



Strategic Deployment of Green Hydrogen Refueling Stations: The Case of the Portuguese Highways

Gonçalo Manuel Silva Lousa

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Supervisors:

Prof. Ana Paula Ferreira Dias Barbosa Póvoa

Prof. Cátia Rafaela Ferreira Medeiros da Silva Coelho

Examination Committee:

Chairperson: Prof. Tânia Rute Xavier de Matos Pinto Varela

Members of Committee: Prof. Ana Paula Ferreira Dias Barbosa Póvoa

Prof. Miguel Vieira

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I declare that this document is an original work of my own authorship and that it fulfils all the requirements of the Code of Conduct and Good Practices of the *Universidade de Lisboa*

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Abstract

In an era characterized by increasing concerns over climate change and the depletion of finite fossil fuel resources, the pursuit of sustainable energy alternatives has become imperative. Among these alternatives, green hydrogen has emerged as a promising solution to address the pressing need for clean energy sources. Hydrogen's unique properties, such as high energy density, zero emissions when used in fuel cells, and versatility, make it a compelling candidate for a wide range of applications, particularly in the transportation sector.

This thesis focuses on the development and application of a model for deploying a hydrogen refueling station network along the primary Portuguese highways, considering ongoing green hydrogen production initiatives. The model considers various factors, including traffic patterns, geographic distribution, infrastructure costs, and potential demand for hydrogen-powered vehicles. By integrating these elements into a cohesive framework, this study aims to provide a blueprint for the implementation of an efficient and sustainable hydrogen refueling infrastructure.

Findings of this thesis reveal a trend in the convergence of hydrogen network costs with hydrogen production costs as economies of scale are reached. This outcome underscores the potential viability of hydrogen as a mainstream transportation fuel for heavy-duty vehicles in Portugal. This research contributes with valuable insights and practical guidance for policymakers, stakeholders, and industry players in advancing the integration of green hydrogen into the country's energy landscape.

Keywords: sustainable energy; green hydrogen; hydrogen supply chain; hydrogen refueling stations; fuel cell vehicles; portuguese highways

Resumo

Numa era caracterizada por crescentes preocupações com as alterações climáticas e pelo esgotamento dos recursos de combustíveis fósseis, a procura de alternativas energéticas sustentáveis tornou-se imperativa. Entre estas alternativas, o hidrogénio verde surgiu como uma solução promissora para responder à necessidade urgente de fontes de energia limpas. As propriedades únicas do hidrogénio, como a elevada densidade energética, emitir zero emissões quando utilizado em células de combustível e a sua versatilidade, tornam-no num candidato atraente para uma vasta gama de aplicações, particularmente no sector dos transportes.

Esta tese centra-se no desenvolvimento e aplicação de um modelo de implantação de uma rede de postos de abastecimento de hidrogénio ao longo das principais autoestradas portuguesas, considerando projetos de produção de hidrogénio verde em curso. O modelo considera vários fatores, incluindo padrões de tráfego, distribuição geográfica, custos de infraestruturas e potencial procura de veículos movidos a hidrogénio. Ao integrar estes elementos num quadro coeso, este estudo visa fornecer um modelo base para a implementação de uma infraestrutura de reabastecimento de hidrogénio eficiente e sustentável.

Os resultados desta tese revelam uma tendência na convergência dos custos da rede de hidrogénio com os custos de produção de hidrogénio à medida que são alcançadas economias de escala. Este resultado sublinha a potencial viabilidade do hidrogénio como principal combustível de transporte para veículos pesados em Portugal. Esta investigação contribui com informações valiosas e orientações práticas para decisores políticos, partes interessadas e intervenientes da indústria no avanço da integração do hidrogénio verde no panorama energético do país.

Palavras-chave: energia sustentável; hidrogénio verde; cadeia de abastecimento do hidrogénio; estações de abastecimento de hidrogénio; veículos com células de combustível; autoestradas portuguesas

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List of abbreviations

Abbreviation	Definition
BBP	Bin-Packing Problem
CCS	Carbon Capture and Storage
CO ₂	Carbon Dioxide
DSS	Decision Supporting Systems
EFTA	European Free Trade Association
EU	European Union
EV	Electric Vehicle
GH ₂	Green Hydrogen
GHG	Greenhouse Gases
GHSC	Green Hydrogen Supply Chain
GIS	Geographic Information Systems
H ₂	Hydrogen
H ₂ O	Water
HRS	Hydrogen Refueling Station
HSC	Hydrogen Supply Chain
HSM	Hydrogen Storage Material
IPCEI	Important Projects of Common European Interest
LULUCF	Land use, land use change, and forestry
NDCs	Nationally Determined Contributions
NG	Natural Gas
O ₂	Oxygen
PEM	Proton Exchange Membrane
PNEC	National Plan for Energy and climate
SMR	Steam-methane Reforming
TSP	Travelling Salesman Problem
UN	United Nations
VRP	Vehicle Routing Problem

1. Introduction

This chapter introduces this master's thesis work dedicated to the topic of green hydrogen (GH₂) transportation and distribution, with a primary focus on its relevance within the unique context of Portugal. The chapter is structured as follows:

- Section 1.1. describes the motivation for this dissertation, outlining the urgent need to transition to a sustainable future and highlighting the critical challenge of establishing an efficient hydrogen (H₂) refueling infrastructure in Portugal.
- Section 1.2. presents this work specific goals and the methodology followed.
- In section 1.3. a brief overview of the thesis structure is provided.

1.1. Motivation

The transition towards sustainable energy sources and the reduction of greenhouse gas emissions have emerged as imperatives in our contemporary world (UNFCCC, 2015). In this context, green hydrogen generated through renewable energy sources has earned substantial attention as a potential game-changer in the quest for a more environmentally friendly and energy-secure future. Portugal is one of the countries that can greatly benefit from this transition, for its wide availability of renewable energy (Presidência do Conselho de Ministros, 2020).

Hydrogen offers a promising alternative for clean energy solutions across different industries. Among the sectors that can potentially benefit, the transportation sector stands out, particularly in Portugal, where the absence of Hydrogen Refueling Stations (HRSs) presents a significant roadblock to the growth of a fuel cell market. The problem at hand is the critical need to establish a HRSs network to facilitate the adoption of hydrogen fuel cell vehicles. Without it, realizing the potential of hydrogen as a clean and efficient transportation fuel remains a distant goal.

Within the broader context of green hydrogen transportation and distribution, there's a specific knowledge gap – the absence of models for deploying HRSs that consider transportation costs, especially within the unique context of Portugal. While hydrogen's potential in the transportation sector is well-documented, the practical steps required to establish an efficient and strategic network of HRSs are underexplored. This work seeks to bridge this gap by developing an optimization model tailored to the Portuguese landscape, aiming to identify the optimal locations for HRSs based on future demand projections, the availability of green hydrogen, and geographic considerations. By doing so, it aims to pave the way for a hydrogen fuel cell market in Portugal, while also contributing to the broader understanding of green hydrogen transportation solutions.

Therefore, this work's significance aims to extend beyond the academic community. It aims to contribute to the global need for a clean energy transition, particularly to the Portuguese case, a nation that already started multiple projects towards decarbonization.

