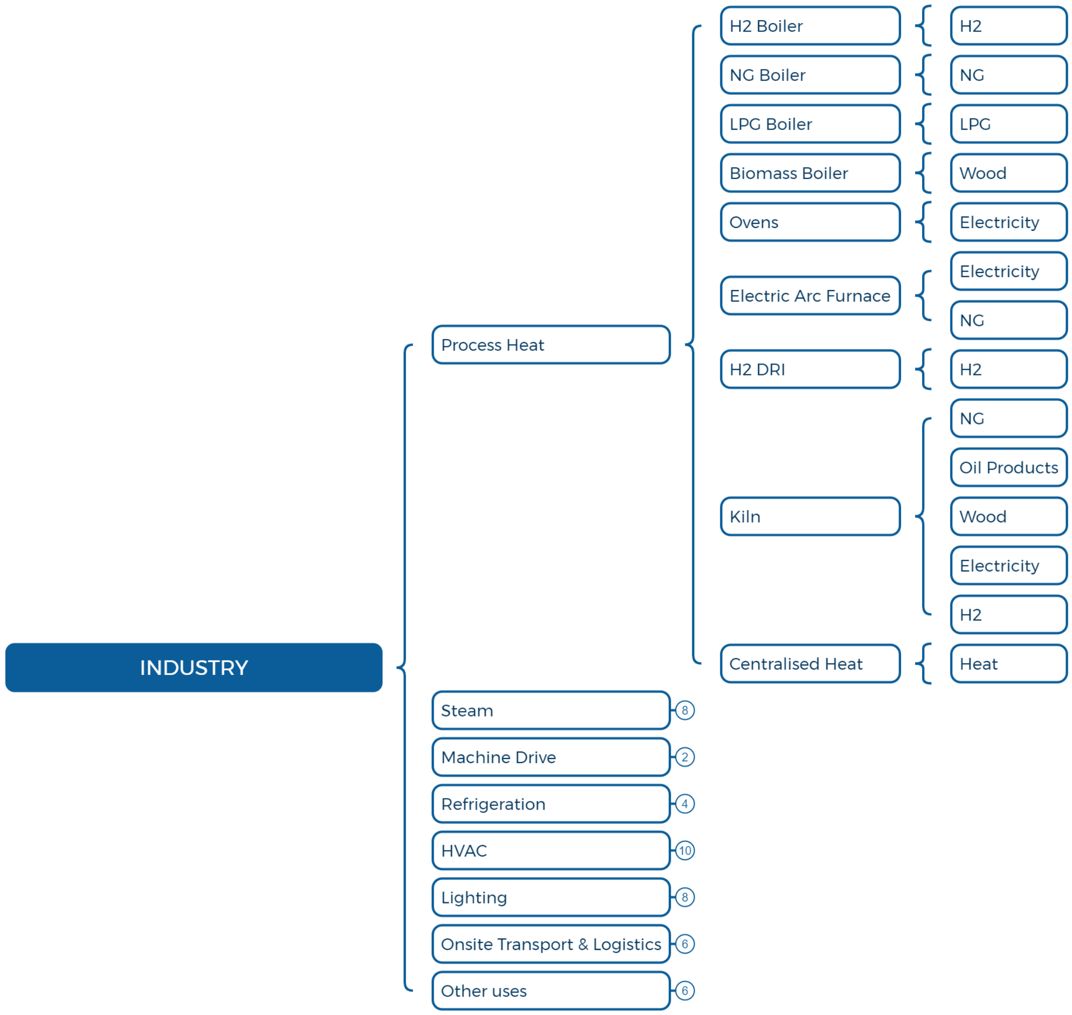

Figure 4.4: Illustration depicting the disaggregation process of the industrial sector.

4.4.2 Buildings sector

The process of disaggregating the buildings sector follows a similar approach to what was explained in the preceding sub-section for the industrial sector. Initially, all the sub-sectors were grouped together under one overarching category, known as the buildings sector. Subsequently, each sub-sector was examined individually, considering its unique set of technologies and diverse sources of fuels associated with each technology. The identified sub-sectors included space heating, space cooling, domestic hot water (DHW), cooking, lighting, washing, drying, cooling, electronics, and other miscellaneous uses. The disaggregation process relied on several key references, notably the JRC database ([52] and [53]), João Madeira's master thesis ([69]), and Ana Neves' PhD dissertation ([67]).

To illustrate this disaggregation process, Figure 4.5 presents an example that visually demonstrates the differentiation of sub-sectors within the buildings sector.

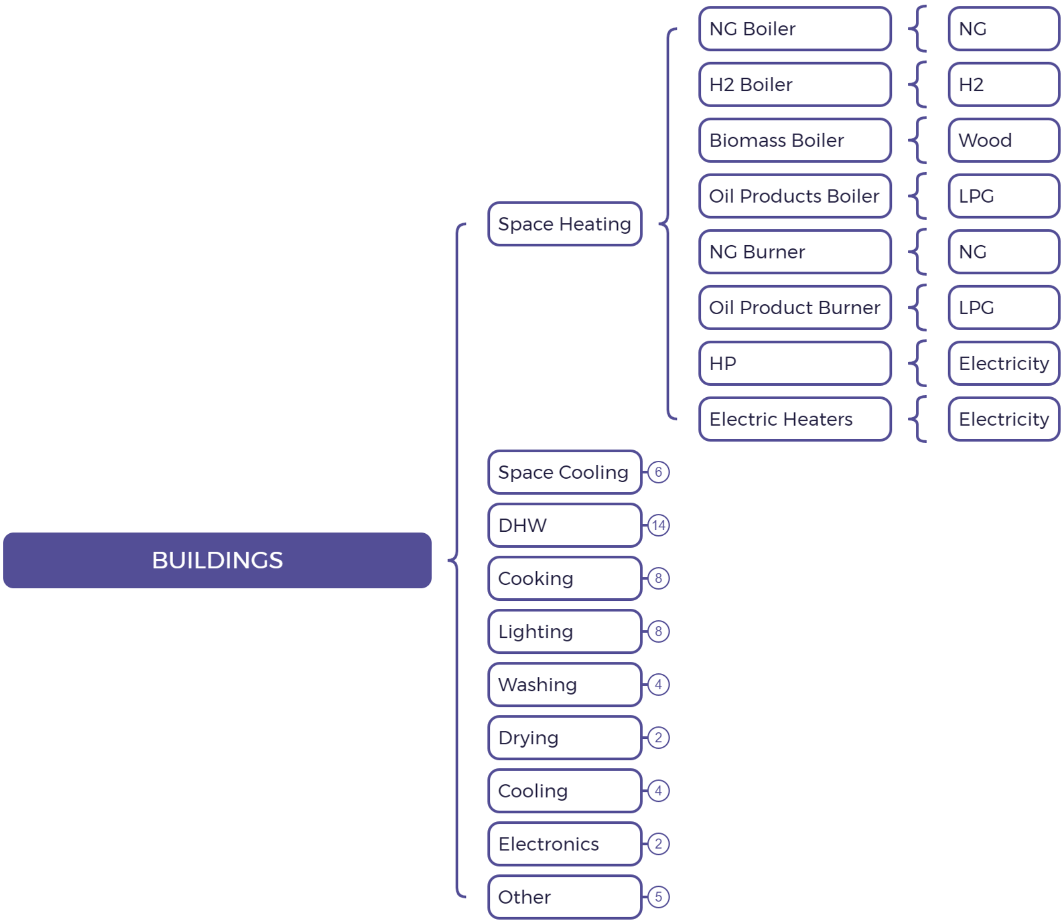

Figure 4.5: Visual representation showcasing the process of disaggregating the buildings sector.

4.4.3 Transport sector

The process of disaggregating the transport sector follows a similar approach to the previously discussed methods. Initially, the transport sector is considered as a whole, which is then further divided into two distinct categories: passenger transport and freight transport. Within each category, a finer breakdown is carried out, taking into account various modes of transportation, including passenger cars, road 2-wheelers, buses, and other relevant means.

To ensure comprehensive analysis, every mode of transportation is examined in terms of the technologies employed, encompassing both existing and potential future advancements. Moreover, this evaluation extends to various energy sources and fuels utilized by each transportation method. In conducting this disaggregation, we relied on specific references, including data from the JRC database, as mentioned in previous sectors ([52] and [53]). Additionally, insights from Ana Neves' PhD dissertation ([67]) and other pertinent statistics were taken into account to complement the analysis. Figure 4.6 illustrates the step-by-step process of disaggregating this sector.

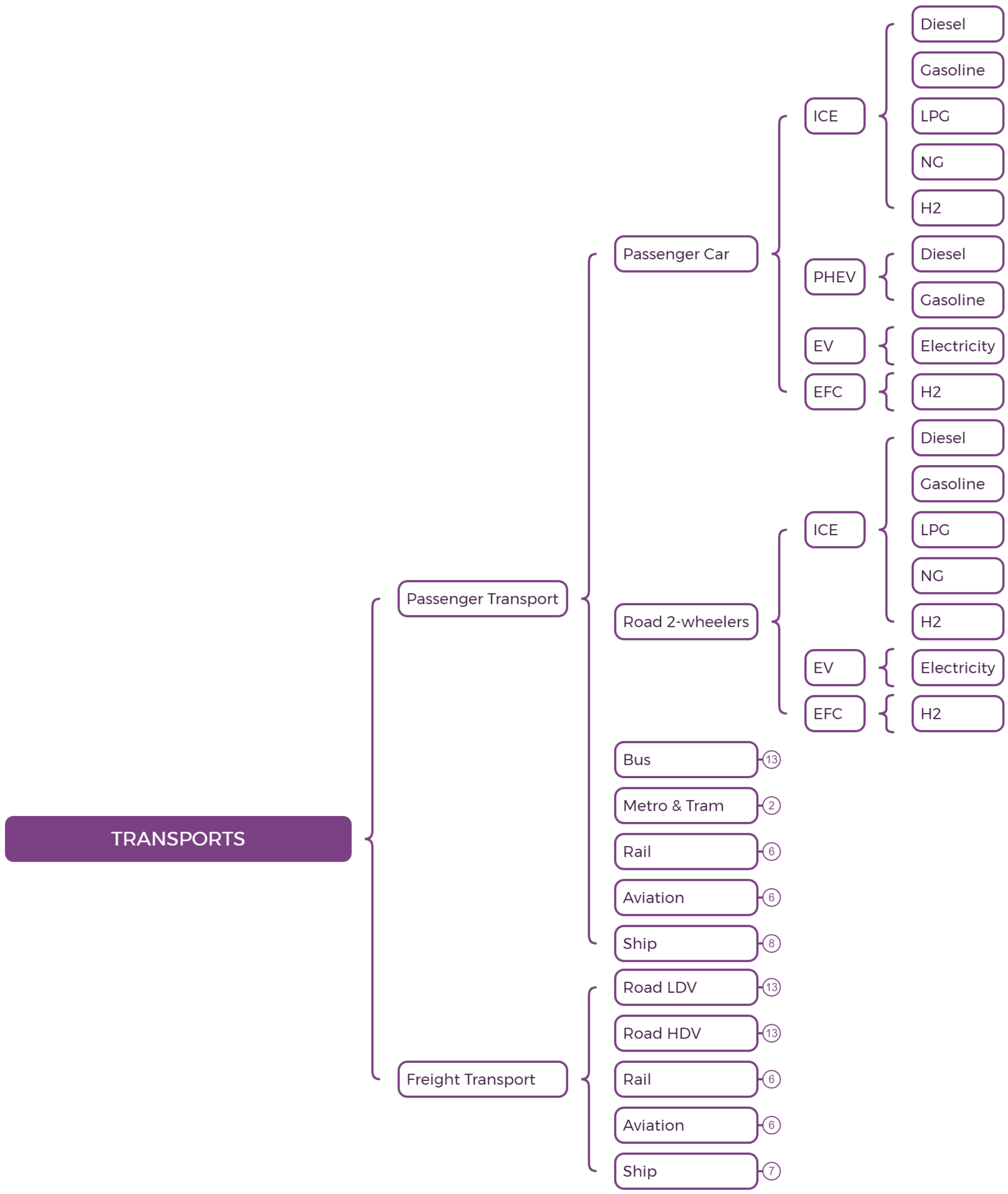

Figure 4.6: Visual representation showcasing the process of disaggregating the transport sector.

4.4.4 Agriculture + fisheries sector

After successfully completing the disaggregation of the three aforementioned sectors, the next step was to apply a similar approach to disaggregate the agriculture and fisheries sector. The process of disaggregation involved starting with a broader sector overview and then dividing it into distinct processes essential to this sector. These processes encompassed irrigation, heating and cooling, lighting, machinery, and other less commonly used operations. For each specific process, various technologies were presented, serving as fuels and energy sources.

The valuable references utilized in this disaggregation endeavor were the comprehensive JRC database ([52] and [53]) and the PhD thesis authored by Ana Neves ([67]). The outcome of this meticulous undertaking is visually presented in Figure 4.7, which provides an overview of the complete disaggregation of the agriculture and fisheries sector.

Due of time constraints, the model does not incorporate disaggregation for agriculture and fisheries.

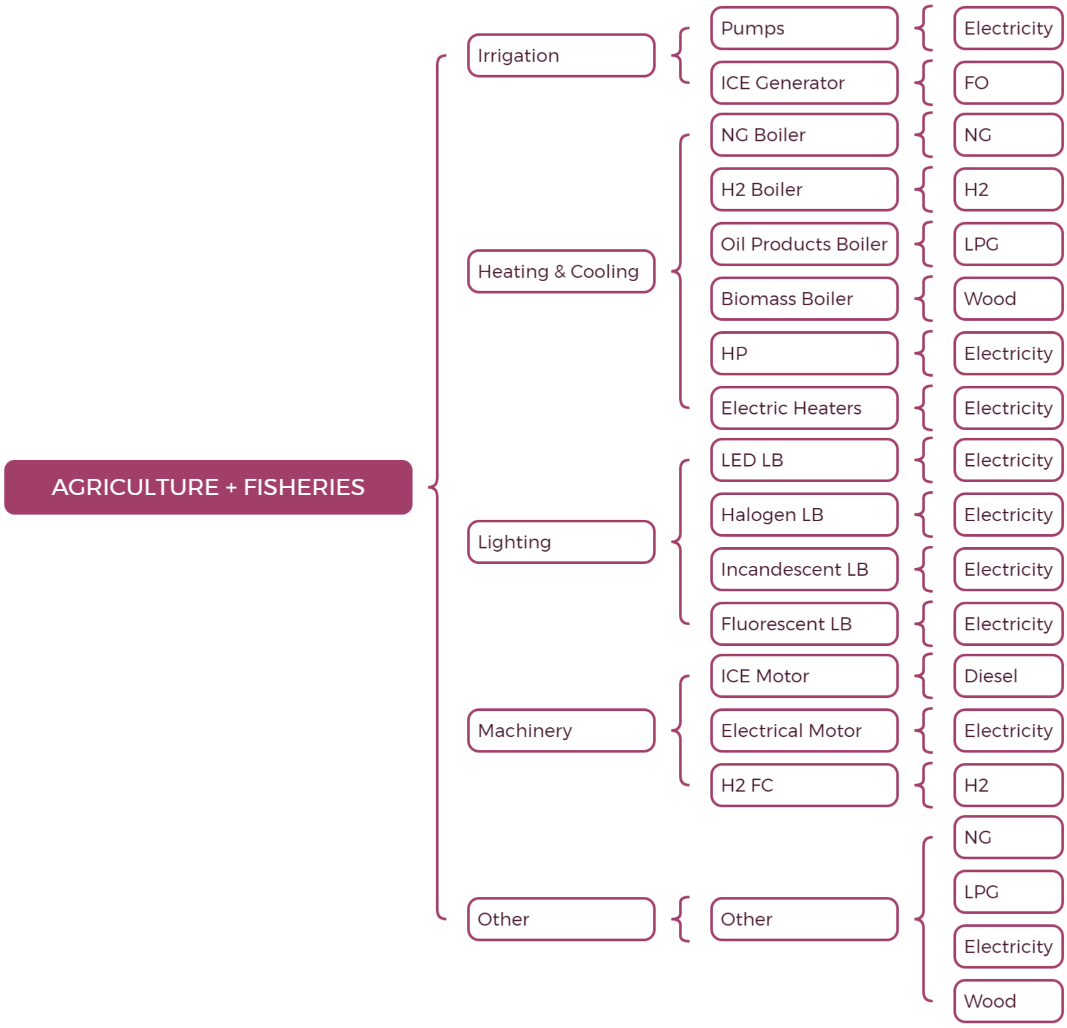

Figure 4.7: Representation of the whole disaggregation of the agriculture and fisheries sector.

4.5 Integration of hydrogen conversion chains into the OSeMOSYS model

After thoroughly defining the hydrogen value chain and gathering essential techno-economic data, the next step involves constructing the model structure and inputting the required information. An Excel spreadsheet was employed for this purpose. The initial stage involves identifying and incorporating the 'fuels' within the model.

These fuels encompass the inputs and outputs (such as energy carriers or sources) associated with each technology and the technologies themselves. The reference energy model already contained certain ‘fuels’ and technologies, as elaborated in the preceding subsection. In order to maintain consistency with the framework used in the reference energy model (REF), ‘fuels’ and technologies were labeled with specific codes, avoiding the inclusion of spaces between words. This approach is illustrated in Table 4.1, where the ’fuel’ and technology names are depicted using the designated codes.

Table 4.1: Example of codes used to identify fuel and technology names in the model

Type	**Name**	**Description**
Fuel	GH2	Hydrogen gas produced
Technology	H2_PEM	Production of hydrogen via PEM electrolysis
Technology	H2_ALK_L_C	Production of hydrogen via electrolysis (ALKALINE) (large size, centralized)

The model solely accounted for hydrogen gas conversion pathways, while the transmission and distribution aspects were limited to the incorporation of new pipelines. This decision was influenced by the existing polyethylene pipeline network in Portugal, which can effectively transport 100% gaseous hydrogen.

Once the remaining fuels and technologies associated with the hydrogen value chain (except for the end-uses) were created in the model, the gathered techno-economic data from the beginning of this work was populated in the Excel sheet. As described in subsection 3.2, OSeMOSYS collects parameters to describe each technology in terms of demand, performance, and technology costs, covering the period from 2015 to 2050. The process began by adding the technology costs, namely ‘CapitalCost’, ‘FixedCost’, and ‘VariableCost’. The available data was incorporated and utilized through linear interpolation to extrapolate costs for specific years between the base years (2015, 2020, 2030, 2050). Subsequently, the next step involved adding performance-related parameters to the model. These parameters encompassed ‘InputActivityRatio’, ‘OutputActivityRatio’, ‘AvailabilityFactor’, ‘CapacityToActivityUnit’, and ‘OperationalLifetime’.

The appendixes C and D contain a comprehensive overview of the hydrogen-related technologies and fuels utilized in the model.

4.6 Incorporating end-use applications within the OSeMOSYS model

After breaking down the end-use sectors, as detailed in section 4.4, the subsequent phase involved the depiction of end-use technologies and applications across various types of fuels. This process in the Excel file closely resembles the one elucidated in the preceding section 4.5. The end-user applications that underwent disaggregation within the model encompassed the industrial sector, both residential and commercial segments of the buildings sector, and the transportation sector. The agricultural and fisheries sector was omitted from the model, as its energy demand is relatively insignificant compared to other sectors, resulting in minimal impact on the overall outcomes.

The process of establishing end-use applications involved integrating technologies and their associated fuels to establish connections within the value chain. In line with the OSeMOSYS model, each technology within the end-use application has both inputs and outputs, with one 'fuel' exiting each final technology. Once the fuels and technologies are firmly defined, the next steps include incorporating the associated costs, such as 'CapitalCost' and 'FixedCost' for the years spanning 2015 to 2050. Additionally, the model requires technical data like 'OperationalLifetime' and efficiency metrics such as 'InputActivityRatio' and 'OutputActivityRatio.'

Furthermore, it is necessary to define the 'ResidualCapacity' for each created technology, a calculation made using available data, along with specifying the 'CapacityToActivityUnit.' Demand-related data is essential on the 'fuels' side, encompassing 'Demand' and 'SpecifiedDemandProfile.' The latter accounts for seasonal and daily variations, covering spring, summer, autumn, and winter.

Most of the required data for the aforementioned categories was sourced from prior research. Specifically, for the industrial sector, the foundation was Gonçalo Oliveira's Thesis [68], while the buildings sector drew from João Madeira's Thesis [69]. In the case of the transport sector, data was derived from the JRC-EU-TIMES model ([52] and [53]), along with other relevant references in the literature (for example [70]). As for data related to hydrogen technologies within these three sectors, it was either obtained from literature sources, presented in the appendices, or estimated through approximations due to the limited availability of comprehensive data for some hydrogen technologies.

Once all the data has been integrated, the model is prepared for simulation. Appendices C and D provide a comprehensive compilation of all the technologies and fuels employed within the model.

4.7 National climate and energy goals

In pursuit of national climate and energy objectives, there are two primary ongoing initiatives: the RNC 2050 (Roteiro para a Neutralidade Carbónica 2050) and the PNEC 2030 (Plano Nacional Energia e Clima).

The RNC 2050 outlines the path to achieving carbon neutrality in Portugal. It sets a greenhouse gas emission reduction target of 85% to 90% by 2050, using 2005 as the baseline year. The remaining emissions are expected to be offset through carbon sequestration, primarily through soil and forest practices. The roadmap also establishes a timeline for emission reduction. By 2030, the goal is to reduce emissions by approximately 45% to 55%, and by 2040, the target is a reduction of about 65% to 75%, all relative to the 2005 emission levels. The ultimate aim is to achieve decarbonization of final energy consumption by progressively incorporating more renewable energy sources and significantly expanding electrification across end-use sectors starting from 2030 onward. By 2050, it is anticipated that electrification will constitute approximately 66% to 68% of final energy consumption. Hydrogen is slated to play a role, contributing around 4% to final energy consumption, especially in heavy passenger and freight transport. The production of this hydrogen is expected to rely on electrolysis, and the corresponding electricity consumption is projected to rise from 5% to 8%.

The PNEC 2030 shares similar goals with the RNC 2050, aiming to decrease emissions, incorporate more renewable energy sources, and boost electricity usage in final energy consumption. Key objectives outlined until 2030 include reducing emissions by 55% compared to 2005 levels and achieving a 35% increase in energy efficiency. Additionally, a fundamental target is to enhance the overall utilization of renewable energy, aiming for 49% of the final gross energy utilization, with a particular emphasis on reaching 23% renewable energy integration within the transport sector. In terms of the targeted greenhouse gas (GHG) emission reductions in final uses by 2030, the report outlines a reduction of 70% in the services sector, 35% in the residential sector, 40% in the transport sector, and 11% in the agriculture sector.

Concerning hydrogen utilization, specific targets have been outlined in several reports, which are summarized in Table 4.2.

Table 4.2: Target percentages of hydrogen penetration in the energy value chain, according to different national perspectives

Roteiro para a Neutralidade Carbónica 2050	Final energy consumption	4% H_2
	Heavy transport sector	40% - 68% H_2
Roteiro e Plano de ação para o hidrogénio em Portugal (for 2050)	Final energy consumption	6,5% H_2
Resolução do Conselho de Ministros n.º 63/2020 (for 2030)	Final energy consumption	1,5% - 2% Green H_2
	Injection in the natural gas grid	10% - 15% Green H_2
	Energy consumption in industry sector	2% - 5% Green H_2
	Energy consumption in transport sector	1% - 5% Green H_2
	Energy consumption in domestic maritime transport	3% - 5% Green H_2
	Final energy consumption	5% H_2
	Energy consumption in industry sector	5% H_2
	Energy consumption in transport sector	5% H_2
	Electrolyzers Capacity	2 - 2,5 GW
Resolução do Conselho de Ministros n.º 63/2020 (for 2050)	Final energy consumption	15% - 20% H_2
	Injection in the natural gas grid	75% - 80% H_2
	Energy consumption in industry sector	20% - 25% H_2
	Energy consumption in transport sector	20% - 25% H_2
	Energy consumption in domestic maritime transport	20% - 25% H_2

4.8 Description and execution of the scenarios

After breaking down the end-uses and integrating various technologies throughout the chains into the Reference Energy System, the model has reached its final state and is now fully prepared for execution. To explore the potential and viability of incorporating hydrogen throughout the chain, five scenarios will be simulated, each imposing different constraints related to demand and the goal of reducing GHG emissions.

The initial scenario (SC1) to be simulated is the BAU (business-as-usual) scenario. No explicit energy demands or GHG constraints will be imposed in this case. The model will optimize based on the current state without any additional limitations. OSeMOSYS will prioritize cost reduction as its primary objective, meaning that the chosen energy pathways will be primarily influenced by minimizing associated costs. To compare the other scenarios, the BAU scenario will act as a baseline. It will establish the current state without any specific energy demands or GHG constraints, providing a reference point to evaluate the outcomes of other scenarios.

In the second scenario (SC2), the model will be simulated according to the RNC 2050 proposed by the Portuguese government. The primary limitations pertaining to GHG emissions and other specific constraints were detailed in the preceding section 4.7.

In the third scenario (SC3), the model will undergo optimization with unique constraints, in alignment with the parameters set forth in the PNEC 2030. This includes the overarching objective of reducing GHG emissions and the incorporation of specific targets outlined in the preceding section 4.7. It will also be subject to the constraint of incorporating 5% hydrogen within the end-use sectors.

In the fourth scenario (SC4), the model will incorporate the constraints imposed by the RNC 2050 scenario. Additionally, it will introduce the requirement of using 25% H_2 in the end-use sectors starting from 2030 onwards.

The fifth scenario (SC5) diverges from the previous ones, as the model has the liberty to determine the extent to which hydrogen technologies are adopted, granting the system full autonomy in its decision-making.

In Table 4.3, an overview of the selected scenarios is presented, highlighting the emissions reduction goals and hydrogen utilization.

Table 4.3: Scenarios comparison for emissions reduction target and hydrogen utilization

Scenario	**Emissions reduction target**	**Hydrogen utilization**
BAU (SC1)	X	X
RNC 2050 (SC2)	85% to 90% by 2050	X
PNEC 2030 with 5% H2 (SC3)	85% to 90% by 2050	5% by 2030
RNC 2050 with 25% H2 (SC4)	85% to 90% by 2050	25% by 2050
RNC 2050 ALT (SC5)	85% to 90% by 2050	Flexible

Regarding the model's utilization of hydrogen in end-use applications in scenarios 3 and 4 (SC3 and SC4), it was generated two distinct outputs for the final-use technologies. One output encompassed technologies that rely on hydrogen consumption, while the other encompassed non-hydrogen-consumer technologies. This approach allowed the model to define varying degrees of hydrogen utilization and enabled it to influence the model's selection of specific technologies.

4.9 Demand

The demand across various sectors remains constant across all scenarios, as it has been predefined. The solver's role is to optimize the model by determining the most suitable technologies to fulfill this demand. The demand is visually represented in Figure 4.8 for all sectors, excluding the transportation sector. The demand is characterized by the total useful energy in the residential, services, and industrial sectors. In the case of the agriculture sector, the demand represents the total final energy use, as the model does not account for further disaggregation. The data utilized to determine the demand was sourced from previous master's dissertations ([68] and [69]).

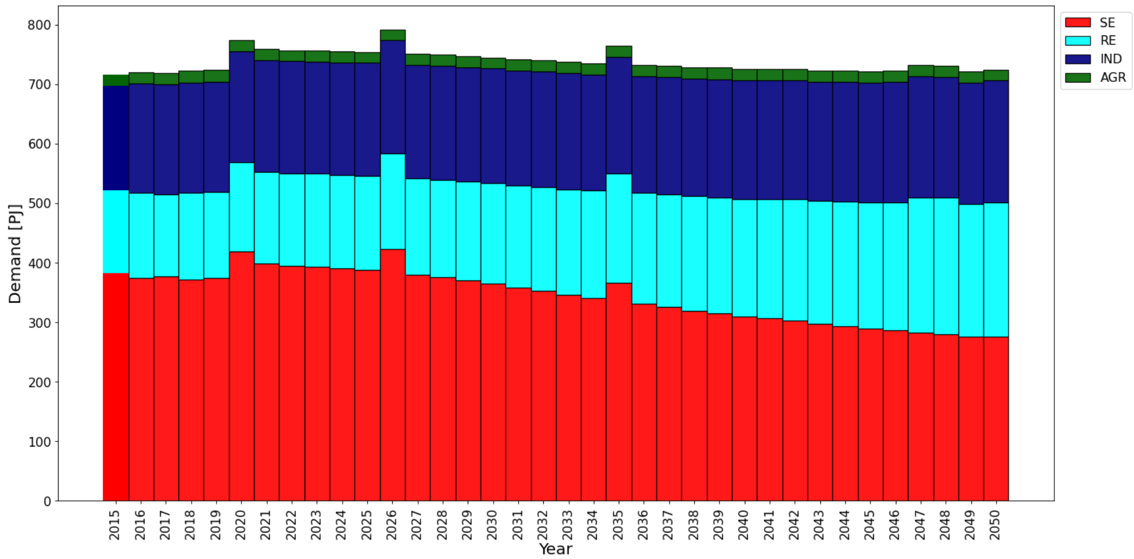

Figure 4.8: Annual Demand by sector

For the transport sector, the process of determining the demand differed. The demand was established using data from JRC-IDEES - Integrated Database of the European Energy System [71], and its variations were aligned with RNBC 2050 (Roteiro Nacional de Baixo Carbono 2050). The demand was segmented into passenger transport and freight transport, with activity serving as the basis for each mode of transportation. To maintain consistency with the respective units (Gpkm and Gtkm), this data was presented in two distinct graphs, as illustrated in Figures 4.9 and 4.10.

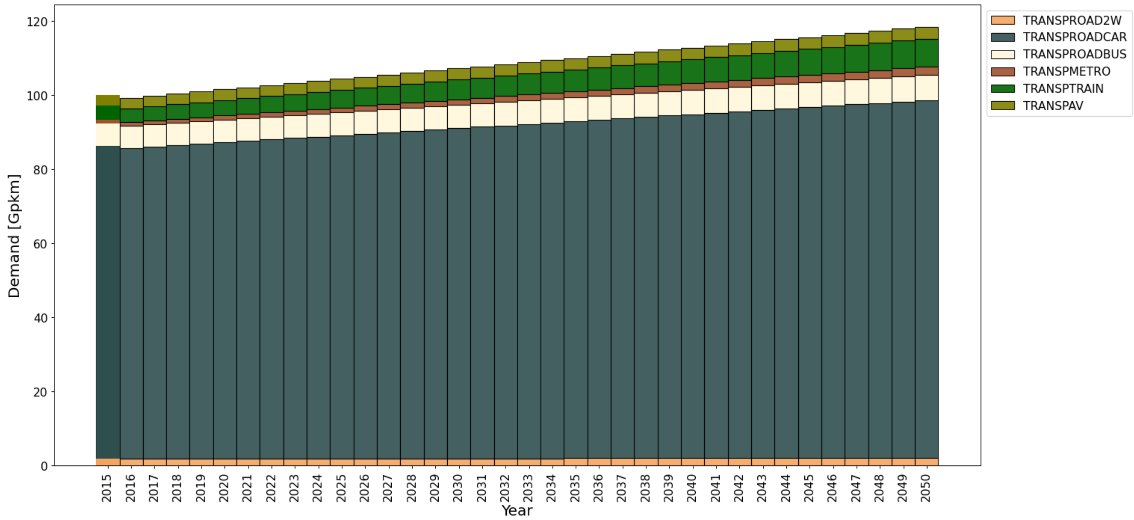

Figure 4.9: Annual Demand for the passenger transport sector

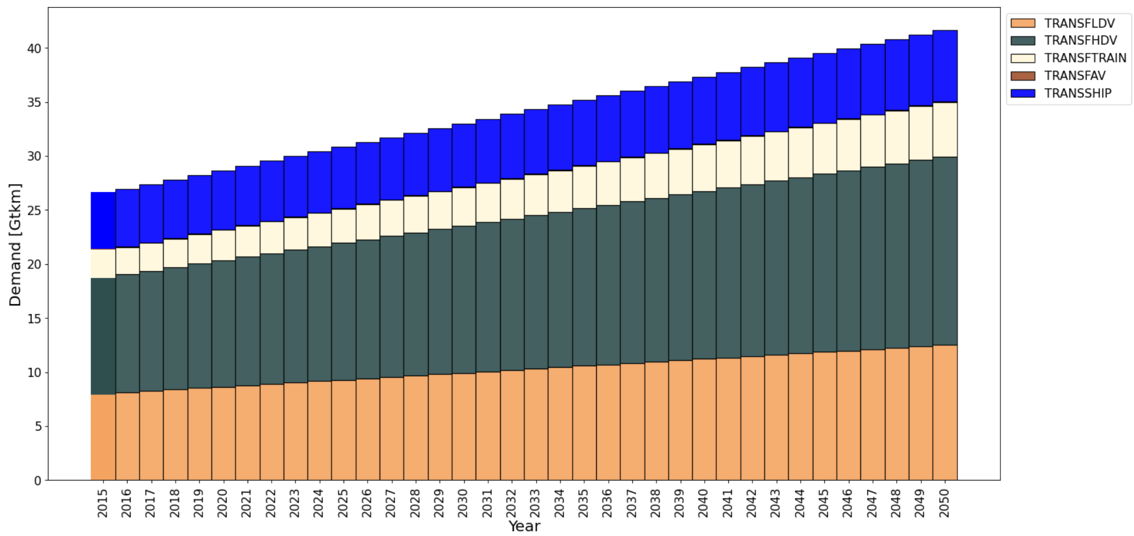

Figure 4.10: Annual Demand for the freight transport sector

4.10 Diverse scenarios analysis in the energy system deployment

In the preceding subsection, after defining the potential scenarios, the focus shifts to their practical execution within the established constraints. With the data from these scenarios now in hand, comparisons can be drawn from the outcomes.

The primary emphasis of this analysis lies in evaluating the available options in terms of the overall efficiency of energy conversion within the systems. This pertains to the transformation of primary energy into useful energy, as employed by end-use applications.

However, the analysis doesn't conclude with efficiency alone. It extends to encompass an exploration of the economic factors at play within the system. This involves a meticulous evaluation of the associated costs across the entirety of the system's operation. By carefully evaluating the efficiency and cost factors, valuable insights are anticipated, shedding light on the optimal avenues for energy utilization and overall system design.

4.11 Running the OSeMOSYS code: A step-by-step process

Once the techno-economic information pertaining to the required parameters for OSeMOSYS was incorporated, the next step involved executing the OSeMOSYS code to ensure the model was appropriately designed and to identify any potential errors. This was accomplished by utilizing the command line interface of Windows, specifically PowerShell 7. The OSeMOSYS execution process employed the otoole interface, as described in Section 3.2. With otoole, the Excel spreadsheet was converted into a text file format. This procedure is outlined in Figures 4.11, and 4.12, depicted below.

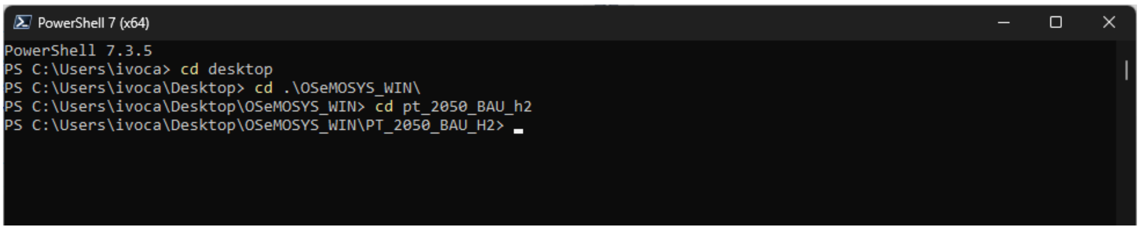

Figure 4.11: Navigating to the folder containing the Excel file.

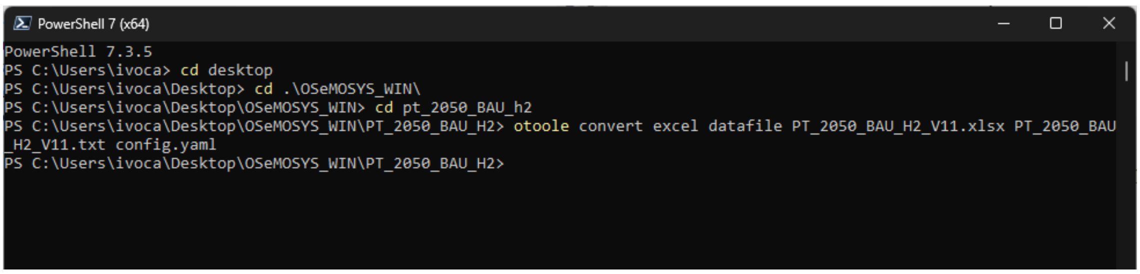

Figure 4.12: Converting the Excel file to a text file using the otoole code.

Following the conversion of the Excel data file to a text file, the OSeMOSYS code was executed using the solver 'Gurobi'. Functioning independently, this very high-performance solver tackles linear, quadratic, and mixed-integer programming, further enhancing the foundational linear programming framework of the OSeMOSYS model. Once the model has successfully processed and solved the given task, it becomes necessary to store the resulting calculations for future reference. To achieve this, the code proceeds by writing the obtained solutions into a collection of Excel files. Additionally, it generates a basic summary of the solution and saves it in a separate text file. The anticipated execution time ranges from 5 to 15 minutes, contingent upon the model's complexity and the imposed constraints.

Chapter 5

Results and Discussion

This chapter presents and discusses the achieved outcomes. Firstly, it delves into the construction of the hydrogen value chain, dissecting it into various components. Subsequently, the focus shifts to the elucidation of the modeled scenarios, as detailed in the preceding subsections 4.8 and 4.10.

5.1 Hydrogen value chain

Having undertaken an exhaustive research effort to unearth and assess the principal production routes, transmission and distribution methods, as well as potential end-use applications, the construction of the hydrogen value chain is now a comprehensive achievement. This synthesized hydrogen value chain will be outlined and partitioned into distinct segments, including hydrogen production and hydrogen-based fuels, hydrogen transmission, distribution and storage, and hydrogen end-use applications, owing to the intricate and expansive nature of this value chain.

5.1.1 Hydrogen production

Regarding the segment of hydrogen production within the hydrogen value chain, the primary sources identified, as mentioned in section 2, encompass natural gas, water, coal, biomass, and diverse electricity sources including wind, solar, hydro, geothermal, tidal, nuclear, and a blend of grid energy from various origins. Furthermore, it encompasses additional sources and technologies, which were not examined in this study. The depiction of hydrogen production within the hydrogen value chain is illustrated in Figure 5.1.

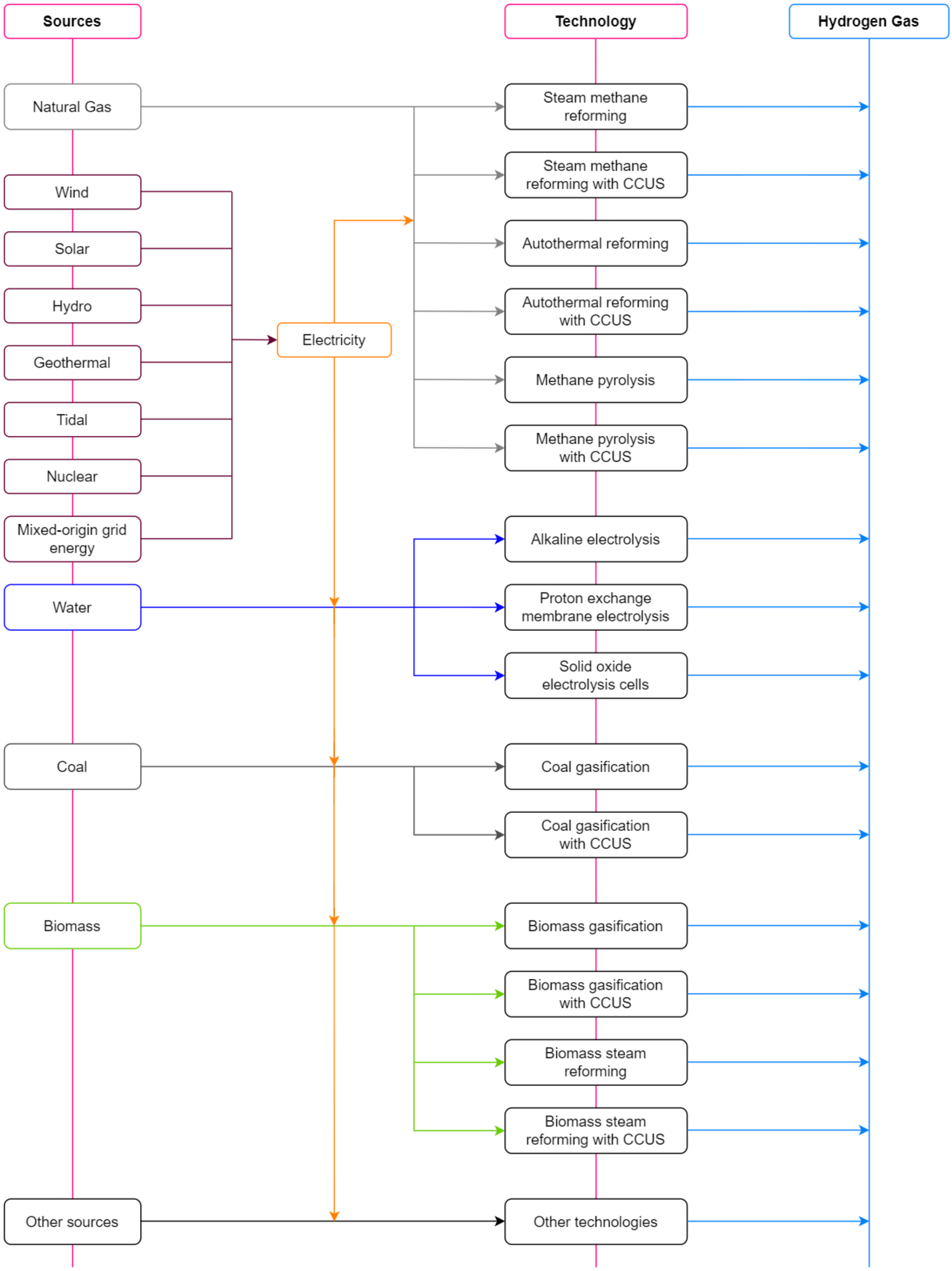

Figure 5.1: Hydrogen production segment

5.1.2 Hydrogen-based fuels and LOHC

Concerning the depiction of hydrogen-based fuels, LOHC (Liquid Organic Hydrogen Carriers), and liquid hydrogen representation, Figure 5.2 provides an illustration of potential conversion pathways. The diagram highlights four primary input sources, including hydrogen gas, and showcases six distinct technologies for generating various fuels: ammonia, synthetic methane, synthetic methanol, kerosene (also referred to as synthetic diesel), LOHC, and liquid hydrogen.

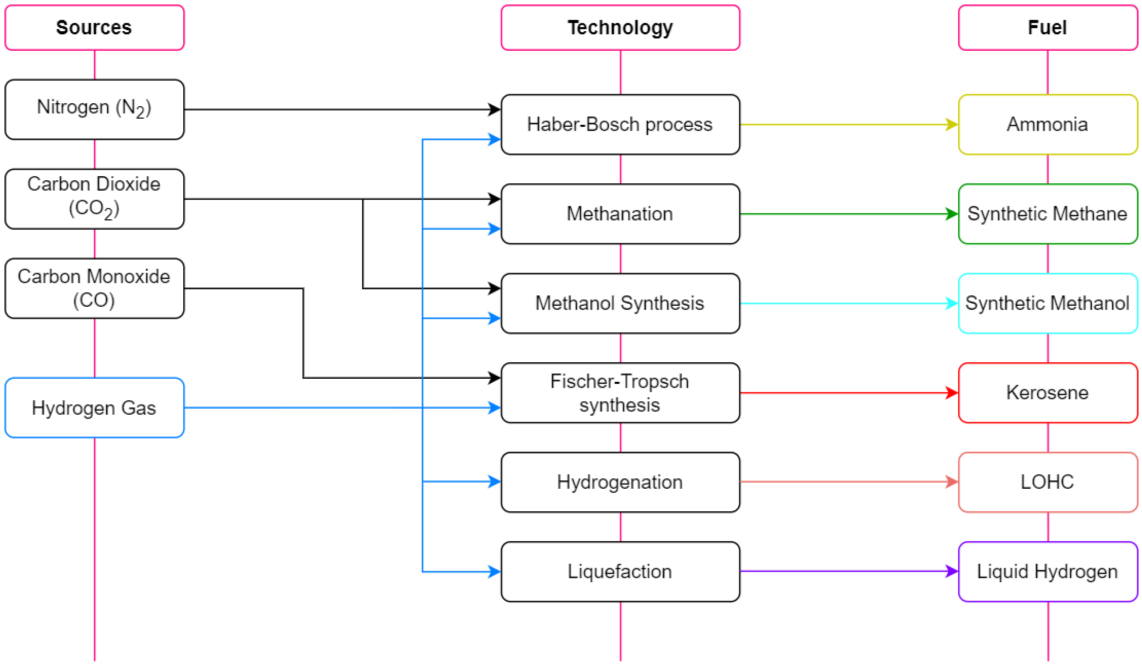

Figure 5.2: Hydrogen-based fuels, LOHC, and liquid hydrogen segment

5.1.3 Hydrogen transmission, distribution, and storage

Between the phases encompassing hydrogen production and the utilization of hydrogen-based fuels on one side, and the final stages of application on the other, lies the essential domain of hydrogen transmission, distribution, storage, and other integral processes. These processes stand as pivotal elements in ensuring the effective operation of the entire conversion process. Figure 5.3 visually outlines the numerous potential pathways and choices for effectively transporting and delivering hydrogen and its associated products to various end-use sectors.