1.2. Objective and Methodology

The objective of this work is to develop and apply an optimization model to identify the optimal locations for HRSs in Portuguese highways, contributing to the broader objective of decarbonizing Portugal in the transportation sector by facilitating the adoption of fuel cell vehicles that use green hydrogen. To achieve this, a methodology was defined containing the following steps:

1. Understand how green hydrogen emerges in the European and Portuguese context.
2. Understand what hydrogen is, its types, distribution and storage modes, and potential uses across different industries.
3. Present current developments of green hydrogen across different European countries and in more detail for Portugal.
4. Elaborate a literature review of the most relevant topics on the problem under study.
5. Model the HRSs deployment.
6. Case study definition and Results analysis
 - a. Define the case study: the Portuguese case.
 - b. Define the data and assumptions used to solve the case study.
 - c. Apply the model and identify best suiting locations for HRSs across the Portuguese highways network.
 - d. Evaluate the costs of such infrastructure.
7. Final Recommendations
 - a. Obtain insights that will sustain the recommendations to hydrogen stakeholders and network planners.
 - b. Elaborate on such recommendations.

1.3. Dissertation structure

This dissertation is structured as follows:

- **1. Introduction** – introduces the topic, highlighting the motivation for this work, its relevance, objectives, and structure.
- **2. Contextualization** – explains what H₂ is, how it emerges, its applications, and the current GH₂ landscape in Europe and Portugal. Done together with Filipa Silva (2023).
- **3. Literature Review** – explores the existing literature on decision support systems on hydrogen supply chain, optimization of hydrogen transport and distribution, and optimization of hydrogen refueling stations' location.
- **4. Model** – presents the optimization model developed.
- **5. Case study: Data collection and treatment** – the case study is presented together with the data and assumptions required to run the optimization model.
- **6. Case study: Results and analysis** – this chapter illustrates the results obtained, and an analysis is performed on the insights that can be retrieved from such results.
- **7. Conclusions and Future Work** – finalizes the dissertation with the main conclusions and reflections on the future work to be developed.

2. Contextualization

In this chapter, the role of green hydrogen in the European energy landscape, its underlying technical aspects, and the current state of hydrogen in European countries will be explored, with a particular focus on Portugal. The aim is to provide a comprehensive understanding of the importance and relevance of H2 as an emerging energy source in this region and to analyze the progress made thus far in its implementation.

The chapter is structured as follows:

- Section 2.1 discusses the broader context of hydrogen in Europe. It outlines its significance in the region's energy systems and policy frameworks, aiming to understand the relevance of H2 as a key component in Europe's transition towards a sustainable energy future.
- In section 2.2. the technical aspects of H2 are explained, covering its production, storage, distribution, and applications. It equips the reader with the necessary background knowledge to better comprehend its role in the energy sector.
- Section 2.3. presents an overview of the current state of hydrogen in various European countries, highlighting the advancements and challenges faced across the region.
- Section 2.4. focuses on the specific case of Portugal, examining its progress in integrating GH2 into its energy systems. The policy frameworks, national strategies, and key projects that have been implemented or are underway will be discussed.
- Finally, section 2.5. addresses the complexities and challenges associated with the hydrogen supply chain and logistics. This section acts as a conclusion, summarizing the previous sections and paving the way for further discussions in the subsequent chapters of this thesis.

2.1. Hydrogen in the European Framework

Nowadays, society faces challenges that require concerted action between energy and climate policies with particular emphasis on the areas of industry and transport. GH2 has emerged as a key element of the energy transition strategy, as the European Union (EU) aims to create a thriving hydrogen economy that can support sustainable growth, job creation, and energy security. It is crucial to define a feasible path toward a carbon-neutral economy and society that simultaneously promotes economic growth, improves the quality of life, and creates opportunities for investment and employment.

For this reason, several EU member states have already announced their national energy and climate plans and, more specifically, their national hydrogen strategies. They are also working on developing hydrogen projects and partnerships, both within Europe and globally. In Portugal, the potential of hydrogen as a clean energy source has also been recognized, and the country has set its targets to reduce emissions and promote renewable energy sources. In this context, the

current state of hydrogen development in Europe will be assessed, including the policy frameworks, technological advancements, and market trends.

2.1.1. Paris Agreement

The energy transition, from fossil fuels to renewable energy, is an increasingly relevant topic and began to gain media attention, especially after 2015 when the Paris agreement was signed by the United Nations (UN). According to it, countries are required to submit Nationally Determined Contributions (NDCs) to reduce the emissions of greenhouse gases (GHG) with the ultimate goal of limiting global warming to well below 2 degrees Celsius above pre-industrial levels and pursue efforts to limit the temperature increase to 1.5 degrees Celsius (UNFCCC, 2015). More specifically, in these NDCs, countries communicate their emissions, the implementation efforts to reduce these GHG, and actions they will take to build resilience to adapt to the impacts of rising temperatures.

2.1.2. European Green Deal

Later, in 2019, the European Commission draws up the European Green Deal, with 3 main goals (European Commission, 2019):

- Zero net emissions of GHG by 2050.
- Economic growth decoupled from resource use.
- No person and no place are left behind.

The plan also aims to increase the EU's climate ambition for 2030, with a proposed target of reducing GHG emissions by at least 55% compared to 1990 levels. It's a key part of the EU's strategy to achieve the goals of the Paris Agreement and lead the global transition to a sustainable and climate-neutral future.

Due to its importance in the decarbonization of European economies, hydrogen is among the several areas to be promoted and supported, both from a regulatory point of view and in terms of financing new technologies and infrastructures.

2.1.3. European Hydrogen Policies

Bearing this in mind, one year after, in July 2020, the forum European Clean Hydrogen Alliance was established to support the large-scale deployment of clean H₂ technologies by 2030. As a result, the EU wants to achieve industry leadership in this domain and accelerate the decarbonization of industry in line with climate change objectives. The members of this alliance come from industry, public authorities, civil society, and other stakeholders (European Commission, n.d.).

At the same time, the EU elaborates on the Hydrogen Strategy for a Climate-Neutral Europe, aiming to accelerate the development of clean hydrogen aligned to achieve carbon neutrality by 2050 and, at the same time, cooperating with Europe's economic recovery generated by the COVID-19 crisis (European Commission, 2020). This strategy aims to:

- By 2024, have 6 GW of GH₂ electrolyzers installed.

- By 2030, have 40 GW of GH2 electrolyzers installed and the production of up to 10 million tons of GH2 in the EU.
- By 2050, GH2 technologies should reach maturity and be deployed on a large scale.
- Create a market for low-carbon hydrogen by promoting demand through policy measures, such as carbon pricing.
- Invest in the necessary infrastructure, including pipelines, storage facilities, and refueling stations.
- Support research and innovation.
- Promote international cooperation to advance the development of a global H2 market.

2.1.4. Fit for 55

In July 2021, the European Commission proposed a package of legislative proposals “Fit for 55” to revise and update the EU legislation. The package is designed to reduce GHG emissions by at least 55% by 2030, compared to 1990 levels, and to bring EU legislation in line with the 2030 goals. It translates the European hydrogen strategy into a concrete European hydrogen policy framework. It also includes new policy measures that can help make the necessary changes in the economy, society, and industry faster to accomplish the goal of climate neutrality by 2050. It incorporates proposed legislation on (European Commission, 2021):

- EU emissions trading system: There should be an overall emission reduction of 61% in the sectors by 2030 compared with 2005 in the existing EU emissions trading system.
- Land use, land use change, and forestry (LULUCF): The EU-level target for net removals of GHG should be at least 310 million tons of carbon dioxide (CO₂) equivalent by 2030, spread among the member states as binding targets.
- Efforts sharing regulation: Member states in sectors that are not covered by the EU emissions trading scheme or the regulation on LULUCF should reduce the EU-level GHG emissions to 40% by 2030, compared with 2005.
- Alternative fuels infrastructure: The implementation of infrastructures for recharging or refueling vehicles with alternative fuels should be accelerated and alternative power supply for ships in ports and stationary aircraft should be considered.
- Carbon border adjustment mechanism: The increase in emissions outside the borders of the EU commission through relocation of production to non-EU countries needs to be prevented.
- Social climate fund: This social and distributional impact of the proposed new emissions trading system for buildings and road transport should be addressed and measures and investments to the benefit of vulnerable households, micro-enterprises, and transport users should be supported by this fund.
- RefuelEU aviation: The aviation sector’s environmental footprint needs to be reduced and this proposal aims to help the EU achieve that.
- FuelEU maritime: The GHG intensity of the energy used onboard by ships needs to be reduced by 75% in 2050, by supporting the use of greener fuels by ships.

- Methane emissions: The methane emissions in the fossil fuels sector need to be tracked and reduced. At the COP26 UN Climate Conference in 2021, over 100 countries committed to reducing their methane emissions by 30% in 2030 compared to 2020 levels.
- CO2 emission standards for cars and vans: Cars or vans with an internal combustion engine will no longer be placed on the market in the EU from 2035 onwards.
- Energy taxation: The taxation of energy products and electricity should be aligned with the EU's energy, environment, and climate policies, and the EU internal market should be preserved and improved by updating the scope of energy products and the structure of rates and by rationalizing the use of tax exemptions and reductions by member states.
- Renewable energy: The current EU-level target of renewable energy sources in the overall energy mix should be increased from 32% to 40% by 2030.
- Energy efficiency: The current EU-level target of at least 32.5% of energy efficiency should be increased to at least 39% for primary energy consumption, and 36% for final by 2030.
- Energy performance of buildings: All new buildings should be zero-emission buildings by 2030 and existing buildings should be transformed into zero-emission ones by 2050.

Investment support has also been provided through the Important Projects of Common European Interest (IPCEIs) on hydrogen. In July 2022, the first IPCEI called "IPCEI Hy2Tech" aimed at developing innovative technologies for the hydrogen value chain to decarbonize industrial processes and the mobility sector, with a focus on end-users. It involves 35 companies and 41 projects from 15 Member States, including Portugal. This predicts 5.4 billion euros of aid, and this public support will crowd in another 8.8 billion euros of private investments (European Commission, 2022).

2.2. Understanding Hydrogen

In the previous section, it was established the significance of hydrogen in shaping Europe's energy future and its contribution towards achieving carbon neutrality goals. But what exactly is hydrogen, and what makes it an attractive option in the quest for sustainable energy solutions? To better understand its potential, it is essential to examine the technical aspects of hydrogen, such as its production, storage, distribution, and applications. In this section, these aspects will be described, exploring how they contribute to making hydrogen a promising energy carrier to help Europe attain its ambitious environmental objectives.

Hydrogen, denoted by the symbol H and atomic number 1, is often represented as H₂ due to its molecular composition, being the lightest chemical element. This notation emphasizes that hydrogen, due to its instability, does not exist in nature as a separate element but rather as diatomic molecules, where two hydrogen atoms are bonded together (Momirlan & Veziroglu, 2005). It is a clean and versatile energy carrier that can be produced from a variety of renewable and non-renewable sources. When used as an energy source, hydrogen produces only water vapor as a byproduct, making it an environmentally friendly option. Furthermore, its potential as a sustainable energy solution, be it the direct use of hydrogen as an energy source or its ability

to store clean energy from other intermittent fonts, makes H₂ increasingly important in the context of climate change and global efforts to transition toward renewable energy sources.

It is the most abundant element in the universe, but on Earth, it is typically found combined with other elements, such as oxygen (O₂) to form water (H₂O) or carbon to form hydrocarbons (Faizollahzadeh et al., 2018) This is because hydrogen is highly reactive and tends to form bonds with other elements. Despite its reactive nature, hydrogen has been used for various applications for centuries, from the first hydrogen-filled balloons in the late 18th century to the use of hydrogen fuel cells in modern vehicles (Davis, 2010).

However, harnessing hydrogen as an energy source also presents challenges, particularly in the areas of production, storage, and distribution. These challenges will be further explored in the following sections.

2.2.1. Hydrogen Production: Methods and Technologies

The pursuit of hydrogen energy began way back in 1671 when it was first obtained and isolated by Robert Boyle while he was experimenting with iron and acids. However, it wasn't until 1766 that Henry Cavendish recognized it as a distinct element (West, 2014). Since then, the technology of obtaining hydrogen has evolved and nowadays the two most common methods for producing hydrogen are steam-methane reforming (SMR) and electrolysis.

2.2.1.1. Steam-methane Reforming - SMR

SMR consists of mixing one molecule of methane with one molecule of H₂O, under high temperature and pressure, resulting in three molecules of hydrogen and one of carbon monoxide (Fowles & Carlsson, 2021). This unsustainable technique produces hydrogen from natural gas (NG) and emits 8.9 kg of CO₂ for every kilogram of H₂. Coal gasification is a similar process that uses coal instead of natural gas and emits 29.33 kg of CO₂ for each kilogram of H₂ (Bairrão et al., 2023).

These techniques account for 96% of current hydrogen production (Erbach & Jensen, 2021). While being cost-effective, this process generates significant CO₂ emissions resulting in 2.3% of total global CO₂ emissions. This is the so-called 'grey hydrogen' if the CO₂ is released, and 'blue hydrogen' if combined with carbon capture and storage (CCS) technologies.

2.2.1.2. Electrolysis

There are different types of electrolysis for hydrogen production, with alkaline electrolysis and proton exchange membrane (PEM) electrolysis being the most common (Stojić et al., 2008). Alkaline electrolysis uses an alkaline solution as an electrolyte and has been a well-established technology for several decades. In contrast, PEM electrolysis uses a solid polymer electrolyte and is a more recent development, offering higher efficiency and power density. Both methods involve decomposing H₂O into its basic components, H₂ and O₂ in their gaseous forms, through the passage of an electric current. Hence, the electric energy is converted into chemical energy. When the electric current comes from renewable resources such as solar or wind power, the

product is called green hydrogen, which has gained a lot of attention in recent years. This is because it promises to be one of the key players in Europe's energy transition and efforts to reach carbon-neutral emissions (European Commission, 2021).

2.2.1.3. Current developments

Other types of hydrogen production are currently being developed, such as turquoise hydrogen which directly splits methane into hydrogen and solid carbon (Hermesmann & Müller, 2022), and, more recently, the direct extraction of hydrogen from seawater (Liu et al., 2022). Nevertheless, this work focuses on green hydrogen.

Worldwide, an average of 120 million tons of hydrogen are produced annually, three times the amount produced in 1980. However, two-thirds of all hydrogen produced is used to create fertilizers, and fuel that can be used for transport (IRENA, 2019). Research and development will play a key role in advancing green hydrogen production technology and reducing costs so that an energy transition plan that includes GH2 becomes more feasible.