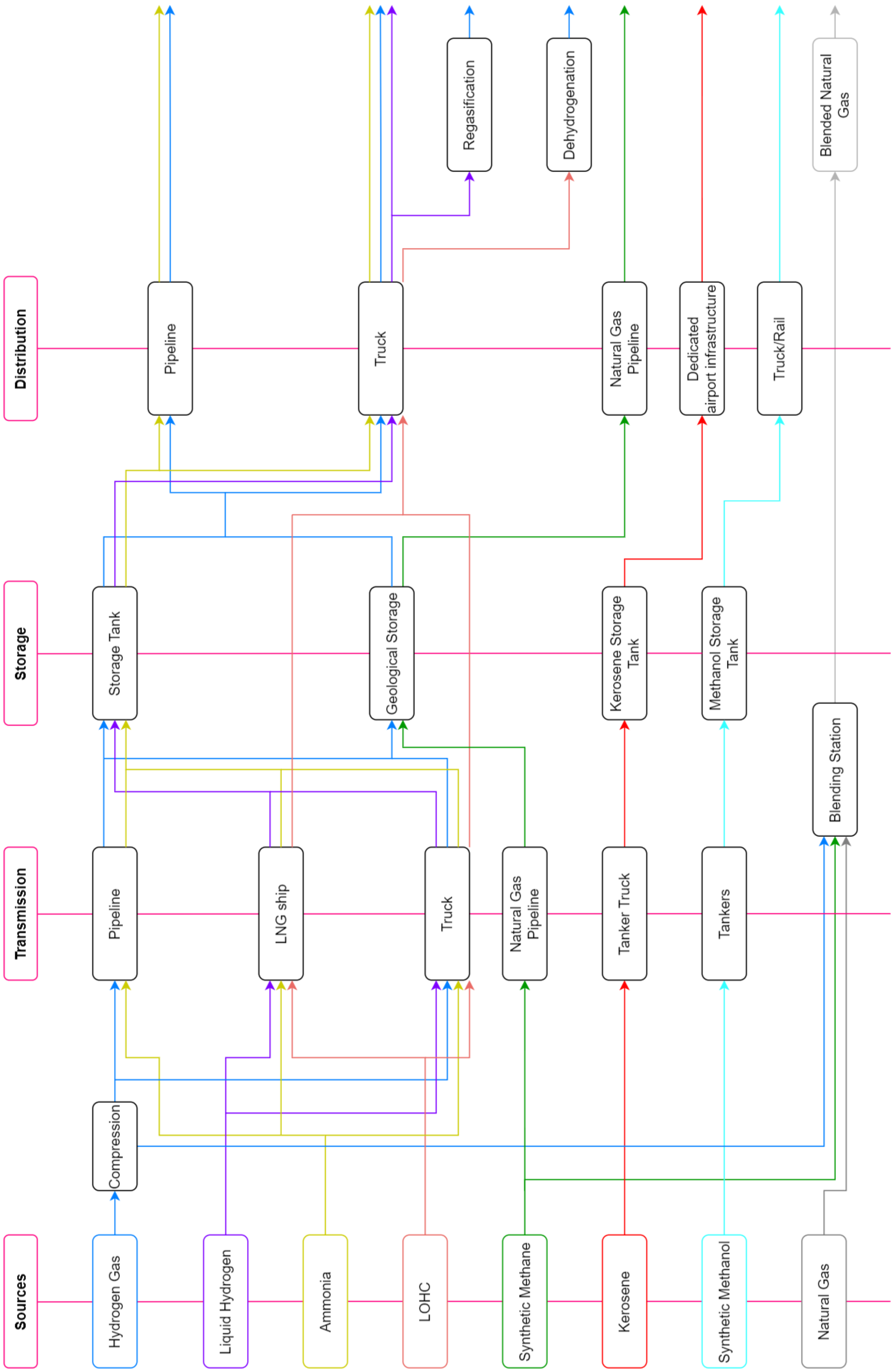

Figure 5.3: Hydrogen transmission, distribution, storage and others segment

5.1.4 Hydrogen end-use applications

A wide array of possibilities exist regarding the potential applications of hydrogen and hydrogen-based fuels, as detailed earlier in Chapter 2 and illustrated in Figure 5.4. This representation includes a more straightforward depiction of the hydrogen value chain, intentionally avoiding excessive complexity for clarity. The utilization of hydrogen is categorized into five primary sectors: Industrial, Transport, Agriculture, Buildings, as well as Power, and Electricity Generation.

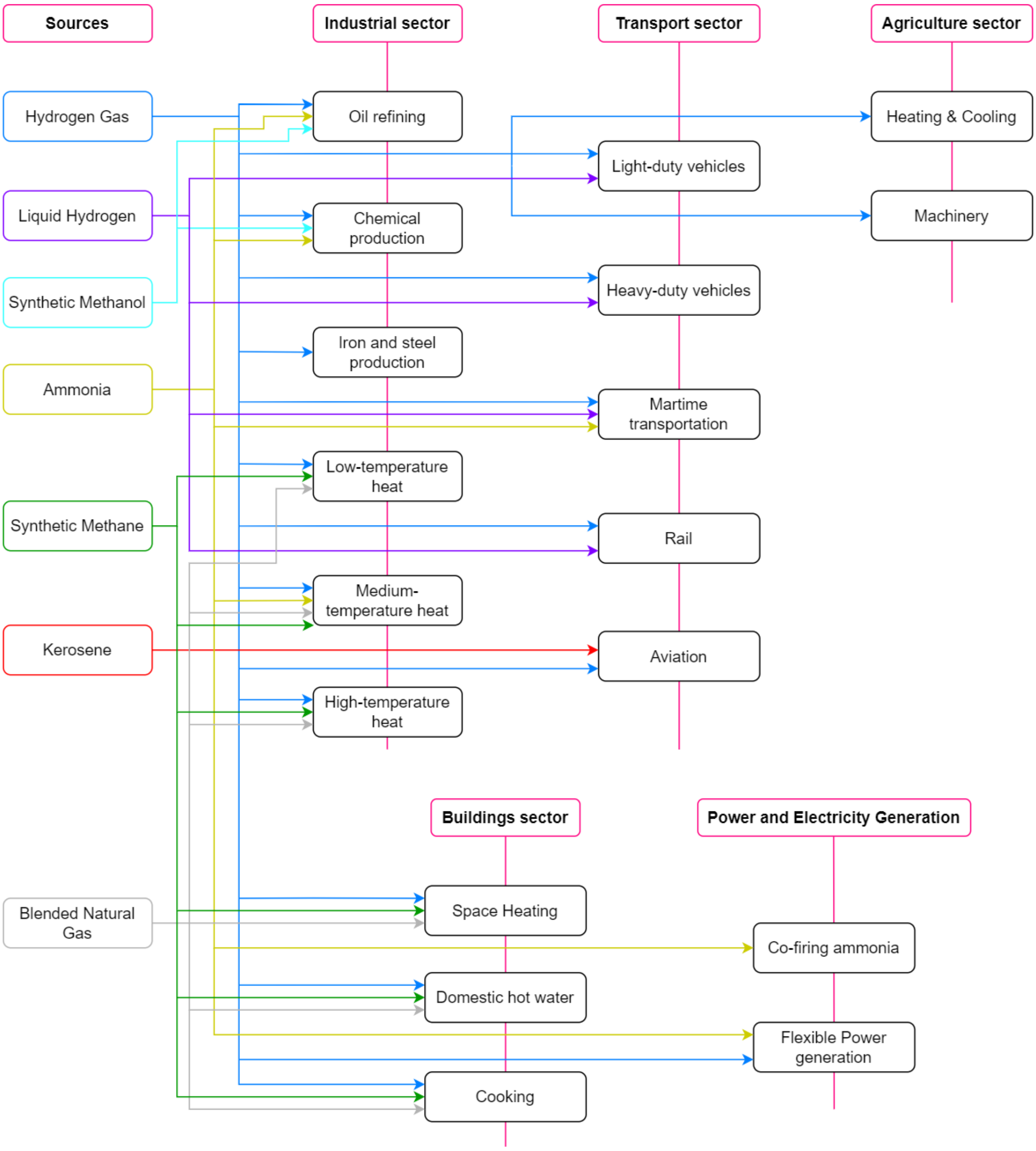

Figure 5.4: Hydrogen end-use applications segment

5.2 Scenario results and calculations

This section presents and discusses the results of the implementation of the energy system model in OSeMOSYS. The discussion is focused on several key aspects, namely on the electricity generation and mix, hydrogen production, and utilization, demand, emissions (i.e., carbon dioxide (CO_2) emissions, nitrogen oxides (NO_x)), as well as various cost considerations - i.e., capital, fixed, and variable costs related to the implementation of different scenarios of hydrogen technology deployment. The outcomes of the analysis will be conveyed through graphical representations and tables for each of the five scenarios detailed in Section 4.8.

5.2.1 Primary resources

An assessment of the primary resource utilization across all the technologies within the system was conducted. The analysis revealed that in the BAU scenario, where there are no restrictions on greenhouse gas (GHG) emissions, the system heavily depends on fossil fuels like coal, crude oil, and natural gas until 2050. Renewable energy sources exhibit only marginal growth in this scenario.

In contrast, for the next four scenarios, which are all characterized by progressively stricter GHG emission limitations, it is possible to observe a consistent trend: a substantial reduction in the reliance on fossil fuels, which are nearly phased out by 2050. Concurrently, there is a significant increase in the adoption of renewable energy sources, particularly wind power. Biomass utilization also experienced steady growth over the years. These trends are visually represented in Figure 5.5.

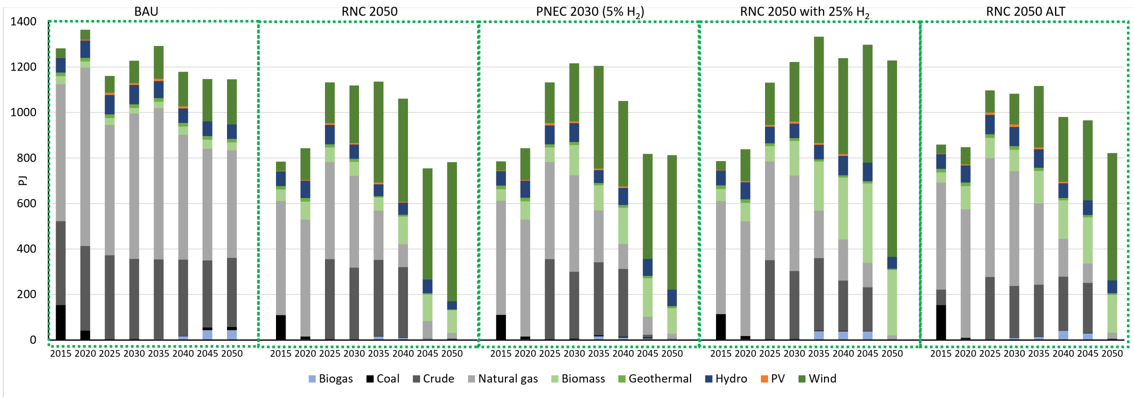

Figure 5.5: Primary resources usage in the system for all the scenarios

5.2.2 Electricity generation

5.2.2.1 Installed Capacity

In relation to the generation of electricity and the technologies employed for this purpose, as illustrated in Figure 5.6, even in the absence of any imposed constraints, certain key trends become apparent.

In the BAU scenario, Wind power plants exhibit a significant increase in their installed capacity during the modeled period. Conversely, coal-fired power plants have phased out their operations completely by the year 2021, which is also a result of the constraints added to the OSeMOSYS model runs. Furthermore, the volume of electricity imports sees a substantial reduction. Again here, this is also likely the result of the restrictions imposed on the model which limits the interconnection capacity to 1.6 GW. Natural gas power plants and cogeneration plants, on the other hand, witness a surge in their installed capacity from 2020 to 2040, followed by a subsequent decline until 2050 in comparison to their 2015 levels. This may be the result of the high demand for heat in the industrial sector and possibly also other sectors. The remaining electricity generation technologies display relatively stable installed capacity levels with only minor fluctuations.

When considering the RNC 2050 scenario, constraints are placed on greenhouse gas (GHG) emissions in accordance with the national goals of reaching carbon neutrality by 2050. In the OSeMOSYS model, only a requirement of reduction of GHG emissions to the level that is considered in the RNC2050 was considered. The optimization results show that the energy system undergoes significant changes in terms of the primary energy mix. Notably, wind power plants experience a substantial increase, contributing to increased shares of electricity production. Furthermore, biomass cogeneration plants also show increased installed capacity from the year 2038 onward. Simultaneously, electricity imports continue to decrease over the years, while coal power plants cease operations as early as 2021 - most likely due to the reasons outlined previously. Natural gas power plants and cogeneration facilities witness a gradual reduction in their installed capacity, nearly phasing out their operations by 2045. Conversely, the other electricity generation technologies demonstrate relatively consistent performance with minor fluctuations throughout the years.

The PNEC 2030 scenario was implemented from the starting point of the BAU, with the addition of specific goals for the incorporation of hydrogen into the energy system, namely 5% of demand in the end-use demand of the different sectors. The analysis of the installed capacity in the PNEC 2030 scenario closely resembles the one conducted for the RNC 2050 scenario. In this scenario, there is a notable increase in the capacity of wind power plants for electricity generation, coupled with the cessation of production from polluting resources before 2050. In part, this increase is due to the necessary support of some of the hydrogen production technologies.

In the context of the RNC 2050 with 25% H_2 scenario, as observed in the previous two scenarios, there is a substantial increase in the installed capacity of wind power plants. Additionally, there is a moderate increase in biomass cogeneration plant capacity. Concurrently, there is a reduction in electricity imports, paralleling the decline in emissions-intensive technologies. For instance, coal power plants cease their operations by 2021, and natural gas power plants gradually phase out of the system, disappearing entirely by 2048.

In the RNC2050_ALT scenario, the installed capacity for electricity generation exhibits a trajectory akin to the previous three scenarios. Notably, wind power plants experience a substantial increase in capacity, while coal power plants cease their operations by 2021. The installed capacity of natural gas power plants and co-generation facilities gradually diminishes over the years until they completely phase out by 2049. Biomass cogeneration plants witness an increase by 2038.

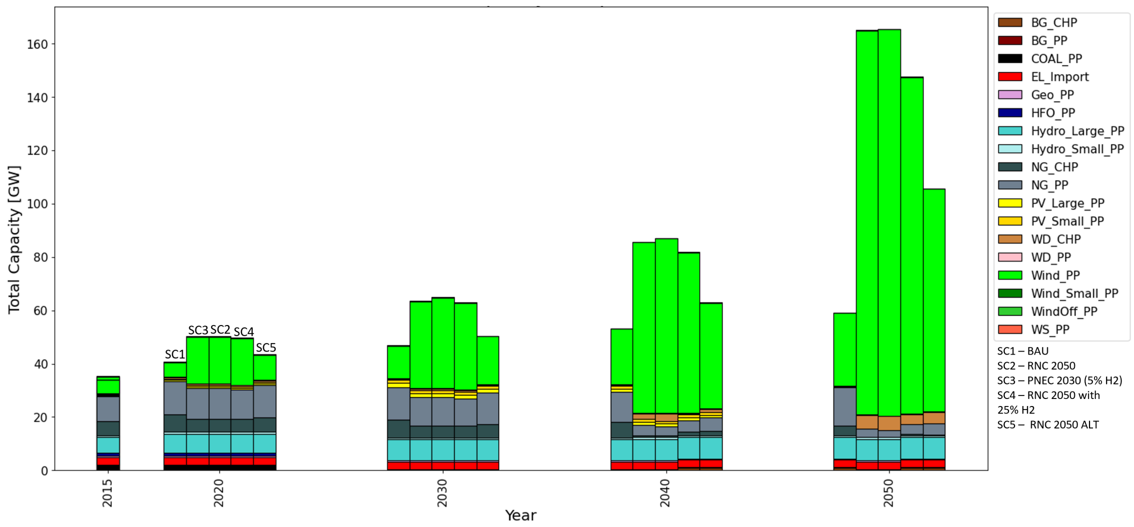

Figure 5.6: Installed capacity for electricity production

Considering the significant growth in the installed capacity of wind power plants and the corresponding investments in them until 2050, it becomes imperative to assess whether Portugal can feasibly meet the capacity requirements outlined by the model. The analysis reveals that until 2050, it falls short of the model's specified values. Consequently, it may be necessary to consider implementing future restrictions to curtail the utilization of wind power plants, by the model.

5.2.2.2 Annual activity

As the annual activity in electricity production is closely tied to the installed capacity designated for electricity generation, the analysis presented in the preceding subsection mirrors the findings in this one. The progression of various scenarios regarding annual electricity production activity is depicted in Figure 5.7.

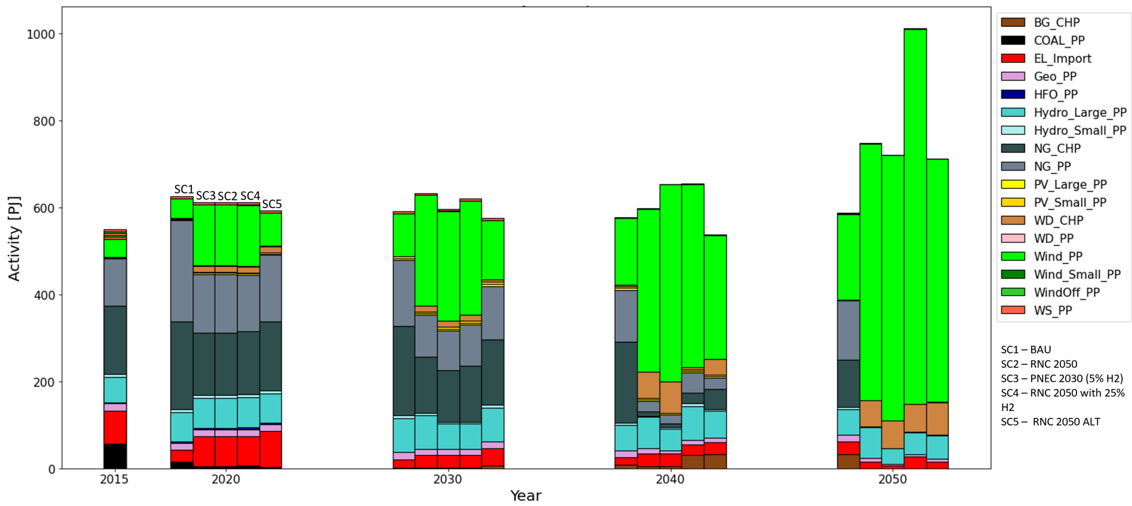

Figure 5.7: Annual activity for electricity production

5.2.3 Hydrogen production and utilization

After analyzing the results for the Business-As-Usual (BAU) scenario, which lacks any imposed restrictions, it becomes evident that the system does not allocate investments towards hydrogen technologies. This is a direct result of the way in which the model was developed, as the system only allocates hydrogen technologies if the demand added for hydrogen is non-null. This is reflected in the absence of hydrogen production and utilization within this scenario.

Similarly, in the context of the RNC 2050 scenario, despite the presence of certain restrictions concerning GHG emissions, the system still does not invest in hydrogen technologies., for the same reasons presented for the BAU scenarios. The results from the optimization also indicate that electricity-based technologies appear more appealing to the system, as once again, hydrogen production and utilization remain at zero.

In the context of the third scenario, PNEC 2030 (or 5% hydrogen in end-use sectors), hydrogen abruptly emerges within the system starting around 2030 - which is the result of restricting their integration into the system only from 2030, as the system starts investing in hydrogen production technologies. The corresponding installed capacity can be observed in Figure 5.8.

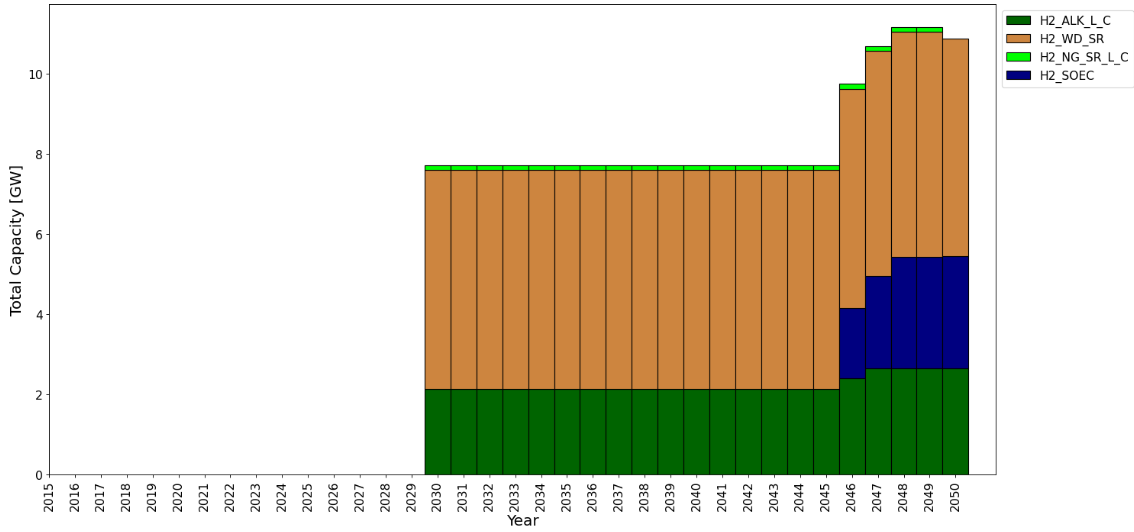

Figure 5.8: Installed capacity for hydrogen production - PNEC 2030 scenario

In the 25% H_2 scenario, where the utilization of hydrogen across end-use sectors is fixed at 25%, the system necessitates increased investment in hydrogen production technologies. Consequently, there is a noticeable escalation in the total installed capacity for hydrogen production. This development is depicted in Figures 5.9.

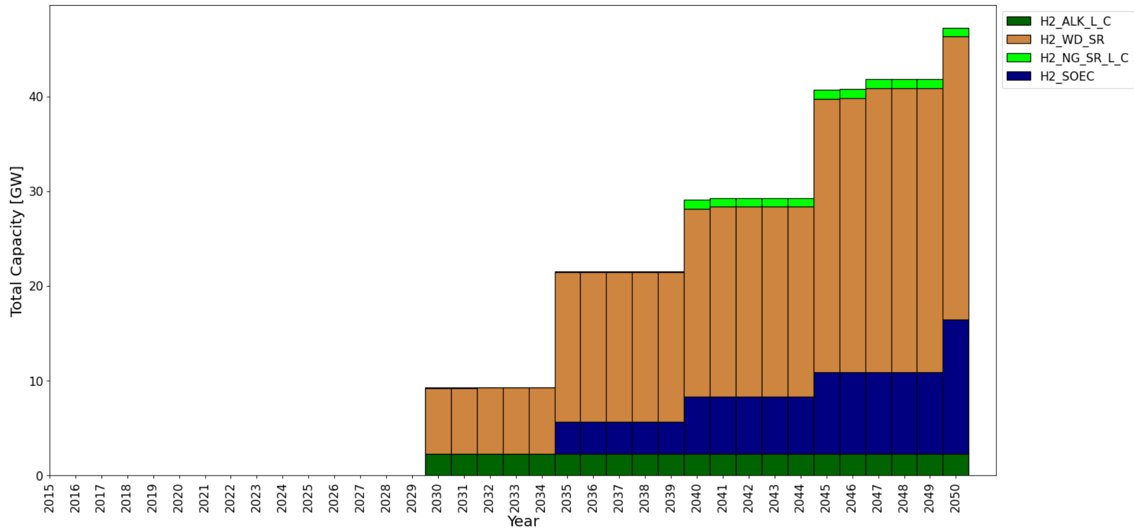

Figure 5.9: Installed capacity for hydrogen production - 25% H_2 scenario

Figure 5.10 illustrates the progression of installed capacity for hydrogen generation in the case of the scenario RNC2050_ALT. As the demand for hydrogen rises, the capacity expands to meet this growing demand.

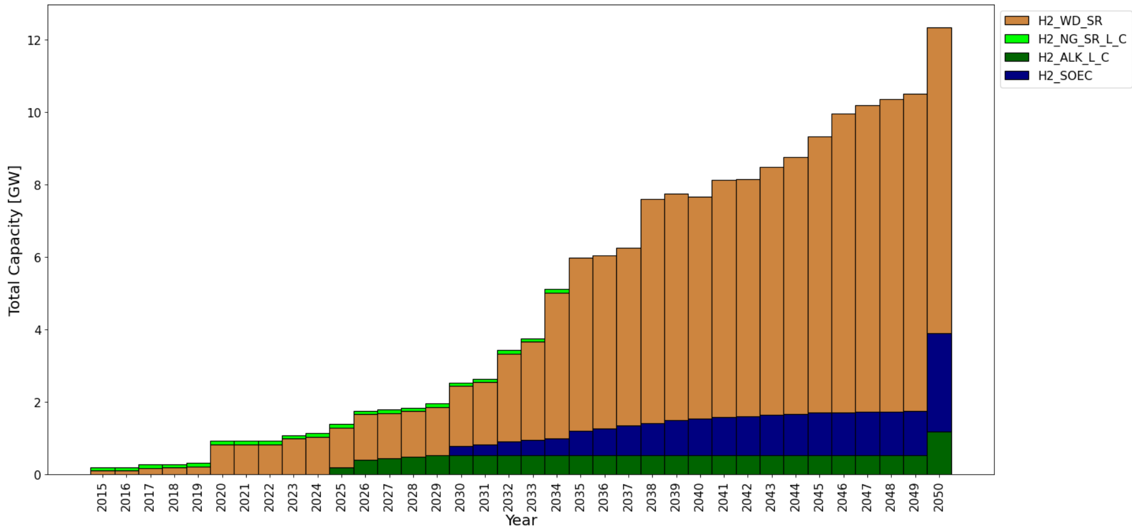

Figure 5.10: Installed capacity for hydrogen production - RNC2050_ALT scenario

Continuing along the trajectory of installed capacity allocated for hydrogen production, Figure 5.11 illustrates the trends observed across the three hydrogen-consumer scenarios. In all these scenarios, a consistent pattern emerges: the gradual increase in SOEC electrolysis over the years, attributed to cost reductions and enhanced efficiency. Additionally, there is a significant presence of biomass steam reforming, while alkaline electrolysis constitutes a smaller fraction of the hydrogen production methods. In the RCN 2050 scenario with a 25% hydrogen composition, the taller bars can be attributed to the substantial demand for hydrogen from end-users.

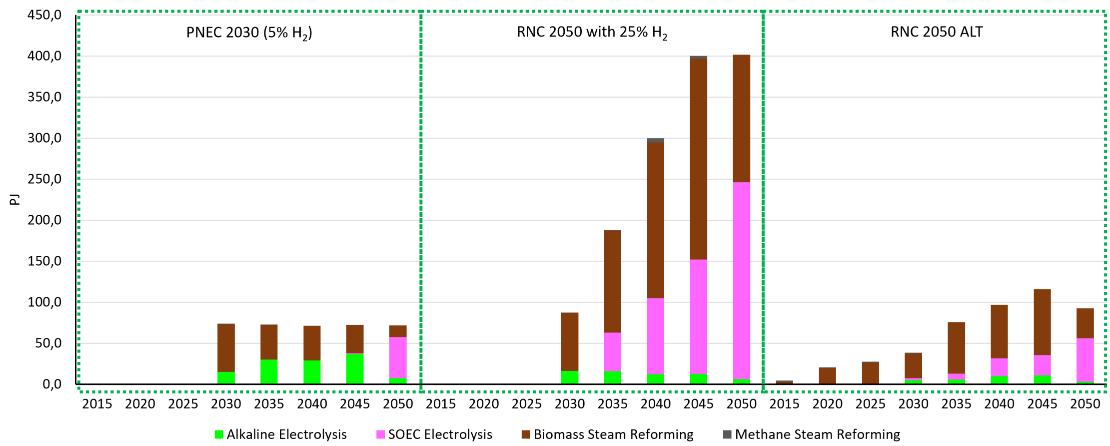

Figure 5.11: Hydrogen production with different technologies

Analyzing Figure 5.12, we can observe that the trends in the RCN 2050 scenario with 25% hydrogen and the RNC2050_ALT scenario exhibit similarities. Both scenarios experience a significant increase in hydrogen demand for residential and service buildings, with a moderate rise in demand for industry and transportation.

In contrast, the PNEC 2030 scenario, with its 5% hydrogen composition, maintains a relatively stable need for hydrogen from 2030 to 2050. This suggests that the system investments in the technologies remain largely consistent over this period.

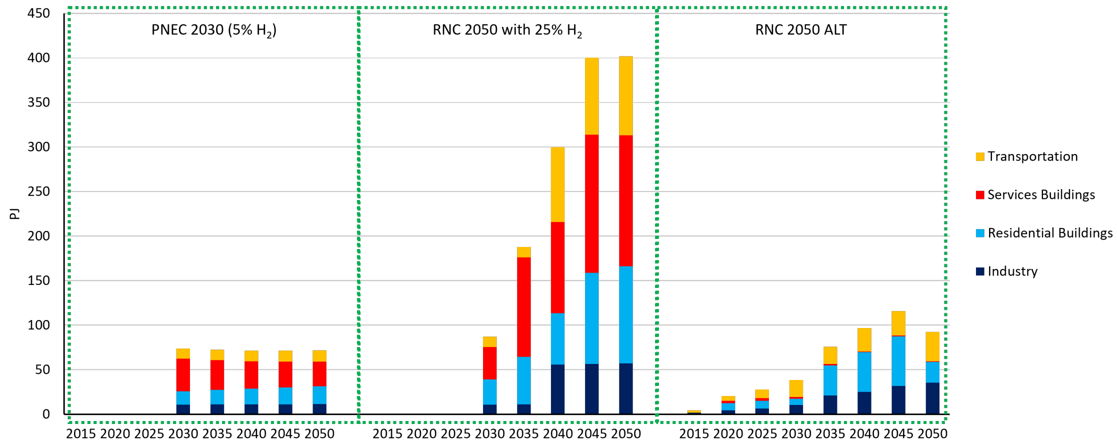

Figure 5.12: Hydrogen utilization in the different end-use sectors

Figure 5.13 illustrates the various technologies employed for end-use hydrogen consumption across different sectors. Examples of these technologies include hydrogen boilers and kilns in the industrial sector, boilers for domestic hot water, as well as hydrogen internal combustion engine cars, among others.

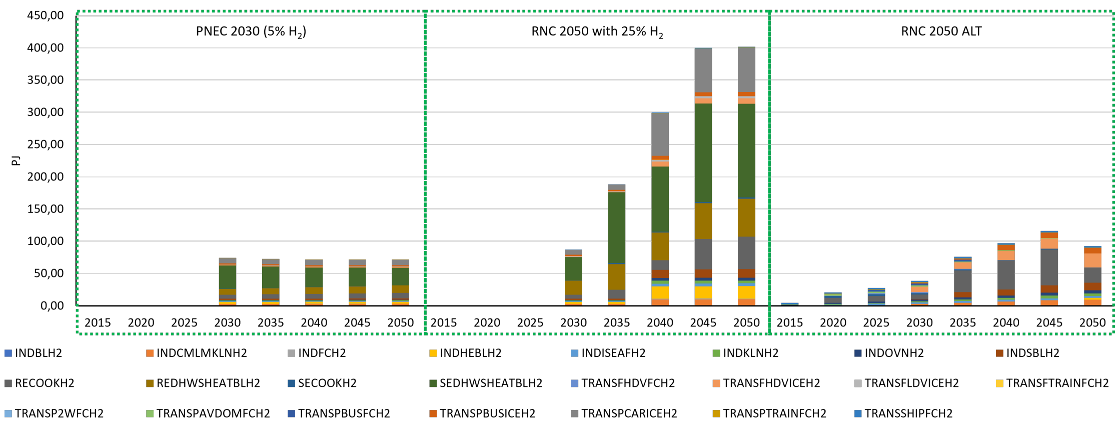

Figure 5.13: Hydrogen utilization in the end-use technologies

5.2.4 Specific uses characterization

In this subsection, it will be provided a detailed examination of specific applications within the end-use sectors, aiming to track the evolution of the technologies employed during the years 2015, 2030, and 2050.

5.2.4.1 Crude steel production

Figure 5.14 provides insight into the dynamics of the system. Notably, in the last three scenarios where hydrogen plays a role, we observe the increasing adoption of the hydrogen-driven technology known as H2 DRI-EAF. In the PNEC 2030 scenario, which has a modest hydrogen utilization constraint of 5%, this technology represents only a minor share. However, in the other two scenarios, by 2050, DRI-EAF nearly monopolizes crude steel production in the fourth scenario and accounts for over half of it in the fifth scenario.

This trend can be attributed to the favorable cost and efficiency assumptions associated with this technology. Even in the fifth scenario, where the system has the liberty to choose from various technologies, it leans significantly towards adopting the hydrogen-driven approach for crude steel production.

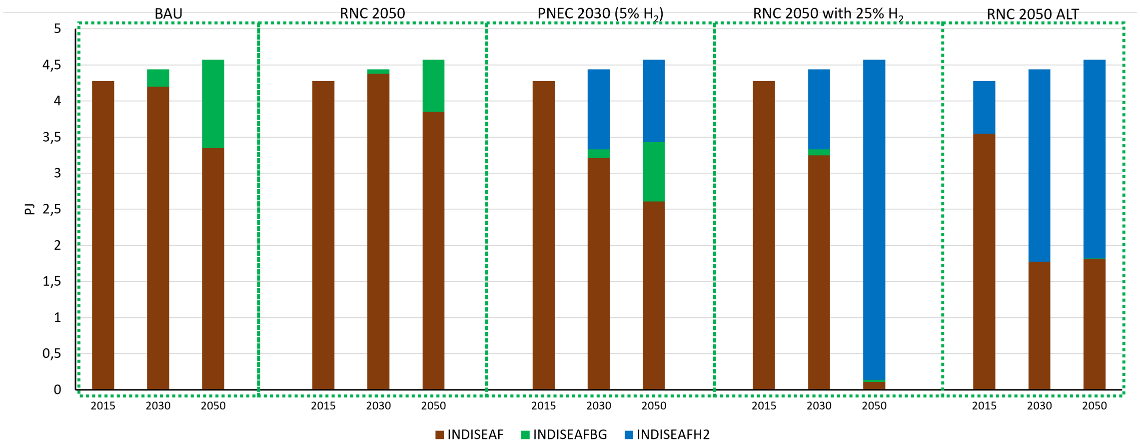

Figure 5.14: Crude steel technologies evolution

5.2.4.2 Industry steam production

Regarding steam production for industrial purposes, in the BAU scenario, it is possible to observe the utilization of coal-based steam boilers in 2050, aligning with the absence of GHG emissions constraints in this scenario. Both in this scenario and the second one, a substantial portion of steam production is generated by heat steam boilers.

For the subsequent scenarios, the prevailing trend remains the use of heat steam boilers. However, with the introduction of hydrogen into the system, hydrogen steam boilers begin to gain traction. In the third scenario, they represent only a minor share. However, as it progresses to the fourth and fifth scenarios, by 2050, hydrogen steam boilers almost entirely dominate industrial steam production. This suggests that as emissions are reduced, hydrogen emerges as a cost-effective and efficient solution for the system. The entire evolution can be observed in Figure

5.15.

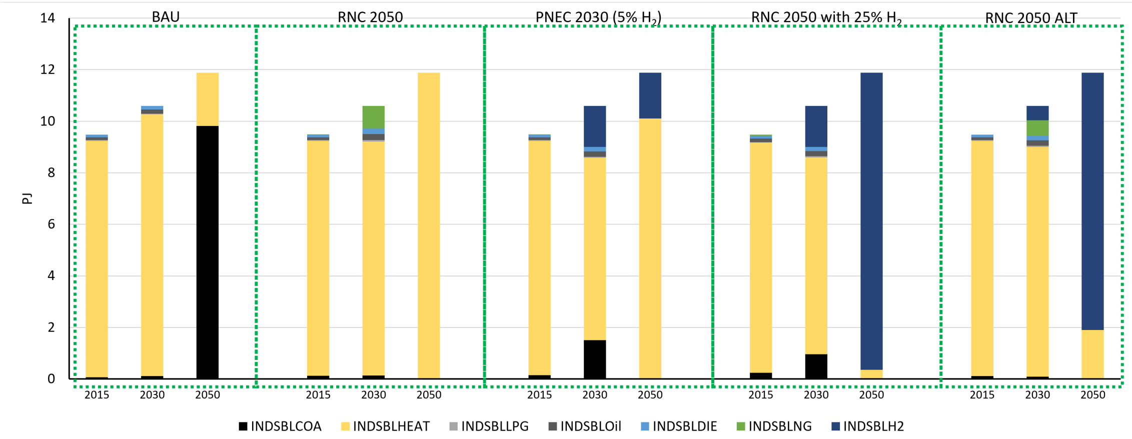

Figure 5.15: Steam production technologies evolution

5.2.4.3 Residential domestic hot water (DHW)

In the context of residential domestic hot water, as depicted in Figure 5.16, hydrogen integration into the system remains minimal. Only a minuscule share is observed in the third and fourth scenarios, primarily due to obligatory hydrogen utilization constraints. Across all scenarios, the dominant technology employed is the oil products boiler. In the scenario where the system enjoys flexibility in technology selection, the oil products boiler overwhelmingly dominates the landscape.

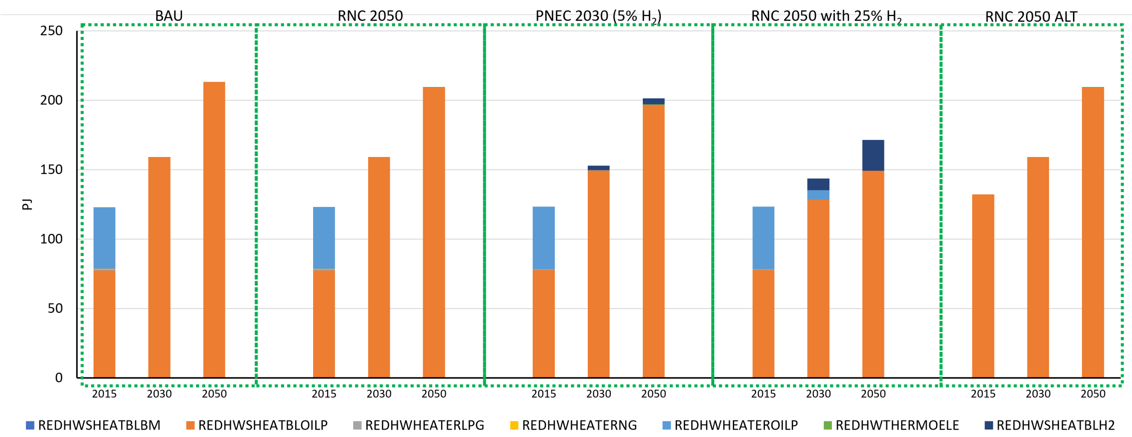

Figure 5.16: Residential DHW technologies evolution

5.2.4.4 Residential heating

The analysis of residential heating closely mirrors that of residential domestic hot water. Hydrogen integration into the system remains limited, and even in the fifth scenario, where there is flexibility in technology choice, the system primarily opts for the oil products boiler, presumably due to its cost-effectiveness and efficiency as the preferred solution. This is visually represented in Figure 5.17.

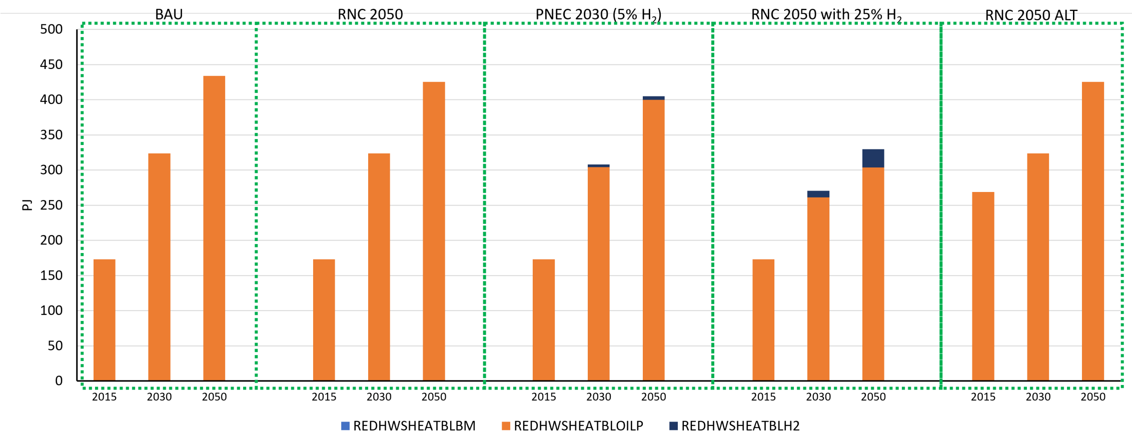

Figure 5.17: Residential heating technologies evolution

5.2.4.5 Freight heavy-duty vehicles (HDV)

Examining Figure 5.18, it is possible to observe that in the BAU scenario and the RNC 2050 scenario, the primary technology employed for freight Heavy-Duty Vehicles (HDV) is the internal combustion engine (ICE) powered by diesel. However, starting from the third scenario, internal combustion engines (ICE) based on hydrogen begin to emerge, albeit in a minor capacity.

As it progresses to the RNC 2050 with 25% hydrogen scenario, the share of hydrogen ICEs gradually increases until 2050, although it does not entirely replace diesel-based counterparts. In the fifth scenario, a noteworthy development occurs. By 2030, the majority of freight HD transportation relies on hydrogen, encompassing both ICE and fuel cell technologies. However, by 2050, fuel cell technology fades away, possibly due to higher associated costs, and the entire market shifts toward hydrogen ICE technology.

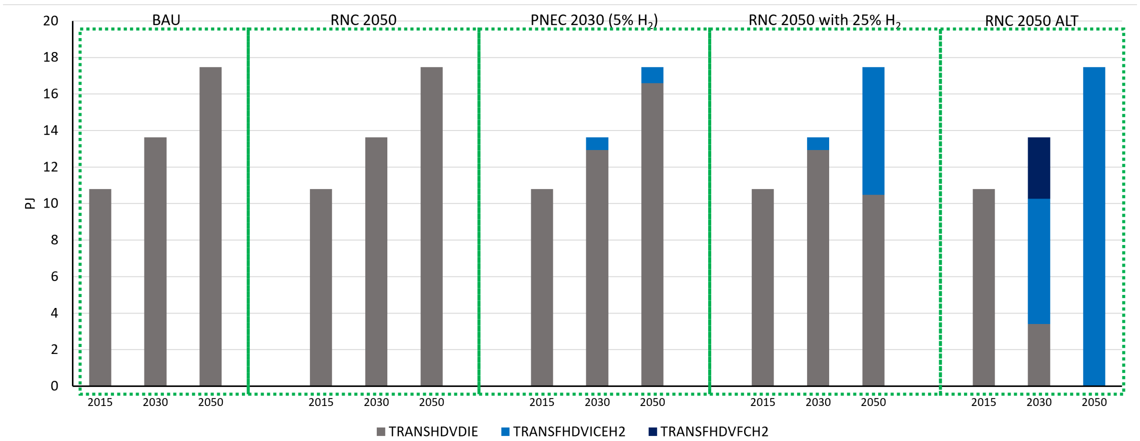

Figure 5.18: Freight HDV technologies evolution

5.2.5 CO_2 and NO_x emissions

In terms of CO_2 emissions, for the BAU scenario, even in the absence of any imposed restrictions on emissions reduction, a notable decrease of approximately 32% is observed. Emissions have diminished from 77 $MtCO_2eq$ to 52 $MtCO_2eq$, which can be attributed to the associated costs of emissions reduction efforts.