In Figure 1, the different types of hydrogen are represented according to the way of production:

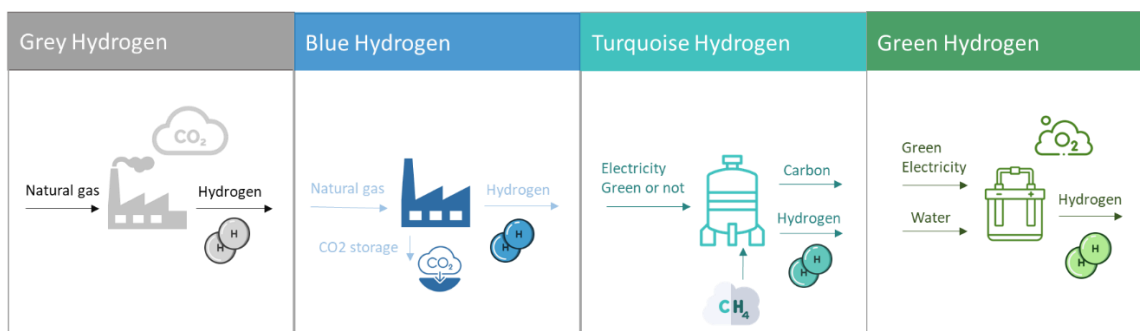


Figure 1: Hydrogen types and respective production method

2.2.2. Hydrogen Storage: Challenges and Solutions

Hydrogen is a highly flammable gas that requires special handling and storage considerations to ensure safety and efficiency. These challenges must be addressed in the design and operation of hydrogen storage systems so that the widespread adoption of hydrogen-based technologies is possible. Several methods for storing hydrogen, each with its advantages and disadvantages, have been developed. The following was retrieved from Langmi et al. (2022).

2.2.2.1. Compressed gas storage:

H₂ gas can be compressed and stored in high-pressure tanks. Two types of vessels serve this purpose, Type III and Type IV. Type III vessels consist of a metal liner, typically aluminum, and are overwrapped with a composite material, such as carbon or glass fiber. Type IV vessels, on the other hand, have a non-metallic liner, usually a polymer, and are fully wrapped with a composite material. Both types of vessels provide increased resistance, but Type IV tanks can hold pressures up to 1000 bar and are lighter due to the absence of a metal liner, making them more suitable for fuel cell vehicles. The main advantage of compressed hydrogen storage is that

it is a well-established technology, but the high cost of the tanks, especially for Type IV which use carbon/glass fiber, is a disadvantage.

Compressed H₂ in the gaseous form can also be stored in large-scale and underground structures that include three classes of storage cavities: porous media storage, salt caverns, and engineered cavities, each with their unique advantages and disadvantages.

2.2.2.2. Liquid hydrogen storage:

H₂ can also be stored as a cryogenic liquid at -253°C, the boiling temperature. It has a higher volumetric density (70g/L) than compressed gas storage (40g/L at 700 bar) meaning it can store more hydrogen in the same volume, however, it requires significant energy to liquefy and keep the hydrogen at the required low temperature. This method of storage is mainly used for industrial applications.

2.2.2.3. Adsorption:

Adsorption storage of hydrogen involves using a solid material called a hydrogen storage material (HSM) to absorb and release hydrogen gas. This is achieved through a process called physisorption, in which hydrogen molecules are adsorbed onto the surface of the HSM, and chemisorption, in which hydrogen molecules are chemically bonded to the HSM.

The advantages of adsorption storage are that it can potentially provide a higher hydrogen storage capacity than other methods, such as compressed or liquid hydrogen storage, and can potentially provide a safer and more stable form of H₂ storage, as the HSM can be designed to release hydrogen at relatively low pressure and temperature.

There are several advantages of physisorption-based storage over chemisorption-based storage: fast hydrogen adsorption/desorption kinetics, complete reversibility, and high stability over many cycles. The most investigated methods are Metal-organic frameworks, Carbon-based materials, and Porous organic materials.

Chemisorption involves the binding of atomic hydrogen chemically within the structure of a material. It can result in relatively high hydrogen storage capacities, but the hydrogen uptake and release kinetics may be slow. The most common ways to achieve this are using Metal hydrides, Liquid organic hydrogen carriers, Ammonia, Formic acid, and Methanol.

Figure 2 summarizes the different hydrogen storage technologies:

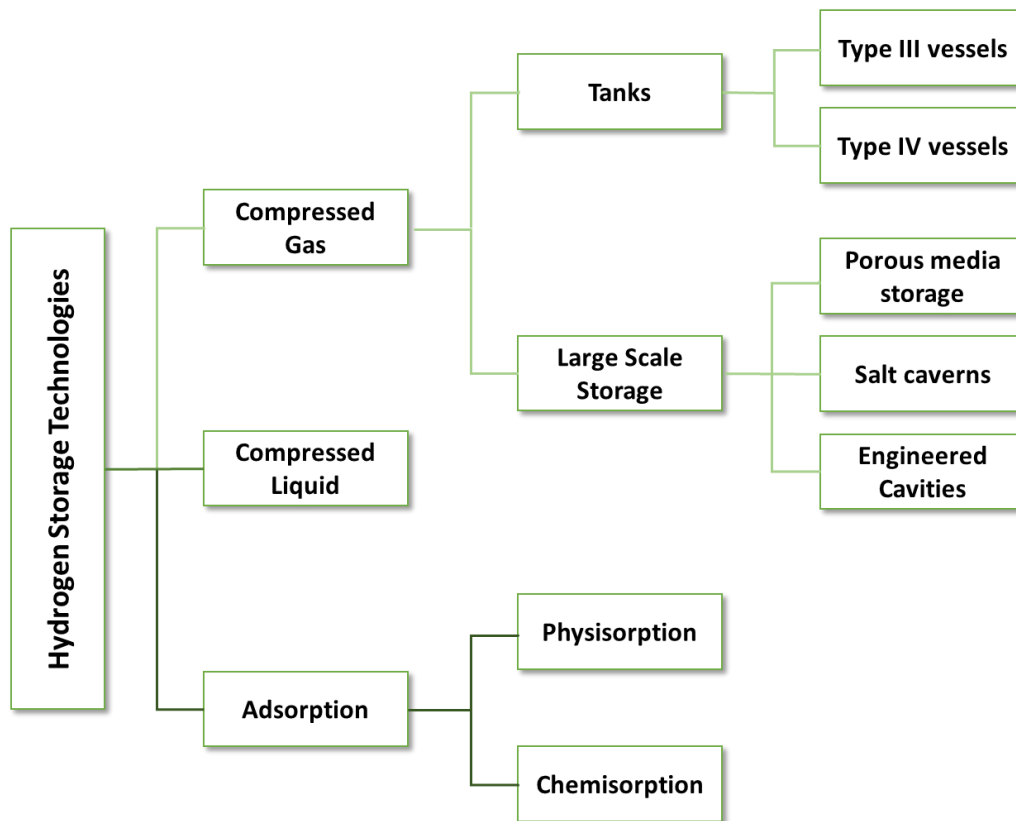


Figure 2: Hydrogen Storage Technologies

2.2.3. Hydrogen Transport and Distribution: Infrastructure and Logistics

Hydrogen needs to be transported and distributed from production sites to end-users. The methods used for this depend on the scale of production, the location of end-users, and the choice between centralized and decentralized distribution approaches. Centralized distribution involves large-scale hydrogen production facilities, with the hydrogen being transported over long distances to end-users, while decentralized distribution focuses on smaller, localized production facilities situated closer to the end-users, reducing transportation distances (Armaroli & Balzani, 2011). Both approaches come with their own set of challenges to ensure the safety, efficiency, and cost-effectiveness of hydrogen transport and distribution.

Hydrogen can be transported from production sites as a compressed gas or liquid directly via pipeline, as a compressed gas in tube trailers, as a compressed liquid in tanker trucks, and as a compressed gas or liquid in ships or rail. In the following sections, we will discuss the advantages and challenges associated with each transportation method and explore how they can be effectively integrated into centralized or decentralized distribution strategies.

2.2.3.1. Centralized distribution

In the centralized distribution approach, hydrogen should be produced in big plants and stored in large amounts in relatively few locations. Large-scale manufacturing of green hydrogen will occur at the location of renewable power production. The centralized distribution would require an infrastructure for hydrogen delivery to secondary storage sites for subsequent distribution to

customers. A modern high-pressure tube trailer is capable of transporting approximately 1000 kg of hydrogen in contrast to gasoline tank trucks, which can transport nearly 14 times the equivalent energy.

Pipeline is the best solution for long-distance distribution of H₂ since it can reach the lowest cost - \$0.10 to \$1.00 per kg per 100km (Tashie-Lewis & Nnabuife, 2021). For short distances tube trailers or tanker trucks can be more cost-efficient, and for international transport ships are the best option. This is a promising intermodal strategy with a first transportation of hydrogen via pipeline and then using trucks for last-mile delivery.

2.2.3.2. Decentralized distribution

The decentralized distribution consists of on-site hydrogen production, where hydrogen is produced directly at the location where it is needed. The electricity required to create green hydrogen could be obtained locally or could come from the grid.

Drawbacks of any kind of on-site production would be the higher cost of hydrogen when produced in small quantities, and safety problems related to the local manufacture of such an explosive gas. Moreover, transferring hydrogen via pipeline is ten times more cost-effective than transporting electricity via cable which makes centralized distribution more attractive. Pipeline capacities (15–20 GW) are more significant than power cable capacities (1–4 GW), so delivering it via pipeline avoids power grid capacity constraints caused by growing renewable electricity output (Bairrão et al., 2023).

2.2.4. Hydrogen Applications: Current and Potential Uses

GH₂ is a versatile and promising energy carrier that has the potential to significantly contribute to the decarbonization of various sectors, including transportation, industrial, chemical, and energy. Many countries, including Portugal, see the widespread adoption of GH₂ leading to significant reductions in GHG emissions, as well as improved energy efficiency and economic benefits. However, the adoption of green hydrogen in each sector is currently facing several challenges, such as high costs, infrastructure limitations, and regulatory barriers. Next, we will explore the most common applications of green hydrogen in each sector and discuss the challenges and opportunities associated with each one.

2.2.4.1. Transportation

The transportation sector is the biggest contributor to GHG and its decarbonization is crucial to meet European goals for 2050 (European Parliament, 2023). A large amount of research has been done trying to find ways to decarbonize the various modes of transportation.

When it comes to hydrogen, the use of fuel cells is the most promising technology. In a fuel cell vehicle, hydrogen is stored in high-pressure tanks and fed into the fuel cell, where it reacts with O₂ from the air to produce electricity that powers the vehicle's electric motor. The only emission is water vapor, and they are quiet when compared to combustion engines, as well as more

efficient, with a conversion efficiency of up to 60%, compared to around 30% for later ones (Leo, 2022). This application of GH₂ is also known as Power-to-Mobility - P2M.

In what concerns road light duty cars, hydrogen failed to be implemented on large scale. Electric cars proved to be a more cost-efficient solution to decarbonize this part of the sector, considering they now offer about 400 km real-world range and the newest generation use 800 V batteries, which can be charged for a range of 200 km in about 15 minutes (Plötz, 2022). There are only two passenger fuel cell car models available from global manufacturers and the infrastructure is still very scarce, especially in Portugal where there's only one hydrogen refueling station (glpautogas, 2023).

However, the European Parliament intends to make green hydrogen in transportation a key player in the process of decarbonization of Europe since it offers a higher driving range than batteries and quick refueling (Erbach & Jensen, 2021). They recognize the difficulties of upscaling the use of fuel cells to light-duty road vehicles or urban buses, however, they see a great opportunity to implement it for heavy vehicles, railways (on non-electrified lines), and vessels.

Currently, the use of Powerfuels, which use green hydrogen in their genesis, are being studied as clean alternatives to power vehicles in aviation and shipping (Gielen et. al., 2020). This application is also called Power-to-Synfuel (P2FUEL), where products derived from crude oil could in principle be produced synthetically with renewable sources, hence decarbonizing air, road, and maritime transport.

2.2.4.2. Industrial & Chemical

As previously stated, these are the sectors that consume most of the hydrogen at the present date, consuming over 90% of H₂ produced worldwide (wha-international, 2023). Hydrogen, which is a highly reactive gas, when combined with nitrogen produces ammonia. This accounts for around 55% of world hydrogen consumption, mostly because ammonia is used to manufacture agricultural fertilizers, but it can also be used for power generation, heating, and cooling (Elbaz et al., 2022).

The second biggest pie in the hydrogen consumption chart, accounting for 25% of its use (wha-international, 2023), corresponds to petroleum refining. Hydrogen here is used to remove sulfur which is naturally contained in fossil fuels. Otherwise, the combustion of these would release sulfur oxides which cause respiratory diseases and air pollution.

The third biggest pie relates to methanol production. It occupies a critical position in the chemical industry as a building block for the manufacture of countless everyday products such as paints, carpeting, and plastics. It is used to synthesize heavier alcohols, gasoline, and many other complex chemicals. There are even innovative ways of using it in internal combustion engines as an alternative to conventional transport fuels (Methanol Institute, 2023). The production of this versatile component is only possible through the hydrogenation of carbon monoxide, in which

hydrogen is crucial. This accounted for around 10% of hydrogen consumption in 2020 (wha-international, 2023).

Hydrogen is also used in Electronics as a carrier gas to produce electronic components, in the glass industry to produce flat glass, in metallurgy to produce mechanical parts or alter their properties, and it enters the composition of textile fibers such as nylon, polyurethane foam, and several plastic materials (Mesguen et al., 2005).

It also has the potential to replace NG as a heat source in the industry, in processes where electrification is not possible or economically inefficient, and in sectors that use high temperatures, e.g., steel and cement). All these applications of GH₂ are also known as Power-to-industry - P2I.

2.2.4.3. Energy & Heating

Hydrogen has a high gravimetric energy content of 143 MJ/kg (Bairrão et al., 2023) being able to store and deliver tremendous amounts of energy. It can then be stored in tanks or pipelines, and later used to generate electricity when needed, either through combustion or fuel cell technology, being attractive for grid storage and a power generation backup, also known as Power-to-Power applications – P2P (Tashie-Lewis & Nnabuife, 2021). One advantage of using hydrogen for grid storage and backup power is that it can be stored for long periods without significant loss of energy, unlike batteries that can lose charge over time. This is one of the main reasons why GH₂ became such an attractive technology for the decarbonization of many countries, allowing the storage of renewable energy for a long time.

Fuel cells were previously explained in the transportation sector. In what concerns combustion, some companies such as Siemens and General Electric are working on the re-electrification of hydrogen by developing hydrogen power plants, where it is burned to move gas turbines and produce electricity (Siemens Energy, n.d.; GE Gas Power, n.d.).

In addition, hydrogen is already being tested as a potential replacement for natural gas systems in some countries, namely Germany, UK, and Portugal – Power-to-Gas, P2G, applications. Natural gas primarily consists of methane, creating CO₂ upon its combustion, and accounts for 19% of worldwide emissions of GHG, hence this transition to hydrogen would have a great impact on the green energy transition. The “H21 pilot project” is being prepared by Northern Gas Networks in Leeds, UK, with ultimate objective of completing energy transition of the city's heating system from natural gas to hydrogen (H21, n.d.).

2.2.4.4. Others

The space industry uses hydrogen as fuel also due to its high specific energy when compared to fossil fuels, being almost 3 times bigger than diesel or gasoline. Nasa even names it “the signature fuel of the American space program” and is used by other countries in the business of launching satellites (NASA, n.d.).