In the RNC 2050 scenario, as anticipated, emissions reduction is far more substantial, reaching approximately 88%. In this scenario, emissions have decreased from roughly 68 $MtCO_2eq$ to a mere 8 $MtCO_2eq$.

Given that the other scenarios followed the same trend as the RNC 2050 scenario in terms of reducing CO2 emissions, the level of reduction is also consistent, ultimately reaching an identical 88% reduction from 2015 levels.

Figure 5.19 showcases the dynamic changes in CO_2 emissions across all the scenarios under review.

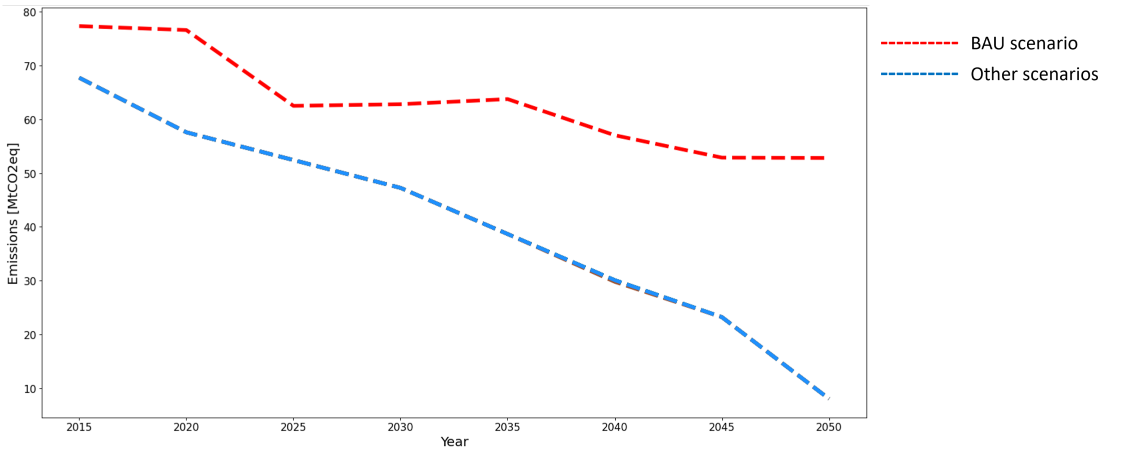

Figure 5.19: Annual CO_2 emissions for the different scenarios

When examining NO_x emissions, the BAU scenario portrays a consistent trend of emissions reduction, culminating in a decrease of approximately 25% by 2050 compared to 2015 levels. Emissions declined from 0.145 $MtNO_xeq$ to 0.109 $MtNO_xeq$ during this period.

In contrast, the RNC 2050 scenario exhibits a less uniform pattern. Emissions initially rose between 2020 and 2025, possibly attributed to heightened natural gas demand in the transportation sector and refineries. Subsequently, emissions undergo a substantial reduction, reaching their lowest point in 2050 at 0.005 $MtNO_xeq$, a significant decline from the 0.036 $MtNO_xeq$ recorded in 2015. The overall reduction in this scenario amounts to approximately 85%.

In the PNEC 2030 scenario, the reduction in NO_x emissions closely aligns with the pattern observed in the RNC 2050 scenario, with a minor deviation noticeable from the year 2025.

In the 25% H_2 scenario, NO_x emissions exhibit a similar trajectory to the previous two scenarios until 2035. However, from 2035 to 2050, the emissions follow a distinct trend, ultimately achieving the same emissions reduction target as the RNC 2050 and PNEC 2030 scenarios by 2050.

In the RNC2050_ALT scenario, NO_x emissions follow a trajectory resembling those observed in the previously mentioned scenarios, except for the BAU scenario. However, there are some distinct patterns, notably with a lower maximum level of emissions compared to the previous scenarios. Nevertheless, all scenarios ultimately converge to the same NO_x level, reflecting an 85% reduction from the 2015 levels.

Figure 5.20 illustrates the progression of NO_x emissions across all the scenarios under examination. The fluctuations in these emissions can be attributed to temporary investments in more pollutant technologies, undertaken to fulfill the demands within the end-use sectors.

Figure 5.20: Annual NO_x emissions for the different scenarios

5.2.6 Costs

This section discussed the OSeMOSYS costs of the system for the different scenarios.

5.2.6.1 Total costs

Figure 5.21 depicts the progression of system costs from 2015 to 2050, which are cumulative in nature. It's worth noting that there is a degree of similarity in the trends observed. However, it's crucial to exercise caution when interpreting this similarity, as some of the technology costs incorporated into the model were determined based on assumptions due to the absence of precise data. Hence, it is advisable to conduct further assessments and seek more accurate values to enhance the model's accuracy.

Despite these considerations, the scenarios with higher costs are the RNC 2050 with 25% hydrogen and the RNC2050_ALT scenarios, which interestingly entail identical cost profiles. This can be attributed to the elevated costs associated with hydrogen-related technologies. Typically, hydrogen-consumer technologies entail substantial investments, and both of these scenarios necessitate a degree of hydrogen utilization, which could account for the comparatively higher system costs.

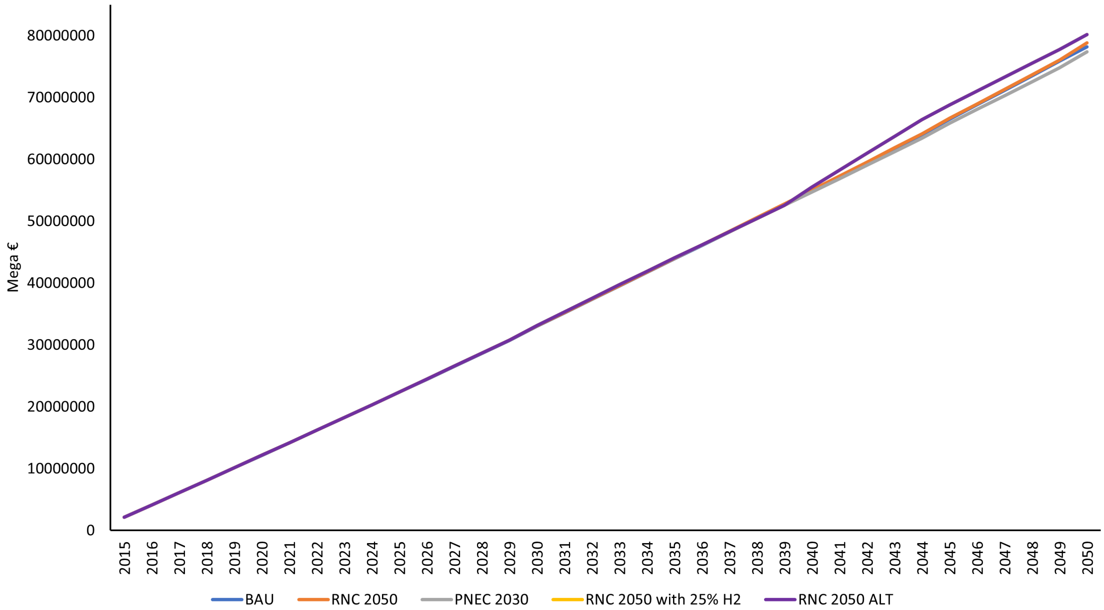

Figure 5.21: Total system costs for the different scenarios

5.2.6.2 Capital, fixed and variable costs across scenarios

Figures 5.22, 5.23, and 5.24 depict the progression of the three distinct cost categories: capital, fixed, and variable costs across all scenarios.

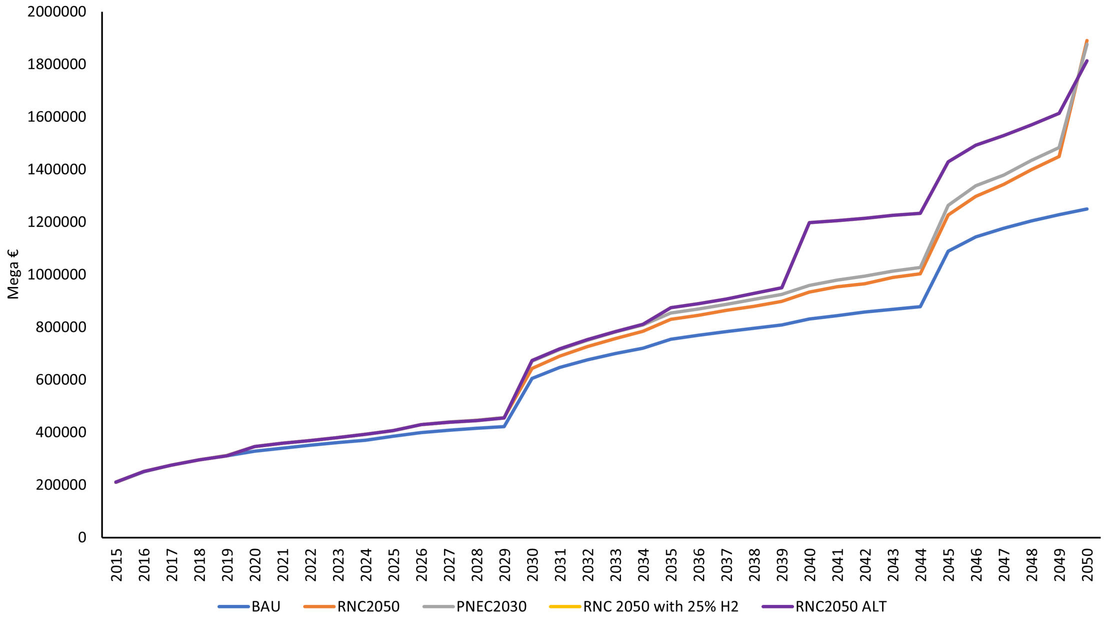

Figure 5.22: Evolution of the capital costs for the different scenarios

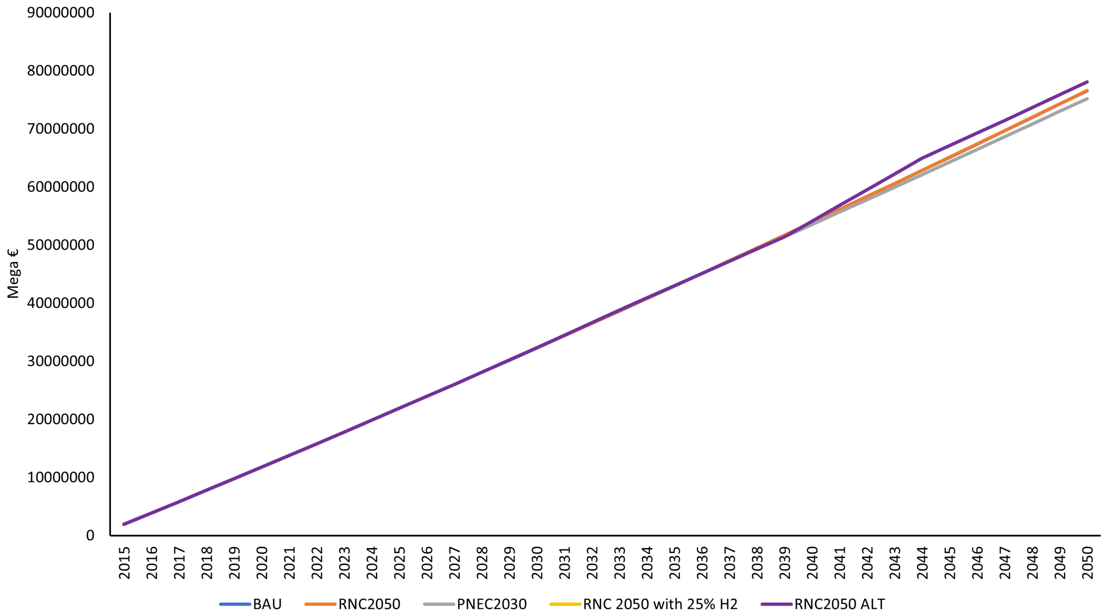

Figure 5.23: Evolution of the fixed costs for the different scenarios

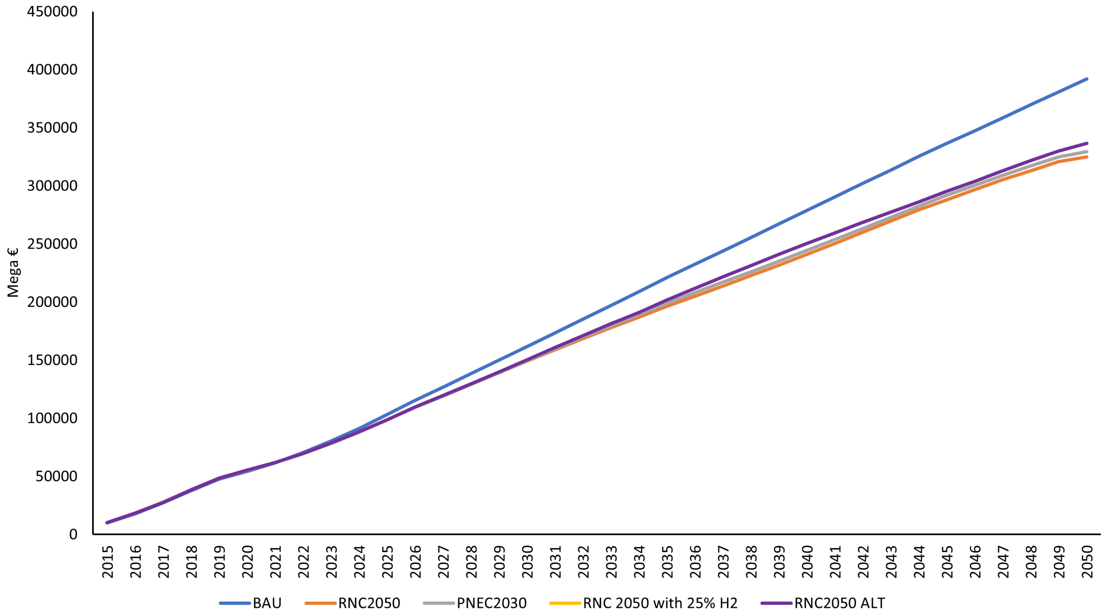

Figure 5.24: Evolution of the variable costs for the different scenarios

Chapter 6

Conclusions

6.1 Main results

One of the primary goals of the thesis was to establish and construct the hydrogen value chain, a fundamental undertaking aimed at enhancing the understanding of the entire process, encompassing hydrogen production, transmission, distribution, storage, and various conversion chains leading to end-user applications. The hydrogen value chain was meticulously developed, facilitating the incorporation of techno-economic data across the various components of these conversion chains.

The other pivotal objective was the creation of a model that incorporates hydrogen technologies while also disaggregating the end-use sectors into distinct categories, including buildings, industry, transport, agriculture, and fisheries. Subsequently, this model was subjected to simulation within five distinct scenarios, each characterized by unique restrictions.

The attainment of this model was made possible by leveraging techno-economic data derived from the constructed hydrogen value chain and drawing upon key information from the literature. This comprehensive approach allowed for the thorough characterization of technologies, spanning from primary sources to their final utilization.

When the goal is to curtail GHG emissions, the system invariably leans towards investing more in renewable energy sources. In the case of Portugal, this implies a need for increased investments in renewables to meet the capacity demands required for substituting fossil fuels.

In the context of hydrogen production, the prevailing technology utilized was SOEC electrolysis, which experienced consistent growth over the years. This trend can likely be attributed to the continuous reduction in investment costs in this particular technology. Additionally, alternative methods such as alkaline electrolysis and biomass steam reforming were also employed to a lesser extent. As for the end-users of hydrogen, it appears that the buildings sector was a significant consumer, accounting for substantial quantities. However, the industrial and transportation sectors also demonstrated noteworthy consumption, and this trend appears to be on the rise in subsequent years.

A key insight from the outcomes of the fifth scenario, wherein the model has the liberty to select the most suitable and cost-effective technologies for emissions reduction, is the ubiquitous presence of hydrogen technologies across various sectors such as industry, buildings, and transportation. Despite the absence of constraints on hydrogen usage, the system consistently opts for investments in hydrogen technologies. This suggests that hydrogen solutions likely offer superior cost-effectiveness in meeting both the demand and emission reduction requirements.

Across all scenarios, a common trend emerges as the total costs escalate exponentially leading up to the year 2050. This underscores one of the persistent challenges on the path to decarbonization. While the costs remain remarkably similar across all scenarios, their environmental impacts vary significantly. Notably, the BAU scenario exhibits a substantially detrimental environmental impact compared to the other four simulated scenarios. The similarity in costs and disparity in environmental impacts can be attributed to the reduction in costs of renewable technologies from 2015 to 2050, which continue to decrease, as well as the absence of carbon-related expenses.

Caution must be exercised when interpreting the results, as the model does not account for certain limitations. For instance, the absence of constraints on the utilization of specific renewable technologies like wind and solar power plants may have influenced the outcomes. Introducing these limitations could yield different results and potentially alter the choice of technologies. Additionally, the model's restriction to using only hydrogen gas within the system has impacted the results, which might have varied had it considered other aspects of the hydrogen value chain, such as hydrogen-based fuels and liquid hydrogen.

6.2 Model assumptions

Energy models hold significant importance for governments and policymakers, enabling them to enhance energy utilization, manage demand, and optimize energy system costs. Nonetheless, these models are not without limitations, primarily stemming from the data they rely upon. A considerable portion of this data is predictive in nature, and given the ever-evolving global economy, its accuracy might not always be optimal.

In this present model, conceived as an initial framework to serve as a foundation for future research and improvements, great care was taken to gather data from reliable sources. The necessity arose to make certain assumptions, such as centralizing all hydrogen production technologies, which provided the foundational basis for the study's scope and objectives. Additionally, given the preliminary nature of the model, another assumption was made to focus solely on hydrogen gas due to its perceived superior potential.

Chapter 7

Future Work

Given the time constraints and the extensive nature of this subject, certain aspects warrant further exploration in the future. These potential areas of focus could make valuable contributions to the ongoing development of this topic, including:

- With regard to the quest for sources and technologies aimed around the hydrogen value chain, the emphasis was placed on the primary ones. Hence, it is important to explore lesser-known technologies, thereby broadening our comprehension of hydrogen generation, transmission, distribution, storage, and applications at the end-user level;
- Continuing from the previous point, there is an opportunity to broaden the hydrogen value chain's construction, aiming to provide a more comprehensive and dependable depiction of the various hydrogen conversion processes;
- Incorporate additional data throughout the hydrogen value chain, ensuring enhanced reliability and consistency, making it more suitable for integration into the Portuguese energy system;
- Concerning the developed model, integrate supplementary technologies encompassing diverse fuels, spanning both centralized and decentralized approaches. Thoroughly populate the model with meticulous attention to detail, aiming to refine it into the most accurate possible representation of the Portuguese energy system.

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Appendix A

Techno-economic data related to hydrogen

A.1 Hydrogen Production

In the context of hydrogen generation, numerous sources and technologies have been highlighted earlier. These sources and technologies are accompanied by primary techno-economic data, which is comprehensively outlined in Tables A.1 to A.8.

Table A.1: Data associated with hydrogen production from water electrolysis [52] [53] [72]

Technology	Efficiency (2015)	Efficiency (2020)	Efficiency (2030)	Availability Factor	Lifetime
PEM Electrolyzer - Proton Exchange Membrane	65,00%	70,00%	75,02%	95%	3 years
Alkaline Electrolyser (large size, centralized)	66,67%	66,67%	-	90%	40 years
Alkaline Electrolyser (medium size, centralized)	61,24%	61,24%	70,62%	90%	20 years
Alkaline Electrolyser (small size, decentralized)	61,73%	61,73%	70,92%	90%	20 years
SOEC - Solid Oxide Electrolyzer Cell	-	90,50%	94,90%	95%	10 years

Table A.2: Costs associated with hydrogen production from water electrolysis [52] [53] [72]

Technology	CAPEX (€/kW) (2015)	CAPEX (€/kW) (2020)	CAPEX (€/kW) (2030)	FIXOM (€/kW) (2015)	FIXOM (€/kW) (2020)	FIXOM (€/kW) (2030)	VAROM (€/GJ) (2015)	VAROM (€/GJ) (2020)	VAROM (€/GJ) (2030)
PEM Electrolyzer - Proton Exchange Membrane	1500,00	1200,00	950,00	45,00	36,00	28,50	-	-	-
Alkaline Electrolyser (large size, centralized)	625,91	625,91	377,20	41,54	40,01	10,39	0,15	0,15	-
Alkaline Electrolyser (medium size, centralized)	1779,05	497,72	444,90	89,92	89,92	10,39	0,06	0,06	0,17
Alkaline Electrolyser (small size, decentralized)	1940,58	865,88	512,48	136,66	136,66	25,42	0,96	0,96	0,17
SOEC - Solid Oxide Electrolyzer Cell	-	785,00	450,00	-	66,00	13,50	-	-	-

Table A.3: Technical data associated with hydrogen production from coal [52] [53]

Technology	Efficiency (2015)	Efficiency (2020)	Efficiency (2030)	Availability Factor	Lifetime
Coal Gasification (large size, centralized)	54,35%	54,35%	60,98%	90%	20 years
Coal Gasification (medium size, centralized)	57,14%	57,14%	-	80%	20 years
Coal Gasification + CCUS (big size, centralized)	53,16%	53,16%	60,86%	90%	20 years
Coal Gasification + CCUS (medium size, centralized)	58,14%	58,14%	-	80%	20 years

Table A.4: Costs associated with hydrogen production from coal [52] [53]

Technology	CAPEX (€/kW) (2015)	CAPEX (€/kW) (2020)	CAPEX (€/kW) (2030)	FIXOM (€/kW) (2015)	FIXOM (€/kW) (2020)	FIXOM (€/kW) (2030)	VAROM (€/GJ) (2015)	VAROM (€/GJ) (2020)}	VAROM (€/GJ) (2030)
Coal Gasification (large size, centralized)	462,46	462,46	350,94	27,50	27,50	22,41	0,16	0,16	0,12
Coal Gasification (medium size, centralized)	573,37	573,37	-	14,33	14,33	-	0,22	0,22	-
Coal Gasification + CCUS (big size, centralized)	570,97	520,40	363,52	41,00	41,00	22,69	0,20	0,20	0,13
Coal Gasification + CCUS (medium size, centralized)	660,83	660,83	-	27,45	27,45	-	0,26	0,26	-

Table A.5: Technical data associated with hydrogen production from biomass [52] [53]

Technology	Efficiency (2015)	Efficiency (2020)	Efficiency (2030)	Availability Factor	Lifetime
Biomass steam reforming (centralized)	71,23%	71,23%	-	90%	20 years
Biomass Gasification (small size, decentralized)	31,25%	31,25%	-	71%	20 years
Biomass Gasification (medium size, centralized)	33,56%	52,52%	-	90%	20 years
Biomass Gasification + CCUS (medium size, centralized)	32,79%	51,36%	-	90%	20 years

Table A.6: Costs associated with hydrogen production from biomass [52] [53]

Technology	CAPEX (€/kW) (2015)	CAPEX (€/kW) (2020)	CAPEX (€/kW) (2030)	FIXOM (€/kW) (2015)	FIXOM (€/kW) (2020)	FIXOM (€/kW) (2030)	VAROM (€/kW) (2015)	VAROM (€/GJ) (2020)	VAROM (€/GJ) (2030)
Biomass steam reforming (centralized)	519,31	519,31	-	20,77	20,77	-	0,18	-	-
Biomass Gasification (small size, decentralized)	4101,10	3099,11	-	81,94	81,94	-	1,83	-	-
Biomass Gasification (medium size, centralized)	2637,55	1290,62	-	131,74	64,50	-	0,93	0,45	-
Biomass Gasification + CCUS (medium size, centralized)	2651,22	1309,21	-	111,52	65,32	-	0,93	0,46	-

Table A.7: Technical data associated with hydrogen production from natural gas (methane) and ethanol [12] [13] [52] [53]

Technology	Efficiency (2015)	Efficiency (2020)	Efficiency (2030)	Availability Factor	Lifetime
Methane Steam Reforming (large size, centralized)	74,63%	74,63%	78,68%	90%	20 years
Methane Steam Reforming (small size, centralized)	62,31%	62,31%	66,67%	90%	20 years
Methane Steam Reforming + CCUS (large size, centralized)	63,69%	63,69%	69,49%	90%	20 years
Methane Steam Reforming + CCUS (small size, centralized)	58,24%	58,24%	69,49%	90%	20 years
Solar Steam Reforming of Methane (centralized)	86,96%	86,96%	-	87%	20 years
Methane Steam Reforming (medium size, decentralized)	62,11%	62,11%	-	86%	20 years
Methane Steam Reforming (small size, decentralized)	53,33%	53,33%	62,50%	90%	20 years
Ethanol Steam Reforming (decentralized)	1,13%	1,13%	-	90%	10 years
Solar Steam Reforming of Methane (decentralized)	51,18%	51,18%	-	33%	20 years
Methane Autothermal Reforming	68,00%	68,00%	68,00%	90%	30 years
Methane Autothermal Reforming + CCUS	66,00%	66,00%	66,00%	90%	30 years
Methane Pyrolysis	-	65,00%	65,00%	90%	30 years
Methane Pyrolysis + CCUS	-	60,00%	60,00%	90%	30 years

Table A.8: Costs associated with hydrogen production from natural gas (methane) and ethanol [12] [13] [52] [53]

Technology	CAPEX (€/kW) (2015)	CAPEX (€/kW) (2020)	CAPEX (€/kW) (2030)	FIXOM (€/kW) (2015)	FIXOM (€/kW) (2020)	FIXOM (€/kW) (2030)	VAROM (€/GJ) (2015)	VAROM (€/GJ) (2020)	VAROM (€/GJ) (2030)
Methane Steam Reforming (large size, centralized)	201,16	201,16	158,25	9,84	9,84	7,65	0,08	0,08	0,05
Methane Steam Reforming (small size, centralized)	431,85	431,85	344,39	16,40	16,40	12,76	0,14	0,14	0,05
Methane Steam Reforming + CCUS (large size, centralized)	284,71	272,77	191,33	14,21	14,21	11,48	0,53	0,53	0,07
Methane Steam Reforming + CCUS (small size, centralized)	590,37	565,23	450,75	29,52	29,52	23,84	0,20	0,20	0,07
Solar Steam Reforming of Methane (centralized)	309,92	309,92	-	21,67	21,67	-	0,11	0,11	-
Methane Steam Reforming (medium size, decentralized)	485,78	485,78	-	28,21	28,21	-	0,04	0,04	-
Methane Steam Reforming (small size, decentralized)	1847,65	1642,94	1157,79	44,55	44,55	22,96	0,65	0,65	0,40
Ethanol Steam Reforming (decentralized)	7379,68	7379,68	-	-	-	-	19,65	19,65	-
Solar Steam Reforming of Methane (decentralized)	851,85	851,85	-	17,14	17,14	-	-	-	-
Methane Autothermal Reforming	467,73	467,73	467,73	23,39	23,39	23,39	-	-	-
Methane Autothermal Reforming + CCUS	901,02	901,02	901,02	45,05	45,05	45,05	-	-	-
Methane Pyrolysis	-	638,43	638,43	-	37,79	37,79	-	-	-
Methane Pyrolysis + CCUS	-	827,47	827,47	-	47,90	47,90	-	-	-

A.2 Hydrogen-based fuels

Concerning the generation of hydrogen-based fuels utilizing hydrogen gas, essential techno-economic information for various production technologies is provided in tables A.9 through A.12.

Table A.9: Production of synthetic methane from hydrogen for different years [55]

Technology	Year	Efficiency	AF	CAPEX (€/kW)	FIXOM (€/kW)	VAROM (€/MW)	Lifetime
Methanation	2020	77%	95%	880	35,2	4,2	30 years
	2030	77%	95%	739	29,6	3,5	30 years
	2050	77%	95%	440	17,6	2,1	30 years

Table A.10: Production of synthetic diesel from hydrogen for different years [55]

Technology	Year	Efficiency	AF	CAPEX (€/kW)	FIXOM (€/kW)	VAROM (€/MW)	Lifetime
Fischer-Tropsch	2020	73%	95%	2050	102,51	5,2	30 years
	2030	73%	95%	1557	77,87	4,1	30 years
	2050	73%	95%	880	44,00	2,0	30 years

Table A.11: Production of ammonia from hydrogen for different years [55]

Technology	Year	AF	CAPEX (€/t_{NH_3}/y)	FIXOM (€/t_{NH_3}/y)	VAROM (€/t_{NH_3}/y)	Lifetime
Haber-Bosch	2020	95%	678	19,67	-	30 years
	2030	95%	678	19,67	-	30 years
	2050	95%	678	19,67	-	30 years

Table A.12: Production of methanol from hydrogen for different years [54]

Feedstock	Year	AF	CAPEX (€/t_{MeOH})	FIXOM (€/t_{MeOH})	VAROM (€/t_{MeOH})	Lifetime
Natural gas	2020	95%	276,96	6,92	-	25 years
	2030	95%	276,96	6,92		
	2050	95%	276,96	6,92		
Natural gas + CCUS	2020	95%	469,04	11,73	-	25 years
	2030	95%	455,64	11,39		
	2050	95%	437,77	10,94		
Coal	2020	95%	670,06	33,50	-	25 years
	2030	95%	670,06	33,50		
	2050	95%	670,06	33,50		
Coal + CCUS	2020	95%	1344,58	67,23	-	25 years
	2030	95%	1295,44	64,77		
	2050	95%	1206,10	60,31		
Biomass	2020	95%	4614,46	230,72	-	25 years
	2030	95%	4614,46	230,72		
	2050	95%	4614,46	230,72		
Electrolysis	2020	95%	705,79	10,59	-	25 years
	2030	95%	531,58	7,97		
	2050	95%	339,50	5,09		

A.3 Hydrogen Transmission and Distribution

Regarding hydrogen, hydrogen-based fuels, and LOHC transmission and distribution, tables A.13 through A.25 showcase the techno-economic data associated with various available choices.

Table A.13: Characteristics of pipelines destined for hydrogen, LOHC, and ammonia transmission (2020) [54]

	Fuel		
	Hydrogen	LOHC	Ammonia
Lifetime (years)	40	-	40
CAPEX (Million €/km)	1,08	2,07	0,49
Utilization	75%	75%	75%

Table A.14: Characteristics of liquefaction of hydrogen (2020) [54]

	Liquefaction
Efficiency (% LHV)	65 - 75%
Capacity CAPEX (Million €)	1250,77
Annual OPEX (Million €)	50,03

Table A.15: Characteristics of conversion of LOHC (2020) [54]

	LOHC
Efficiency (% LHV)	90 - 95%
Plant CAPEX (Million €)	205,48
Annual OPEX (Million €)	8,22

Table A.16: Costs of two different hydrogen injection stations (2020) [22]

	Power	
	1 MW	100 MW
CAPEX (Million €)	1,30	2,77
OPEX (Million €)	0,10	0,22

Table A.17: Characteristics of a hydrogen export terminal (2020) [54]

	Fuel		
	Hydrogen	LOHC	Ammonia
CAPEX/tank (Million €)	259,09	37,52	60,75
Annual OPEX (Million €)	10,36	1,50	2,43
Boil off rate (%/day)	0,2	-	-
Flash rate (%)	0,1	-	-

Table A.18: Characteristics for seaborne transport (2020) [54]

	Fuel		
	Hydrogen	LOHC	Ammonia
CAPEX/ship (Million €)	368,08	67,90	75,94
Annual OPEX (Million €)	14,72	2,72	3,04
Boil off rate (%/day)	0,2	-	-
Flash rate (%)	1,3	-	-

Table A.19: Characteristics for a hydrogen import terminal (2020) [54]

	Fuel		
	Hydrogen	LOHC	Ammonia
CAPEX/tank (Million €)	285,89	31,27	86,66
Boil off rate (%/day)	0,1	-	-

Table A.20: Characteristics of reconversion back to hydrogen (2020) [54]

	Fuel	
	LOHC	Ammonia
Efficiency (% LHV)	65	80
Capacity CAPEX (Million €)	598,58	410,97
Annual OPEX (Million €)	23,94	16,44

Table A.21: Characteristics of high-pressure pipelines destined for hydrogen, LOHC, and ammonia distribution (2020) [54]

	Fuel		
	Hydrogen	LOHC	Ammonia
Lifetime (years)	40	40	40
CAPEX/km (Million €)	0,45	0,89	0,22

Table A.22: Characteristics of low-pressure pipelines destined for hydrogen, LOHC, and ammonia distribution (2020) [54]

	Fuel		
	Hydrogen	LOHC	Ammonia
Lifetime (years)	40	40	40
CAPEX/km (Million €)	0,27	-	-

Table A.23: Characteristics of trucks destined for hydrogen, LOHC, and ammonia distribution (2020) [54]

	Fuel		
	Hydrogen	LOHC	Ammonia
Depreciation period (years)	12	12	12
CAPEX (Thousand €)	165,28	165,28	165,28
Annual OPEX (Thousand €)	19,83	19,83	19,83

Table A.24: Characteristics of trailers destined for hydrogen, LOHC, and ammonia distribution (2020) [54]

	Fuel		
	Hydrogen	LOHC	Ammonia
Depreciation period (years)	12	12	12
CAPEX (Thousand €)	LH2: 893,41 GH2: 580,72	151,88	196,55
Annual OPEX (Thousand €)	LH2: 17,87 GH2: 11,61	3,04	3,93

Table A.25: Characteristics of refueling stations destined for hydrogen, LOHC, and ammonia (2020) [54]

	Fuel		
	Hydrogen	LOHC	Ammonia
Lifetime (years)	10	10	10
CAPEX (Million €)	0,80 - 1,07	3,13	1,97
OPEX (Million €)	0,04 - 0,05	0,16	0,10
Boil off	LH2: 3% GH2: 0,5%	0,5%	1,50%

A.4 Hydrogen Storage

Concerning the storage of hydrogen, you can find detailed techno-economic information in Table A.26 for long-term and large-scale storage of hydrogen and ammonia. Additionally, Tables A.27 and A.28 provide data on various short-term storage methods for 2015 and 2025.

Table A.26: Long-term and large-scale storage characteristics (2020) [54]

Technology	CAPEX (power) (€/kW)	OPEX (power) (€/kW)	CAPEX (energy) (€/kWh)	OPEX (energy) (€/kWh)	Round-trip efficiency	Lifetime
Compressed hydrogen storage	1626,00	65,22	0	0	37%	20 years
Ammonia storage	2537,28	38,42	0	0	22%	20 years

Table A.27: Day/Night and seasonal storage characteristics (2015) [52] [53]

Technology	Efficiency	AF	CAPEX (€/kWh)	FIXOM (€/kWh)	VAROM (€/kWh)	Lifetime
Centralised Hydrogen Underground Storage	100%	100%	3,53	0,30	-	30 years
Centralised Hydrogen Gas Tank Storage	100%	98%	16,58	0,76	-	22 years
Distributed Hydrogen Gas Tank Storage	100%	98%	9,55	0,44	-	22 years

Table A.28: Day/Night and seasonal storage characteristics (2025) [52] [53]

Technology	Efficiency	AF	CAPEX (€/kWh)	FIXOM (€/kWh)	VAROM (€/kWh)	Lifetime
Centralised Hydrogen Underground Storage	100%	100%	2,71	0,23	-	30 years
Centralised Hydrogen Gas Tank Storage	100%	98%	12,97	0,60	-	22 years
Distributed Hydrogen Gas Tank Storage	100%	98%	7,47	0,34	-	22 years

A.5 Hydrogen End-use applications

When considering the industrial utilities of hydrogen, specifically within the steel sector, Table A.29 outlines key techno-economic details concerning the hydrogen-based Direct Reduced Iron (DRI) - Electric Arc Furnace (EAF) technology.

Table A.29: Data associated with Hydrogen-based DRI-EAF technology [54]

	Year	2020	2030	2050
Hydrogen-based DRI-EAF	CAPEX (€/$t_{\text{crude steel}}$)	844,27	763,86	674,52
	Annual OPEX (€/$t_{\text{crude steel}}$)	135,08	137,50	134,90
	Electricity consumption (GJ/$t_{\text{crude steel}}$)	14,7	13,9	13,2
	Biomass consumption (GJ/$t_{\text{crude steel}}$)	1,9	1,9	1,9

Concerning the field of transportation, Tables A.30 to A.41 display key technical and economic information pertaining to various transportation modes and diverse fuel types.

Table A.30: Technical data associated with different modes of transportation and fuel type [52] [53]

Mode of transportation	Fuel type	Efficiency (2015)	Efficiency (2020)	Efficiency (2030)	Efficiency (2050)	Lifetime
Car	Hydrogen gas (IC)	38,38%	38,38%	42,53%	52,21%	15 years
	Liquid hydrogen (IC)	40,31%	40,31%	44,67%	54,84%	15 years
	Hydrogen gas (FC)	60,64%	60,64%	67,19%	82,49%	15 years
Bus	Hydrogen gas (FC)	82,88%	-	86,20%	90,61%	15 years
Truck HD	Hydrogen gas (FC)	75,96%	-	79,00%	83,04%	15 years
Truck LD	Hydrogen gas (IC)	51,18%	51,18%	56,71%	62,83%	15 years
	Liquid hydrogen (IC)	53,75%	53,75%	59,55%	65,99%	15 years
	Hydrogen gas (FC)	80,85%	80,85%	89,58%	99,26%	15 years

Table A.31: Costs associated with different modes of transportation and fuel type [52] [53]

Mode of transportation	Fuel type	CAPEX (€) (2015)	CAPEX (€) (2020)	CAPEX (€) (2030)	CAPEX (€) (2050)	FIXOM (€) (2015)	FIXOM (€) (2020)	FIXOM (€) (2030)	FIXOM (€) (2050)
Car	Hydrogen gas (IC)	24530	-	24130	24080	740	-	720	720
	Liquid hydrogen (IC)	24530	-	24130	24080	740	-	720	720
	Hydrogen gas (FC)	33600	24350	22527	20540	1010	730	680	620
Bus	Hydrogen gas (FC)	507570	-	415680	293170	10150	-	8310	5860
Truck HD	Hydrogen gas (FC)	219410	-	209820	197020	4390	-	4200	3940
Truck LD	Hydrogen gas (IC)	24530	-	24130	24080	740	-	720	720
	Liquid hydrogen (IC)	24530	-	24130	24080	740	-	720	720
	Hydrogen gas (FC)	33600	24350	22527	20540	1010	730	680	620

Table A.32: Techno-economic data related to hydrogen bikes (2020) [22]

Hydrogen Bike	Power output (kW)	0,1 - 0,25
	Fuel consumption (kg H_2/100km)	0,035
	Range (km)	100 - 150
	CAPEX/acquisition cost (€)	4467 - 6700
	Lifetime (years)	5

Table A.33: Techno-economic data related to hydrogen scooters (2020) [22]

Hydrogen Scooter	Power output (kW)	3 - 4
	Fuel consumption (g H_2/100km)	0,3 - 0,8
	Range (km/tank)	120 - 200
	CAPEX/acquisition cost (€)	3037 - 11614
	Lifetime (years)	5

Table A.34: Techno-economic data associated with hydrogen forklifts (2020) [22]

Hydrogen Forklift	Power output (kW)	2,5 - 4,5
	Fuel consumption (kg H_2/hour)	0,15
	Range (km/tank)	8
	CAPEX/acquisition cost (€)	12507 - 26802

Table A.35: Techno-economic data associated with hydrogen cars (2020) [22]

Hydrogen Car	Power output (kW)	70 - 130
	Fuel consumption (kg H_2/100km)	0,8 - 1
	Range (km/tank)	500 - 700
	CAPEX/acquisition cost (€)	50030 - 76833
	Lifetime (years)	5

Table A.36: Techno-economic data related to hydrogen vans (2020) [22]

Hydrogen Van	Power output (kW)	45 - 150
	Fuel consumption (kg H_2/100km)	3,0 - 9,0
	Range (km/tank)	300 - 400
	CAPEX/acquisition cost (€)	-

Table A.37: Techno-economic data associated with hydrogen buses (2020) [22]

Hydrogen Bus	Power output (kW)	100
	Fuel consumption (kg H_2/100km)	8,0 -14,0
	Range (km/tank)	250 - 450
	CAPEX/acquisition cost (€)	607518

Table A.38: Techno-economic data associated with hydrogen trucks (2020) [22]

Hydrogen Truck	Power output (kW)	250 - 750
	Fuel consumption (kg H_2/100km)	7,5 - 16
	Range (km/tank)	1200
	CAPEX/acquisition cost (€)	312693
	Fuel cell efficiency	55%

Table A.39: Techno-economic data for marine applications (2020) [22]

Marine applications	Power output (kW)	12 - 2500
	Fuel consumption (kg H_2/nm)	3,4
	Range (hours)	50 - 90, 8 - 12
	CAPEX/acquisition cost (€)	10,7 - 14,7 M
	Lifetime (years)	25

Table A.40: Techno-economic data related to hydrogen trains (2020) [22]

Hydrogen Train	Power output (kW)	400
	Fuel consumption (kg H_2/100km)	33
	Range (km/tank)	600 - 800
	CAPEX/acquisition cost (€)	11,6 M

Table A.41: Techno-economic data associated with aviation, based on the HY4 project (2020) [22]

Aviation	Power output (kW)	80
	Fuel consumption (kg H_2)	170
	Range (km)	750 - 1500
	CAPEX/acquisition cost (€)	-
	Lifetime (years)	-

Concerning the field of buildings, Tables A.42 to A.45 display the primary technologies utilized for heating both spaces and water.

Table A.42: Techno-economic data related to space and water heating in buildings (2020) [72]

Sector	Feed	Technology	Efficiency	CAPEX (€/kW)	VAROM (€/GJ)	Heat to power ratio	Lifetime
Residential	Natural Gas blend	PEM	39,0%	9000	5,0	1,46	20 years
	Natural Gas blend	Solid Oxide	50,0%	3964	4,8	0,88	20 years
	Pure H2	PEM	50,0%	9000	6,7	0,96	20 years
	Pure H2	Solid Oxide	55,0%	3000	4,5	0,78	20 years
Commercial	Natural Gas blend	PEM	39,0%	4000	12,5	1,33	20 years
	Natural Gas blend	Solid Oxide	60,0%	1850	2,2	0,57	20 years
	Pure H2	Solid Oxide	50,0%	350	5,6	0,9	20 years

Table A.43: Technical and economic data associated with different technologies for space and water heating (2030) [55]

Technology	Efficiency	CAPEX (€/kW)	OPEX (€/kW/y)	Lifetime
Hydrogen Boiler	85 - 95%	211,5	6,3	15 years
Hydrogen Hybrid Heat Pump	220 - 320%	380,6	11,4	15 years
Hydrogen Fuel Cell	75 - 95%	2960,3	88,8	15 years

Table A.44: Techno-economic data associated with hydrogen burners (2010) [52]

Technology	Efficiency	CAPEX (€/kW)	FIXOM (€/kW)	Lifetime
Hydrogen Burner	86%	1827,3	104,4	20 years

Table A.45: Techno-economic data for fuel-cell technologies with CHP [52]

Technology	Year	CAPEX (€/kW)	VAROM (€/kW)	Electrical Efficiency	Thermal Efficiency	Heat To Power	Lifetime
PEM Fuel Cell	2010	50000	55,6	36,0%	52,0%	1,44	20 years
	2020	15000	31,9	37,0%	52,0%	1,41	20 years
	2030	11500	19,4	38,0%	52,0%	1,37	20 years
	2040	8500	13,9	39,0%	52,0%	1,33	20 years
	2050	7800	12,5	39,0%	52,0%	1,33	20 years
SO Fuel Cell	2010	18000	33,3	53,0%	32,0%	0,60	20 years
	2020	6300	18,1	53,0%	32,0%	0,60	20 years
	2030	4000	6,9	55,0%	32,0%	0,58	20 years
	2040	2550	2,8	59,0%	34,0%	0,58	20 years
	2050	1850	2,2	60,0%	34,0%	0,57	20 years

Two primary options for co-firing in electricity generation are accessible, and pertinent technical and economic information can be found in Table A.46.