Other hydrogen applications include turning unsaturated fats into saturated oils and fats, and it is being studied as therapeutic gas for some different diseases. It may have anti-inflammatory and antioxidant properties, and it is being investigated as a possible treatment for conditions such as sepsis, stroke, and neurodegenerative diseases (Huang et al., 2010).

The different applications of GH2 described in this chapter are represented accordingly with their value chain in Figure 3¹:

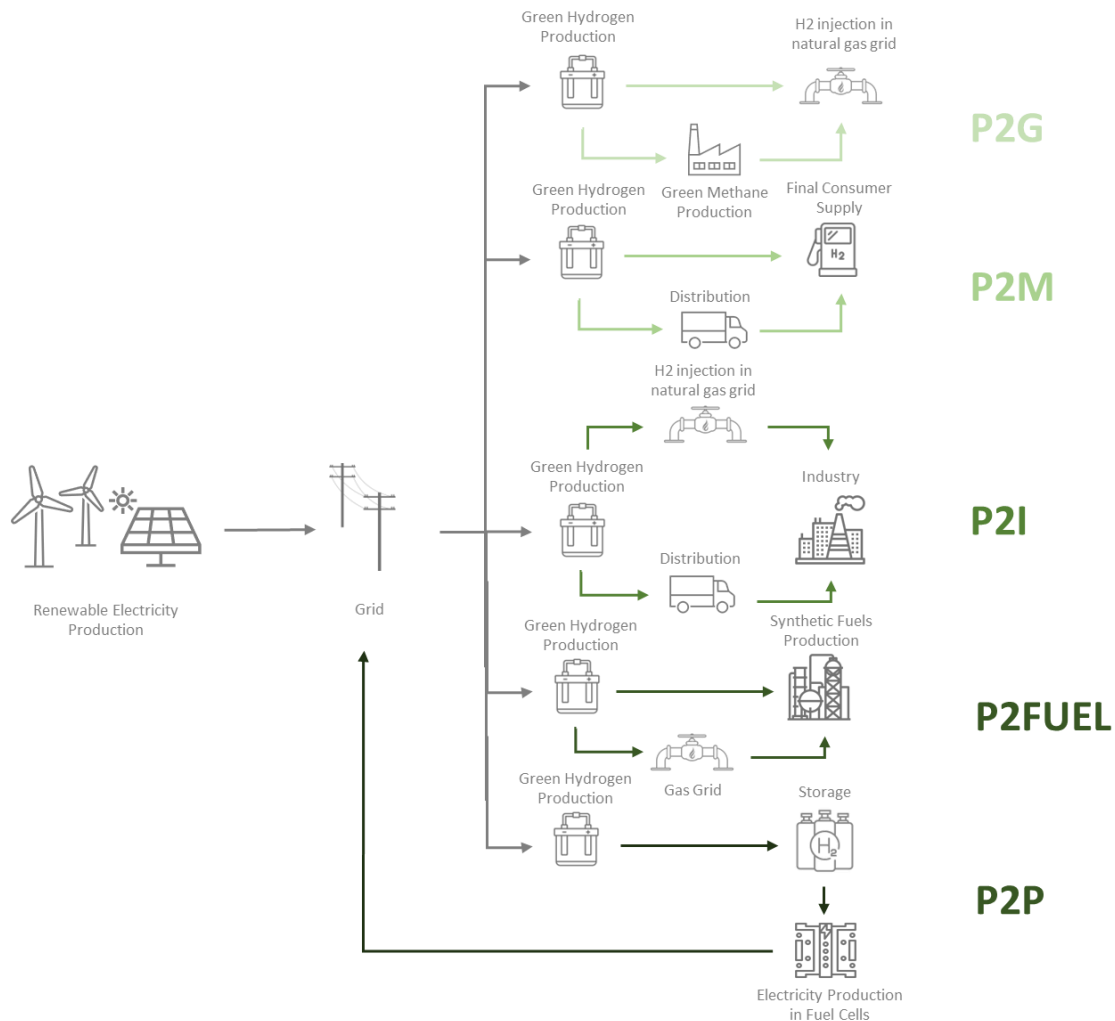


Figure 3: Hydrogen Applications

2.3. Current State of Hydrogen in European Countries

Now that the technical aspects of hydrogen have been explored, it is crucial to examine how these elements translate into the real-world context across European countries. In this section, the current state of hydrogen in various European nations will be assessed, highlighting the progress made, as well as the challenges faced in implementing hydrogen-based solutions.

¹ The renewable electricity production represented in this figure could also go directly to the electrolyzers without having to go first to the grid for the different value chains.

2.3.1. General situation of H2 in Europe

By the end of 2020, it was identified as being in operation 504 hydrogen production sites, with a total production capacity of 11.4 MT per year². Germany, Netherlands, Poland, Italy, and France alone account for 55% of the total hydrogen production capacity of the EU, European Free Trade Association (EFTA), and the United Kingdom (FCHO, 2022). Below is a graphic³ (Figure 4) that represents the hydrogen production capacity per country (Hydrogen Europe, 2022):

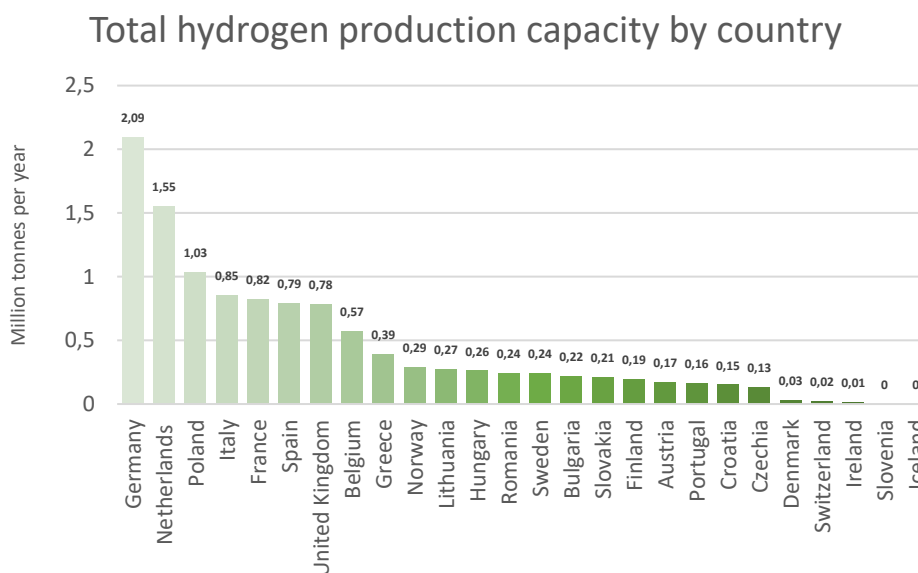


Figure 4: H2 production by country

In the European hydrogen market in 2020, 95.7% of total hydrogen production capacity was represented by the conventional production SMR methods, which include reforming, partial oxidation, gasification, by-product production from refining operations, and by-product production from ethylene and styrene. SMR with CCS (known also as “blue” hydrogen) contributed 0.5% of total hydrogen production capacity. The electrolysis process, which includes the production of hydrogen from electrolysis as the main product or as a by-product (capacity from chlorine and sodium chlorate production) accounted for 3.8% (Hydrogen Europe, 2022). However, it’s important to notice that almost all the hydrogen obtained by electrolysis probably was not from renewable energy. Below, is represented a graphic⁴ (Figure 5) with the five countries with the largest production capacity in the EU, EFTA, and the UK plus Portugal by production process:

² This is without having in account the by-product hydrogen from coke oven gas

³ This graphic was adapted from Clean Hydrogen Monitor report

⁴ The data from Fuel Cells and Hydrogen Observatory was used to create this graphic

Total Hydrogen Production Capacity by Production Process

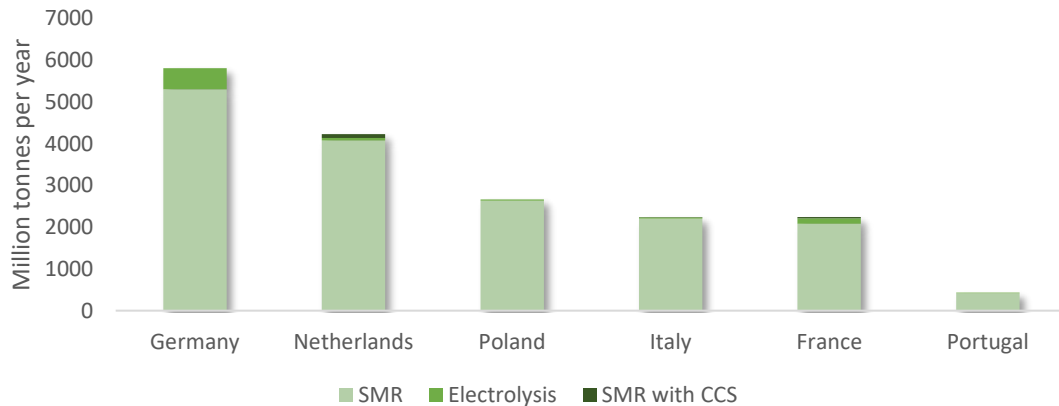


Figure 5: Total hydrogen production capacity by production process

The composition of this capacity depends on the industries in each country, but it is possible to observe a common trend between all of them: captive reforming capacity in the refining and ammonia sectors domains and all the other production processes.

On the other hand, the total demand for hydrogen in 2020 has been estimated at 8.7 Mt. The biggest share of hydrogen demand comes from refineries, which were responsible for 50% of total hydrogen use (~4.4 Mt), followed by the ammonia industry with 29% (~2.5 Mt). Together, these two sectors consumed 79% of the total hydrogen consumption in the EU, EFTA, and the UK. Germany, Netherlands, Poland, and Spain alone account for 51% of the total hydrogen production capacity of the EU, EFTA, and the UK, with respectively 20%, 15%, 9%, and 7% (Hydrogen Europe, 2022). However, only 8.7% of global hydrogen demand in 2020 is represented by the total hydrogen consumption in the EU, EFTA, and the UK (IRENA, 2022).

Hydrogen produced only by water electrolysis⁵ has been emerging as a future technology for large-scale hydrogen production. It has almost doubled its capacity from 85 MW in 2019 to 162 MW in 2022 in the EU, EFTA, and the UK. To reach the 2030 climate targets, several projects on water electrolysis were planned. Between 2022 and 2030, the average tracked capacity growth rate is as high as 111% annually, which, if achieved, would result in 138 GW of installed water electrolysis capacity by 2030. As presented in Figure 6, the country with the highest planned capacity of water electrolysis by 2030 is Spain with 74,174 MW, followed by the Netherlands with 10,149 MW, Germany with 7,295 MW, and Denmark with 6,288 MW (Hydrogen Europe, 2022).

⁵ Water electrolysis produced with electricity both from renewable and non-renewable energy sources.

Planned capacity of water electrolysis by 2030

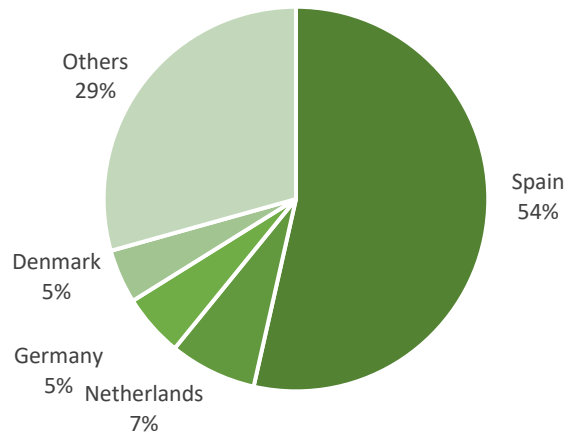


Figure 6: Planned capacity of water electrolysis by 2030

These four countries together represent around 70% of the planned capacity in Europe. Therefore, due to the importance of these countries in hydrogen development, the next GH2 targets and main improvements for each of them will be analyzed.

2.3.2. H2 in Germany

Germany is at the lead of the green hydrogen revolution, and the country is making significant investments in the development of this clean energy source. It has a target of producing 5 GW of electrolysis capacity by 2030 (Federal Ministry for Economic Affairs and Energy, 2020).

This country is a pioneer in the creation and use of fuel cell vehicles, which run on hydrogen as their fuel. Major German manufacturers are investing in fuel cell technology, and hydrogen refueling stations are already operational in several locations. In fact, in 2022, the number of these stations was 93 (Statista, 2022). These automakers include BMW, Daimler, and Volkswagen. The government has set a target of having 400 hydrogen refueling stations in operation by 2025, which will support the deployment of fuel cell vehicles across the country (European Alternative Fuels Observatory, 2022).

Another field where Germany is advanced is the use of hydrogen in industry. Numerous significant industrial conglomerates, including Siemens, ThyssenKrupp, and Linde, are based in the nation and are making investments in the creation of green hydrogen technologies.

Germany is also making investments in the creation of massive hydrogen storage systems, which can be used to hold extra renewable energy and offer a reliable source of power. Investments in the creation of heating and cooling systems and the creation of tractors and harvesters that run on hydrogen fuel are also a priority for the country, which can help to lower GHG pollution and enhance air quality.

Additionally, Germany is working to develop a hydrogen pipeline network to transport hydrogen to end-users. There is already a plan to convert 5 900 km of its natural gas pipelines to hydrogen - around 15% of the total national network-, with the first 1 200 km to be completed by 2030 (Martin, 2020).

One of the biggest green hydrogen projects in Germany is the AquaVentus project. It aims to create a 10 GW offshore wind park in the North Sea that will produce green hydrogen using electrolysis powered by wind turbines. The project intends to produce up to 1 million tons of green hydrogen per year by 2030 (AquaVentus, n.d.).

2.3.3. H2 in The Netherlands

The Netherlands is already Europe's second largest hydrogen producer and is aiming to become a major producer and exporter of green hydrogen, with a target of producing 500 MW of electrolysis capacity by 2025 and 3-4 GW by 2030 (Government of the Netherlands, 2019). To enable large-scale production of green hydrogen, Dutch are aiming to have installed 4 GW of electrolyzer capacity by 2030. Northern Netherlands' goal is to have an annual production of green hydrogen of 65 Petajoules (PJ) by 2030 (Netherlands Enterprise Agency, 2022).

The Netherlands considers that investing in offshore wind power is a crucial enabler of scaling up the production of green hydrogen. In the Dutch sector of the North Sea, there are already planned projects that add up to 11 GW of offshore wind capacity by 2030 (Netherlands Enterprise Agency, 2022). Additionally, the Netherlands already has over 1,000 km of dedicated hydrogen pipeline. The current natural gas grid can be adapted to transport hydrogen at an acceptable cost, accelerating the development of a 'national hydrogen backbone' that can be ready by 2026 (Netherlands Enterprise Agency, 2022).

As an advantage, the country is located at the heart of the European hydrogen infrastructure proposed by 11 European grid operators (Netherlands Enterprise Agency, 2022).