Table A.46: Technical and economic data related to electricity generation through co-firing in existing fossil thermal plants (2020) [55]

Technology	Parameter	Values
Natural Gas Combined Cycle plant	Modification to H_2 combustion (€/MWh)	1,44
	LNG price (€/MWh)	16,9 - 24,5
	OPEX (excluding fuel) (€/MWh)	1,7
	Efficiency	51%
Coal Ultra-Supercritical plant	Modification to NH_3 combustion (€/MWh)	0,93
	Coal price (€/MWh)	5,9 - 11,8
	OPEX (excluding fuel) (€/MWh)	3,4
	Efficiency	44%
Hydrogen Fuel	Price (€/kg)	1,3 - 2,1
Ammonia Fuel	Price (€/t)	253,7 - 422,9

Appendix B

Disaggregation of the end-use sectors

This chapter will present a comprehensive breakdown of the end-use sectors, including the industrial sector, buildings sector, and transport sector. Refer to Figures B.1 to B.5 for visual representation.

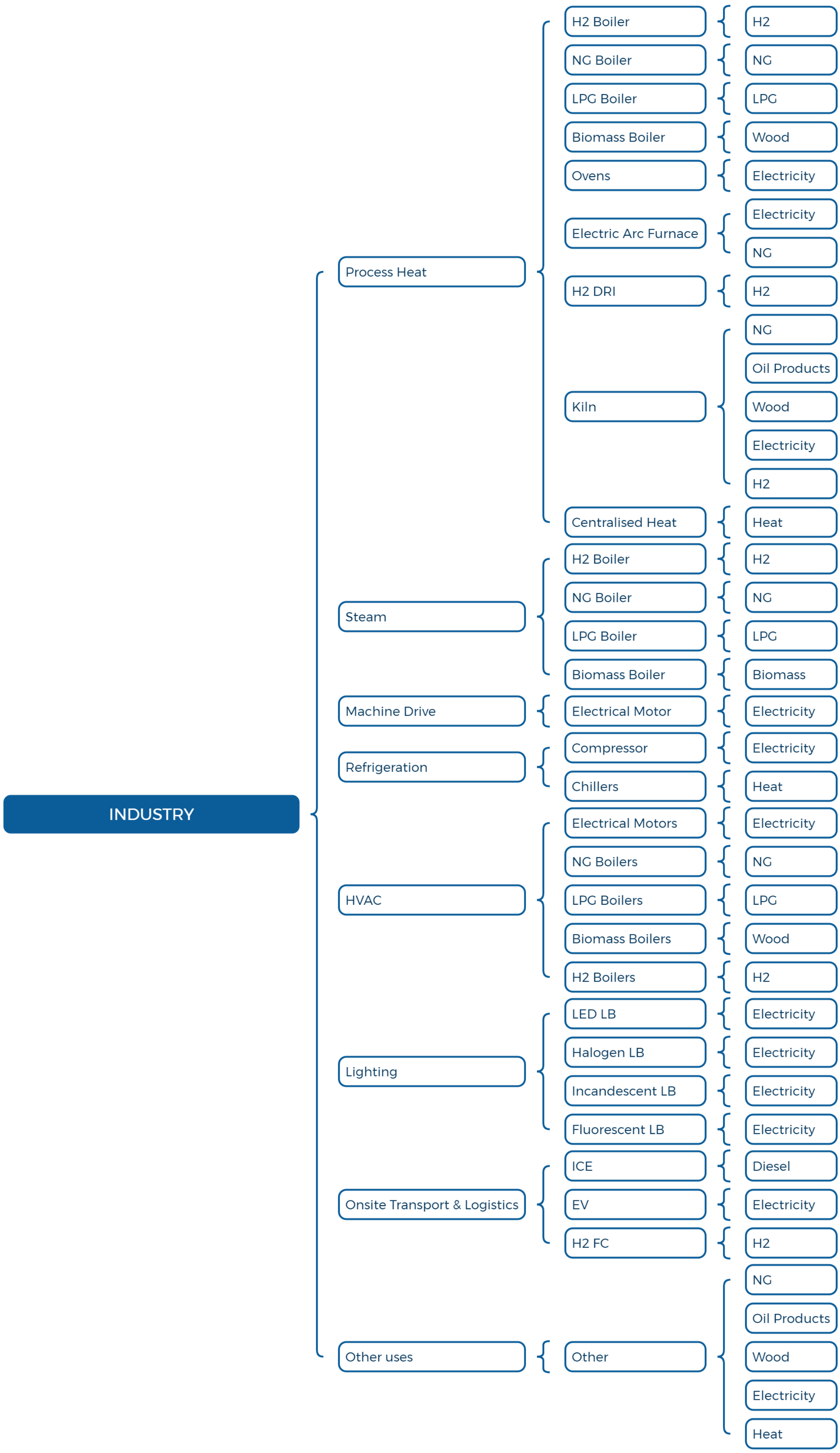

Figure B.1: Visual Representation showcasing the complete breakdown of the industrial sector.

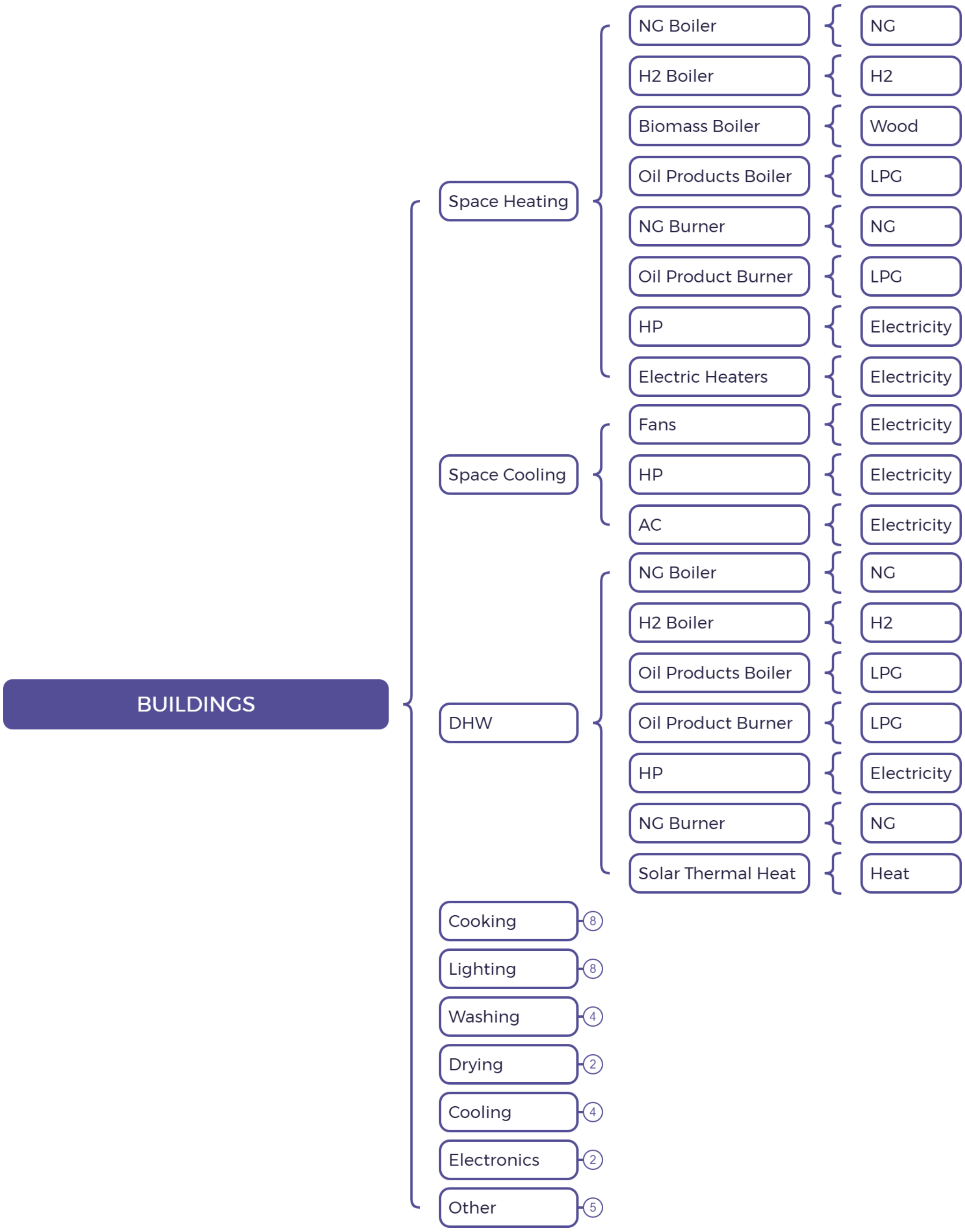

Figure B.2: Visual depiction illustrating the progressive disaggregation of the buildings sector (part 1).

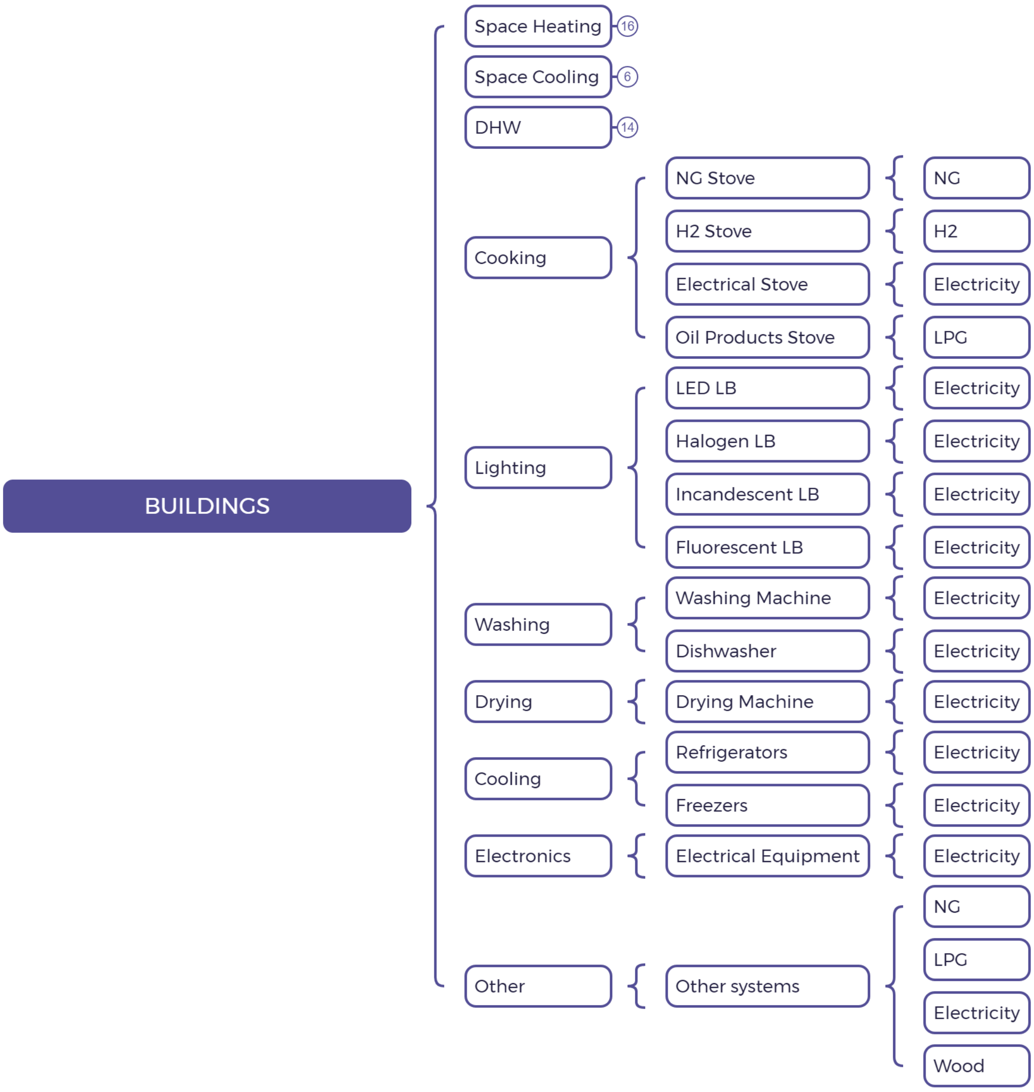

Figure B.3: Visual depiction illustrating the progressive disaggregation of the buildings sector (part 2).

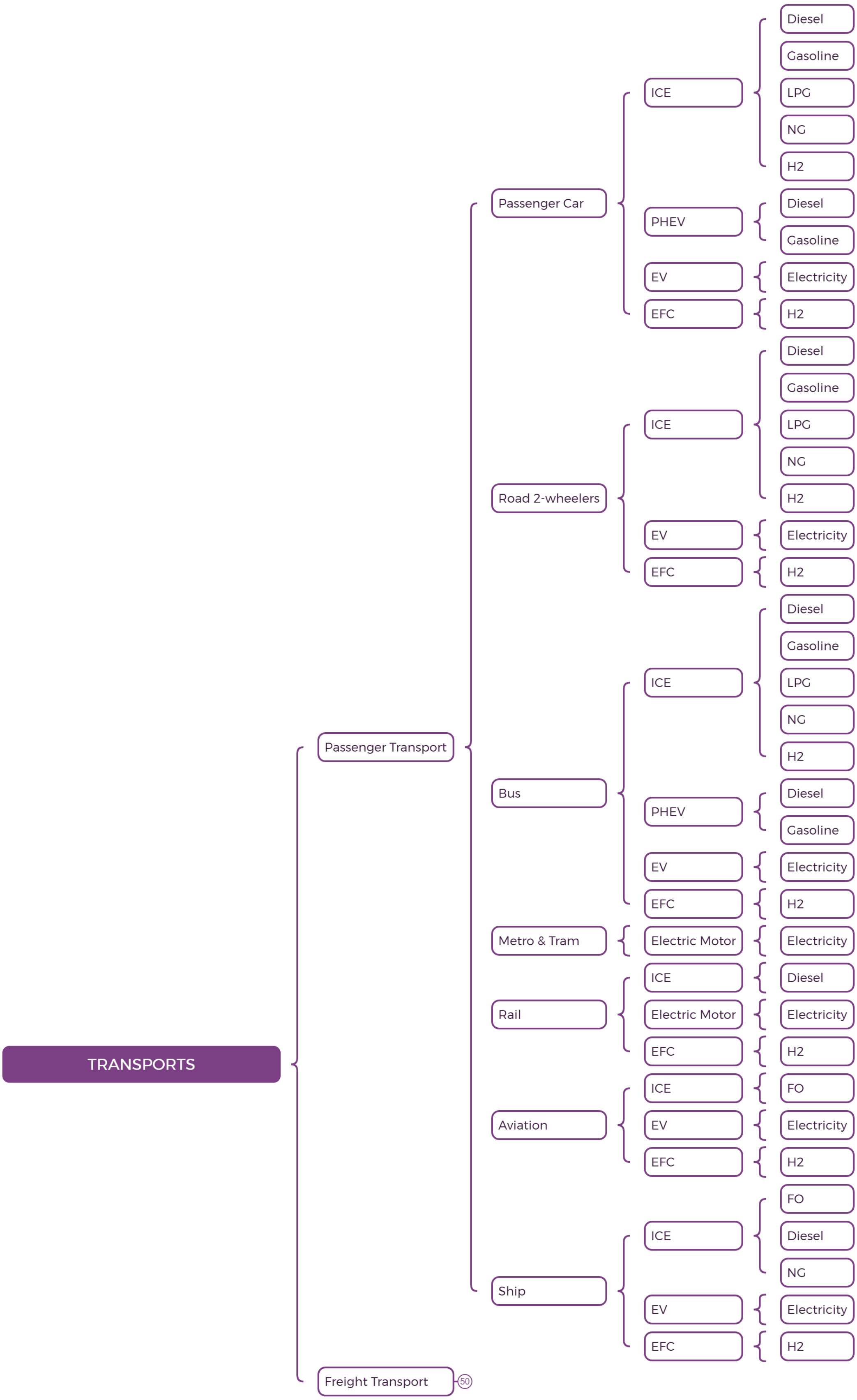

Figure B.4: Illustration presenting the comprehensive disaggregation of the entire transport sector (part 1).

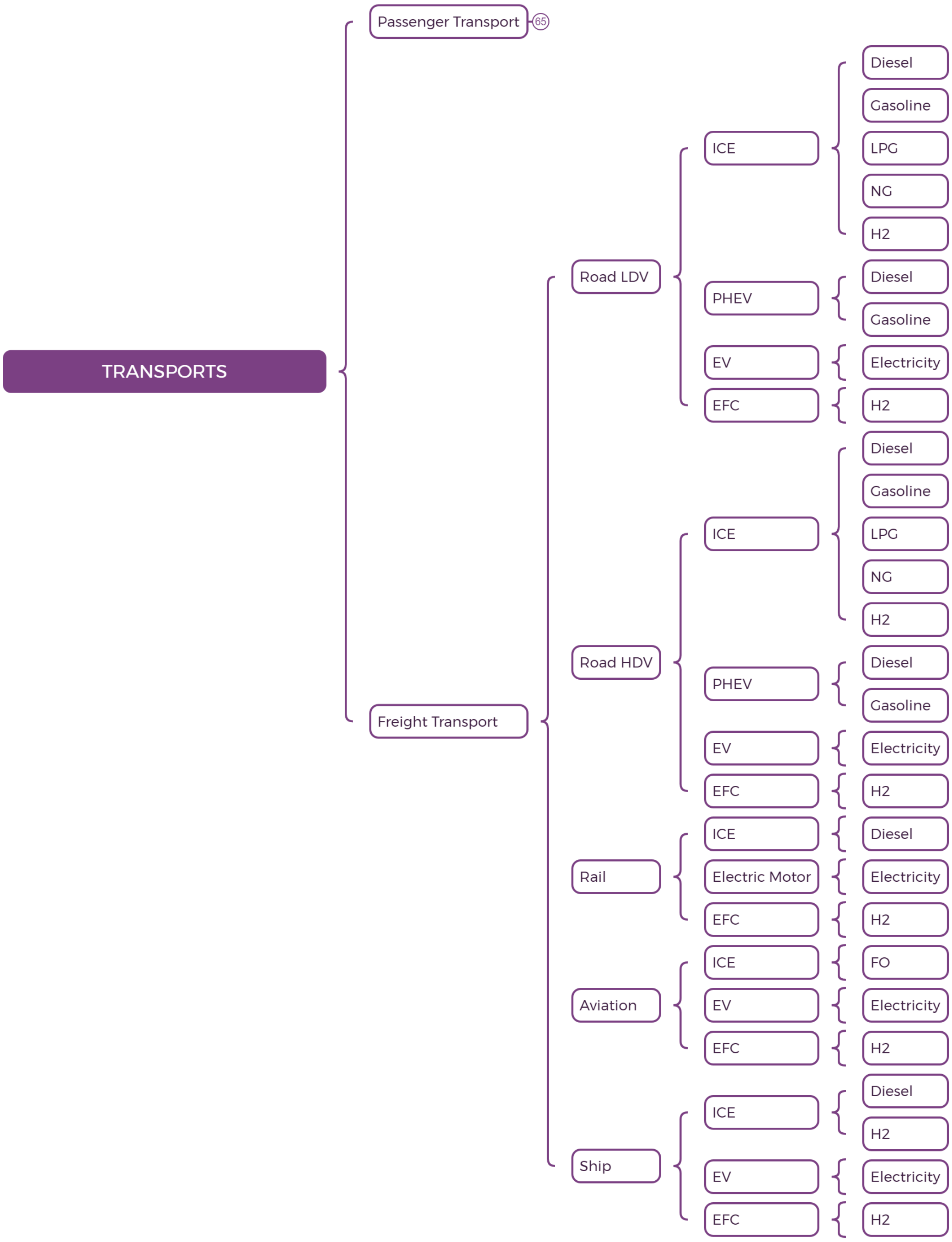

Figure B.5: Illustration presenting the comprehensive disaggregation of the entire transport sector (part 2).

Appendix C

List with description of the technologies used in the model

Table C.1 displays a comprehensive list of the technologies utilized in the model, along with brief descriptions.

Table C.1: List of technologies with a brief description

#	Name	Description
1	BG_CHP	Biogas cogeneration plant
2	BG_PP	Biogas power plant
3	COAL_PP	Coal power plant
4	Geo_PP	Geothermal power plant
5	GH2_Compression	Compression of hydrogen gas
6	GH2_Dist_Pipelines	Hydrogen gas transmission through pipelines
7	GH2_Trans_Pipelines	Hydrogen gas distribution through pipelines
8	H2_ALK_L_C	Production of hydrogen via electrolysis (ALKALINE) (large size, centralized)
9	H2_ALK_M_C	Production of hydrogen via electrolysis (ALKALINE) (medium size, centralized)
10	H2_COAL_GAS_CCUS_B_C	Production of hydrogen via coal gasification + CCUS (big size, centralized)

11	H2_COAL_GAS_CCUS_M_C	Production of hydrogen via coal gasification + CCUS (medium size, centralized)
12	H2_COAL_GAS_L_C	Production of hydrogen via coal gasification (large size, centralized)
13	H2_COAL_GAS_M_C	Production of hydrogen via coal gasification (medium size, centralized)
14	H2_NG_SR_CCUS_L_C	Production of hydrogen via methane steam reforming + CCUS (large size, centralized)
15	H2_NG_SR_CCUS_S_C	Production of hydrogen via methane steam reforming + CCUS (small size, centralized)
16	H2_NG_SR_L_C	Production of hydrogen via methane steam reforming (large size, centralized)
17	H2_NG_SR_S_C	Production of hydrogen via methane steam reforming (small size, centralized)
18	H2_PEM	Production of hydrogen via PEM electrolysis
19	H2_SOEC	Production of hydrogen via Solid Oxide Electrolyzer Cell (SOEC)
20	H2_WD_GAS_CCUS_M_C	Production of hydrogen via biomass gasification + CCUS (medium size, centralized)
21	H2_WD_GAS_M_C	Production of hydrogen via biomass gasification (medium size, centralized)
22	H2_WD_SR	Production of hydrogen via biomass steam reforming
23	HFO_PP	Fuel oil power plant
24	Hydro_Large_PP	Hydro large power plant
25	Hydro_Small_PP	Hydro small power plant
26	INDAC	Air conditioner to HVAC

27	INDBLBG	Biogas boiler
28	INDBLBGSH	BG boiler for space heating
29	INDBLBM	Biomass boiler
30	INDBLCOA	Coal boiler
31	INDBLH2	H_2 boiler
32	INDBLLPG	LPG boiler
33	INDBLLPGSH	LPG boiler for space heating
34	INDBLNG	NG boiler
35	INDBLNGSH	NG boiler for space heating
36	INDBLOILP	Oil boiler
37	INDBLOilPSH	OilP boiler for space heating
38	INDCHAMP	Advanced membrane production Chemical Industry
39	INDCHAMPI	Advanced membrane production Improvement
40	INDCHPAC	Plasma arc decomposition Chemical Industry
41	INDCHPACBG	Plasma arc decomposition with biogas instead of NG
42	INDCMLM_DPE	Dry process equipment (cement)
43	INDCMLM_FCPE	Finished cement production equipment
44	INDCMLMKLNBG	BG kiln Cement & Lime Industry
45	INDCMLMKLNCOA	Coal kiln Cement & Lime Industry
46	INDCMLMKLNH2	H_2 kiln Cement & Lime Industry
47	INDCMLMKLNNG	NG kiln Cement & Lime Industry
48	INDCMLMKLNOilP	Oil kiln Cement & Lime Industry
49	INDCMLMQLP	Quick lime production equipment
50	INDCMPELE	Compressor for refrigeration use
51	INDCRGLFPE	Flat glass production equipment in Ceramic and Glass industry
52	INDCRGLFPEBG	Flat glass production equipment with BG instead of NG
53	INDCRGLFPEHR	Glass flat production equipment with heat recovery
54	INDCRGLFPEHRBG	Glass flat production with heat recovery with BG instead of NG

55	INDCRGLGHE	Flat glass production equipment in Ceramic and Glass industry
56	INDCRGLGHEBG	Hollow glass production equipment with BG instead of NG
57	INDCRGLGHEHR	Glass hollow equipment heat recovery
58	INDCRGLGHEHRBG	Glass hollow equipment heat recovery with BG instead of NG
59	INDCRGLGLRE	Recycling glass production equipment in Ceramic and Glass industry
60	INDCRGLGLREBG	Recycling glass production equipment with BG instead of NG
61	INDCRGLGLREIM	Glass recycling equipment improved melting
62	INDCRGLGLREIMBG	Glass recycling equipment improved melting with BG instead of NG
63	INDEVELE	Electric vehicle to on-site transportation use
64	INDFCH2	H_2 vehicle to on-site transportation use
65	INDFLRTELE	Fluorescent light bulb for lighting use
66	INDHEBLBG	High efficiency BG boiler
67	INDHEBLBM	High efficiency biomass boiler
68	INDHEBLH2	High efficiency H_2 boiler
69	INDHEBLNG	High efficiency NG boiler
70	INDHEBLOilP	High efficiency OilP boiler
71	INDHLGELE	Halogen light bulb for lighting use
72	INDHPELE	Heat pump for HVAC use
73	INDICEDIE	Diesel internal combustion engine for onsite transportation use
74	INDINCTELE	Incandescent light bulb for lighting use
75	INDISEAF	Electric arc furnace in Iron and Steel Industry
76	INDISEAFBG	Electric arc furnace with BG instead of NG
77	INDISEAFH2	DRI-EAF with H_2
78	INDISISPT	Iron and Steel production technologies

79	INDISISPTBG	Iron and Steel production techs with BG instead of NG
80	INDKLNBG	BG kiln (other industries)
81	INDKLNBM	BM kiln (other industries)
82	INDKLNELE	ELE kiln (other industries)
83	INDKLNH2	H_2 kiln (other industries)
84	INDKLNNG	NG kiln (other industries)
85	INDKLNOilP	OilP kiln (other industries)
86	INDLEDELE	LED light bulb for lighting use
87	INDMTRELE	Motors for machine drive use
88	INDNFMFAP	Finished aluminium production equipment
89	INDNFMFAPBG	Finished aluminium production equipment with BG instead of NG
90	INDNFMIA	Inert anodes to produce Al Crude
91	INDNFMIABG	Inert anodes to produce Al Crude with BG instead of NG
92	INDOTHERBG	Other industrial uses BG
93	INDOTHERBM	Other industrial uses BM
94	INDOTHERCOA	Other industrial uses Coal
95	INDOTHERELE	Other industrial uses ELE
96	INDOTHERHEAT	Other industrial uses Heat
97	INDOTHERLPG	Other industrial uses LPG
98	INDOTHERNG	Other industrial uses NG
99	INDOTHEROilP	Other industrial uses OilP
100	INDOVNBG	Biogas oven
101	INDOVNBM	Biomass oven
102	INDOVNCOA	Coal oven
103	INDOVNDIE	Diesel oven
104	INDOVNELE	Eletric oven
105	INDOVNH2	H_2 oven
106	INDOVNNG	NG oven
107	INDOVNOilP	OilP oven
108	INDPPCPP	Chemical pulp production
109	INDPPHQPE	High-quality paper equipment
110	INDPPHQPEAD	High-quality paper production equipment with advanced drives

111	INDPPLQPE	Low-quality paper equipment
112	INDPPLQPEAD	Low-quality paper production equipment with advanced drives
113	INDPPMPP	Mechanical pulp production
114	INDPPMPPAD	Mechanical pulp production airless drying in PP industry
115	INDPPMPPADBG	Mechanical pulp production airless drying with BG instead of NG
116	INDPPMPPBG	Mechanical pulp production
117	INDPPRPP	Recycling pulp production
118	INDSBLBG	BG steam boiler
119	INDSBLCOA	Coal steam boiler
120	INDSBLDIE	Diesel steam boiler
121	INDSBLH2	H_2 steam boiler
122	INDSBLHEAT	Heat steam boiler
123	INDSBLLPG	LPG steam boiler
124	INDSBLNG	NG steam boiler
125	INDSBLOil	Oil steam boiler
126	INDVHEBLBG	Very-high efficiency BG boiler
127	INDVHEBLBM	Very-high efficiency biomass boiler
128	INDVHEBLH2	Very-high efficiency H_2 boiler
129	INDVHEBLNG	Very-high efficiency NG boiler
130	INDVHEBLOilP	Very-high efficiency OilP boiler
131	NG_CHP	NG cogeneration plant
132	NG_PP	NG combined cycle power plant
133	NUC_PP	Nuclear power plant
134	PV_Large_PP	PV centralized generation site
135	PV_Small_PP	PV decentralized generation
136	RECLOWASHEELE	Clothes washer and dryer high eff.
137	RECLOWASLEELE	Clothes washer and dryer low eff.
138	RECOOKELE	Electrical stove
139	RECOOKH2	H_2 stove
140	RECOOKLPG	OILP stove
141	RECOOKNG	NG stove
142	REDHWHEATERBM	BM heater
143	REDHWHEATERH2	H2 heater

144	REDHWHEATERLPG	LPG heater
145	REDHWHEATERNG	NG heater
146	REDHWHEATEROILP	OILP heater
147	REDHWSHEATBLBM	BM boiler
148	REDHWSHEATBLH2	H_2 boiler
149	REDHWSHEATBLLPG	LPG boiler
150	REDHWSHEATBLNG	NG boiler
151	REDHWSHEATBLOILP	OILP boiler
152	REDHWSOLTHERM	Solar thermal
153	REDHWTHERMOELE	Thermoaccumulator
154	REDISHWHEELE	Dishwasher high efficiency
155	REDISHWLEELE	Dishwasher low efficiency
156	RELIGHTFLUORELE	Fluorescent lightbulbs
157	RELIGHTHALELE	Halogen lightbulbs
158	RELIGHTINCANELE	Incandescent lightbulbs
159	RELIGHTLEDELE	LED
160	REREFHEELE	Refrigerator high efficiency
161	REREFLEELE	Refrigerator low efficiency
162	RESAPPLELE	Small appliances
163	RESCOOLACELE	AC
164	RESCOOLCACELE	Centralized AC
165	RESHEATAPPL	Small heating equipment
166	RESHEATCFPBM	Closed BM fireplace
167	RESHEATCOOLHPELE	Heat pump
168	RESHEATOFPBM	Open BM fireplace
169	SECLOWHEELE	Clothes washer and dryer high eff.
170	SECLOWLEELE	Clothes washer and dryer low eff.
171	SECOOKELE	Electrical stove
172	SECOOKH2	H_2 stove
173	SECOOKLPG	LPG stove
174	SECOOKNG	NG stove
175	SEDHWHEATERBM	BM heater
176	SEDHWHEATERH2	H_2 heater
177	SEDHWHEATERLPG	LPG Heater
178	SEDHWHEATERNG	NG heater
179	SEDHWHEATEROILP	OILP heater
180	SEDHWSHEATBLBM	BM boiler

181	SEDHWSHEATBLH2	H_2 boiler
182	SEDHWSHEATBLLPG	LPG boiler
183	SEDHWSHEATBLNG	NG boiler
184	SEDHWSHEATBLOILP	OILP boiler
185	SEDHWSOLTHERM	Solar thermal
186	SEDHWTHERMOELE	Thermoaccumulator
187	SEDISHWHEELE	Dishwasher high efficiency
188	SEDISHWLEELE	Dishwasher low efficiency
189	SEFREEZHEELE	Compressor high efficiency
190	SEFREEZLEELE	Compressor low efficiency
191	SELIGHTFLUORELE	Fluorescent lightbulbs
192	SELIGHTHALELE	Halogen lightbulbs
193	SELIGHTINCANELE	Incandescent lightbulbs
194	SELIGHTLEDELE	LED
195	SEREFHEELE	Refrigerator high efficiency
196	SEREFLEELE	Refrigerator low efficiency
197	SESAPPELE	Small appliances
198	SESCOOLACELE	AC
199	SESCOOLCACELE	Centralized AC
200	SESHEATCFPBM	Closed fireplace
201	SESHEATHPELE	Heat pump
202	Solar_Thermal	Solar thermal for DHW
203	TRANSFAVDEUEVELE	Freight Aviation Domestic + Intra-EU EV
204	TRANSFAVDEUFCH2	Freight Aviation Domestic + Intra-EU FC
205	TRANSFAVDEUFO	Freight Aviation Domestic + Intra-EU FO ICE
206	TRANSFHDVFCH2	Freight HDV FC H_2
207	TRANSFHDVICEH2	Freight HDV H_2 ICE
208	TRANSFLDVDIE	Freight LDV Diesel ICE
209	TRANSFLDVEV	Freight LDV EV
210	TRANSFLDVFCH2	Freight LDV FC H_2
211	TRANSFLDVGAS	Freight LDV Gasoline ICE
212	TRANSFLDVICEH2	Freight LDV H_2 ICE
213	TRANSFLDVLPG	Freight LDV LPG ICE
214	TRANSFLDVNG	Freight LDV NG ICE

215	TRANSFTRAINDIE	Freight Train Diesel ICE
216	TRANSFTRAINELE	Freight Train EV
217	TRANSFTRAINFCH2	Freight Train FC H_2
218	TRANSHDVDIE	Freight HDV Diesel ICE
219	TRANSP2WELE	Passenger Transport 2-Wheeler EV
220	TRANSP2WFCH2	Passenger Transport 2-Wheeler FC H_2
221	TRANSP2WGAS	Passenger Transport 2-Wheeler
222	TRANSPAVDOMEVELE	Passenger Aviation Domestic EV
223	TRANSPAVDOMFCH2	Passenger Aviation Domestic FC H_2
224	TRANSPAVDOMFO	Passenger Aviation Domestic FO ICE
225	TRANSPBUSEVELE	Passenger Bus EV
226	TRANSPBUSFCH2	Passenger Bus FC H_2
227	TRANSPBUSICEDIE	Passenger Bus Diesel ICE
228	TRANSPBUSICEGAS	Passenger Bus Gasoline ICE
229	TRANSPBUSICEH2	Passenger Bus H_2 ICE
230	TRANSPBUSLPG	Passenger Bus LPG ICE
231	TRANSPBUSNG	Passenger Bus NG ICE
232	TRANSPCAREVELE	Passenger Car EV
233	TRANSPCARFCH2	Passenger Car FC H_2
234	TRANSPCARHYBPIDIE	Passenger Car Hybrid Plug-In DIE
235	TRANSPCARHYBPIGAS	Passenger Car Hybrid Plug-In GAS
236	TRANSPCARICEDIE	Passenger Car Diesel ICE
237	TRANSPCARICEGAS	Passenger Car Gasoline ICE
238	TRANSPCARICEH2	Passenger Car H_2 ICE
239	TRANSPCARICELPG	Passenger Car LPG ICE
240	TRANSPCARICENG	Passenger Car NG ICE
241	TRANSPMETROELE	Passenger Metro & Tram EM
242	TRANSPTRAINDIE	Passenger Train Diesel ICE
243	TRANSPTRAINELE	Passenger Train EV
244	TRANSPTRAINFCH2	Passenger Train FC H_2
245	TRANSPTRAINHSELE	Passenger Train EV High Speed
246	TRANSSHIPFCH2	Domestic Shipping FC H_2 (coastal)
247	TRANSSHIPICEDIE	Domestic Shipping Diesel ICE (coastal)
248	TRANSSHIPICEFO	Domestic Shipping FO ICE (coastal)
249	Wave_PP	Wave generation installation
250	WD_CHP	Biomass cogeneration plant
251	WD_PP	Biomass power plant

252	Wind_PP	Onshore wind large installation
253	Wind_Small_PP	Onshore wind decentralized generation
254	WindOff_PP	Offshore wind large installation
255	WS_PP	Waste power plant (MSW)

Appendix D

List with description of the fuels used in the model

Table D.1 exhibits an inventory of the fuels incorporated within the model, accompanied by concise descriptions.

Table D.1: List of fuels with a brief description

#	Name	Description
1	BG	Biogas Primary Source
2	BG_Agr	Biogas for agriculture and fisheries sector at the end-user level
3	BG_Distribution	Biogas at Distribution Level
4	BG_Ind	Biogas for industry sector at the end-user level
5	BG_Res	Biogas for residential sector at the end-user level
6	BG_Ser	Biogas for services sector at the end-user level
7	BG_Trans	Biogas for transport sector at the end-user level
8	COAL	Coal Primary Source
9	COAL_Ind	Coal for Industrial sector at the end-user level
10	CRUDE	Crude Oil Primary Source
11	DIE_Agr	Diesel for agriculture and fisheries sector at the end-user level
12	DIE_Ind	Diesel for industry sector at the end-user level

13	DIE_Res	Diesel for residential sector at the end-user level
14	DIE_Ser	Diesel for services sector at the end-user level
15	DIE_Trans	Diesel for transport sector at the end-user level
16	EL_Agr	Electricity for agriculture and fisheries sector at the end-user level
17	EL_Distribution	Electricity at Distribution Level
18	EL_Ind	Electricity for industry sector at the end-user level
19	EL_Res	Electricity for residential sector at the end-user level
20	EL_Ser	Electricity for services sector at the end-user level
21	EL_Trans	Electricity for transport sector at the end-user level
22	EL_Transmission	Electricity from PP to Transmission Level
23	FO_Agr	Fuel oil for agriculture and fisheries sector at the end-user level
24	FO_Ind	Fuel oil for industry sector at the end-user level
25	FO_Res	Fuel oil for residential sector at the end-user level
26	FO_Ser	Fuel oil for services sector at the end-user level
27	FO_Trans	Fuel oil for transport sector at the end-user level
28	GA_Trans	Gasoline for transport sector at the end-user level
29	GH2	Hydrogen gas at production Level
30	GH2_Compressed	Compressed hydrogen gas
31	GH2_Distribution	Hydrogen gas at Distribution Level
32	GH2_Transmission	Hydrogen gas at Transmission Level
33	H2_Ind	Hydrogen gas for industry sector at the end-user level

34	H2_Trans	Hydrogen gas for transport sector at the end-user level
35	Heat_Distribution	Heat at Distribution Level
36	Heat_Ind	Heat for industry sector at the end-user level
37	Heat_Res	Heat for residential sector at the end-user level
38	Heat_Ser	Heat for services sector at the end-user level
39	Heat_Transmission	Distributed Heat from PP to Transmission Level
40	INDCHAM	Ammonia produced in the chemical industry
41	INDCHCL	Chlorine produced in the chemical industry
42	INDCMLMCLK	Clinker produced in the cement and lime industry
43	INDCMLMCMT	Cement produced in the cement and lime industry
44	INDCMLMLM	Lime produced in the cement and lime industry sector
45	INDCRGLGF	Glass flat produced in th C&G Industry
46	INDCRGLGH	Glass hollow produced in th C&G Industry
47	INDHVAC	Industrial HVAC
48	INDISCSTEEL	Crude Steel produced in the Iron and Steel Industry
49	INDISCSTEELH2	Crude Steel produced in the Iron and Steel Industry with H_2
50	INDISSTEEL	Steel produced in the Iron and Steel Industry
51	INDLIGHT	Lighting
52	INDMD	Machine Drive
53	INDNFMAL	Aluminum produced in the Non Ferrous Metal Industry
54	INDNFMCAL	Crude Aluminum produced in the Non Ferrous Metal Industry
55	INDOST	On Site Transportation in Industry

56	INDOSTH2	On Site Transportation in Industry with H_2
57	INDOTHERTHERM	Other uses thermal
58	INDOTHERUELE	Other uses electric
59	INDPHEATBL	Process Heat Boilers
60	INDPHEATBLH2	Process Heat Boilers with H2
61	INDPHEATCMKILN	Process Heat Kilns in Cement and Lime industry
62	INDPHEATCMKILNH2	Process Heat Kilns in Cement and Lime industry with H_2
63	INDPHEATKILN	Process Heat Kilns
64	INDPHEATKILNH2	Process Heat Kilns with H_2
65	INDPHEATOV	Process Heat Ovens
66	INDPHEATOVH2	Process Heat Ovens with H_2
67	INDPPHQP	High Quality Paper produced in the Pulp and Paper industry
68	INDPPLQP	Low Quality Paper produced in the Pulp and Paper industry
69	INDPPPULP	Pulp produced in the Paper and Pulp industry
70	INDRFR	Refrigeration
71	INDSTEAM	Steam production
72	INDSTEAMH2	Steam production with H_2
73	LPG_Agr	LPG for agriculture sector at the end-user level
74	LPG_Ind	LPG for industry sector at the end-user level
75	LPG_Res	LPG for residential sector at the end-user level
76	LPG_Ser	LPG for services sector at the end-user level
77	LPG_Trans	LPG for transport sector at the end-user level
78	NG	Natural Gas Primary Source
79	NG_Agr	Natural gas for agriculture and fisheries sector at the end-user level
80	NG_Distribution	Natural gas at Distribution Level

81	NG_Ind	Natural gas for industry sector at the end-user level
82	NG_Res	Natural gas for residential sector at the end-user level
83	NG_Ser	Natural gas for services sector at the end-user level
84	NG_Trans	Natural gas for transport sector at the end-user level
85	OilProd_Distribution	Refined Oil Products at Distribution Level
86	OilProd_Transmission	Refined Oil Products at Transmission Level
87	RECLOTH	Residential Clothes Washing & Drying
88	RECOOK	Residential Cooking
89	RECOOKH2	Residential Cooking with H_2
90	RECOOL	Residential Space cooling
91	REDHW	Residential DHW
92	REDHWH2	Residential DHW with H_2
93	REDHWST	Residential DHW with Solar Thermal
94	REDISH	Residential Dishwashing
95	RELIGHT	Residential Lighting
96	REREF	Residential Refrigeration
97	RESHEAT	Residential Space heating
98	RESHEATH2	Residential Space heating H_2
99	RESMALLAPPL	Residential Small Appliances
100	SECLOTH	Services Clothes Washing & Drying
101	SECOOK	Services Cooking
102	SECOOKH2	Services Cooking with H_2
103	SECOOL	Services Space cooling
104	SEDHW	Services DHW
105	SEDHWH2	Services DHW with H_2
106	SEDHWST	Services DHW with Solar Thermal
107	SEDISH	Services Dishwashing
108	SEFREEZ	Services Freezing
109	SELIGHT	Services Lighting
110	SEREF	Services Refrigeration

111	SESHEAT	Services Space heating
112	SESHEATH2	Services Space heating with H_2
113	SESMALLAPPL	Services Small Appliances
114	TRANSFAV	Freight Aviation Transportation
115	TRANSFAVH2	Freight Aviation Transportation with H_2
116	TRANSFHDV	Freight Heavy Duty Transportation
117	TRANSFHDVH2	Freight Heavy Duty Transportation with H_2
118	TRANSFLDV	Freight Light Duty Transportation
119	TRANSFLDVH2	Freight Light Duty Transportation with H_2
120	TRANSFTRAIN	Freigh train Transportation
121	TRANSFTRAINH2	Freigh train Transportation with H_2
122	TRANSPAV	Passenger Aviation Transportation
123	TRANSPAVH2	Passenger Aviation Transportation with H_2
124	TRANSPMETRO	Passenger Metro Transportation
125	TRANSPROAD2W	Passenger 2 wheelers Road Transportation
126	TRANSPROAD2WH2	Passenger 2 wheelers Road Transportation with H_2
127	TRANSPROADBUS	Passenger Bus Road Transportation
128	TRANSPROADBUSH2	Passenger Bus Road Transportation with H_2
129	TRANSPROADCAR	Passenger Car Road Transportation
130	TRANSPROADCARH2	Passenger Car Transportation with H_2
131	TRANSPTRAIN	Passenger Train Transportation
132	TRANSPTRAINH2	Passenger Train Transportation with H_2
133	TRANSSHIP	Ship Transportation
134	TRANSSHIPH2	Ship Transportation with H_2
135	UR	Uranium Primary Source
136	WD	Biomass Primary Source
137	WD_Agr	Biomass for agriculture and fisheries sector at the end-user level
138	WD_Ind	Biomass for industry sector at the end-user level

139	WD_Res	Biomass for residential sector at the end-user level
140	WD_Ser	Biomass for services sector at the end-user level
141	WS	Waste Primary Source
142	WS_Ind	Waste for industrial sector at the end-user level