One big project for the Netherlands is the Hystock project which implies the construction of a green hydrogen production plant in the northern city of Groningen. The hydrogen will be used to decarbonize the chemical industry in the region and will be transported by a pipeline network to industrial customers (Hystock, n.d.).

2.3.4. H2 in Denmark

Denmark has established electrolysis capacity goals of 4 - 6 GW by 2030 (Danish Ministry of Climate, Energy and Utilities, 2021). The nation is making significant investments in the creation of green energy sources, especially wind energy. More than 40% of Denmark's electricity requirements are met by wind turbines (Danish Energy Agency, n.d.), making it a global leader in wind energy and an advantage for green hydrogen production.

Large-scale green hydrogen initiatives are currently being worked on in Denmark. The Green Fuels for Denmark project, which seeks to generate green hydrogen using offshore wind power, is one of the most noteworthy. Off the coast of Denmark, the project entails the installation of a

total electrolysis capacity of 1,300 MW. Buses, trucks, and ships will all use the hydrogen that is generated as fuel. (Ørsted, 2022).

Denmark has plans to invest in hydrogen refueling sites and in 2022 there were already 7 hydrogen stations for road vehicles working (Statista, 2022). Additionally, the country is investing in the creation of a green hydrogen infrastructure. To investigate the use of green hydrogen in the transportation industry, the nation has also started several pilot initiatives, including the use of hydrogen fuel cell buses in Copenhagen.

Denmark is looking into using green hydrogen in the industrial sphere in addition to transportation. The nation is currently testing the use of hydrogen in the manufacture of steel and chemicals through some experimental projects.

2.3.5. H2 in Spain

Spain is making significant investments in the creation of renewable energy sources to support its goal of producing 4 GW of green hydrogen by 2030 (Secretaría de Estado de Energía, 2020). To support this target, the country is investing heavily in the development of renewable sources, particularly wind and solar energy as they have significant potential for it by being the second-largest producer of wind energy in Europe and the fifth-largest producer of solar energy.

The use of green hydrogen in the industrial and transportation industries is something that Spain is also looking into. To investigate the use of hydrogen in the transit industry, the nation has started several pilot projects, including the use of hydrogen fuel cell buses in Barcelona and Madrid. The nation is also working to build a hydrogen refueling infrastructure for fuel cell cars and has started already by having 3 hydrogen refueling stations in operation in 2022 (Statista, 2022).

Spain is investigating the commercial use of hydrogen in the chemical and steel sectors. To lower carbon emissions and improve energy efficiency, the nation is currently testing the use of green hydrogen in many different sectors.

Finally, a big project for Spain is the Green Hysland project. This project will involve solar power to produce green hydrogen for transportation and energy storage through the development of a green hydrogen ecosystem on the Spanish island of Mallorca. The project aims to create a model for the use of green hydrogen in island communities and has the potential to be scaled up to other regions (Green Hysland, n.d.).

2.4. Hydrogen in Portugal

Portugal, due to its geographic location, the high and growing penetration of renewables in its electrical system, the competence of its industrial sector, the excellence of its human resources in the area of engineering, and the competitive advantage in the low-cost production of renewable electricity, presents very favorable and competitive conditions for the production of green hydrogen and for the development of zero-emissions value chains based on hydrogen for the domestic market and export.

The country has made significant progress in building a robust green hydrogen ecosystem, including developing a national strategy, implementing pilot projects, and collaborating with international partners, which reflect efforts to incorporate this gas in the decarbonization of the country.

2.4.1 Portuguese efforts to reach Carbon Neutrality

In July 2019, the Portuguese Roadmap to Carbon Neutrality 2050 was approved, aiming for a reduction of GHG emissions for Portugal between 85% and 90% by 2050, compared to 2005 levels, and offsetting the remaining emissions through carbon sequestration through the use of soil and forests (Governo de Portugal, 2019).

Following this, in July 2020, the National Plan for Energy and climate (PNEC 2030) is approved as well. This establishes the goals and objectives and implements the policies and measures for the horizon of 2030, in which green hydrogen is a key player to achieve these goals:

- Reduce GHG emissions between 45% and 55% related to 2005 levels.
- Incorporate 47% of RE in the final energy consumption.
- Reduce 35% of primary energy consumption.
- Reach 15% interconnections of electricity.
- Reduce GHG emissions: 70% in the services sector; 35% in the residential sector; 40% in the transports sector; 11% in agriculture sector; 30% in waste and wastewater.

PNEC 2030 includes H₂ as a mechanism to accelerate decarbonization. Thanks to its properties, such as high gravimetric energy, compatibility with natural gas networks, and long life storage of renewable energy, the Portuguese government sees many advantages in this gas: (i) reducing decarbonization costs; (ii) security of supply; (iii) reducing imports and energetic dependence; (iv) reducing GHG emissions; (v) promotes efficiency in production and consumption of energy; (vi) promoting economic growth and job creation; (vii) promoting investigation and technological development (Presidência do Conselho de Ministros, 2020).

2.4.2 National Strategy for Hydrogen

Following the PNEC 2030, in August 2020 Portugal approves its National Strategy for Hydrogen, EN-H₂, aiming to establish Portugal as a leading player in the hydrogen industry, both in Europe and globally, and at the same time contributing to achieving PNEC 2030 goals.

EN-H₂ macro goals to reach until 2030 (Presidência do Conselho de Ministros, 2020):

- 10 % to 15 % of green hydrogen injection in natural gas networks.
- 2 % to 5 % of green hydrogen in the energy consumption of the industry sector.
- 1 % to 5 % of green hydrogen in the energy consumption of road transportation.
- 3 % to 5 % of green hydrogen in the energy consumption of domestic maritime transportation.
- 1,5 % to 2 % of green hydrogen in the final energy consumption.
- 2 GW to 2,5 GW of electrolyzers capacity installed.

- Creation of 50 to 100 hydrogen filling stations.
- 7000-9000 M€ invested in new projects.
- 400-450 M€ in support of investment from European funds.
- 500-550 M€ in support of production.
- 380-740 M€ reduction in Natural Gas imports.
- 180 M€ reduction in Ammonia imports.
- 8500 to 12000 jobs created.
- 6 – 8 Mt of CO2 emissions reduction.
- 1% of residual treated H2O used.

When it comes to GH2 production, the strategy will involve a combination of large-scale centralized production (e.g. Sines' project) with decentralized production on a variable scale associated with various sectors and forms of use.

When it comes to storage and distribution, the following combinations are stated in EN-H2 as the most likely to be used:

- i) Distribution by road or rail, or both in an intermodal solution, in the form of liquefied/compressed gas, ending with a liquid-to-liquid refueling process for liquid cryogenic hydrogen storage systems, in liquid-to-gas form and gas-to-gas at various scales,
- ii) Hydrogen distribution by ships in the form of liquefied hydrogen, including delivery for final use with gas pipelines and road transport.
- iii) Hydrogen gas distribution by a pipeline system.
- iv) Mixing of hydrogen with natural gas in the current natural gas infrastructure.

Out of the H2 applications previously mentioned in Section 2.1.4., EN-H2 predicts that the most relevant uses of hydrogen in Portugal will include P2G, P2M, P2I, P2FUEL, and P2P applications and states projects that were underway in each one:

P2G: Up to the date of the report, there were two projects already on board in Portugal for this application. The implementation of a Solar Plant with local H2 production and the research of H2's role in the decarbonization of the national economy by conducting feasibility studies capable of assessing the technical, economic, environmental, and social impact of hydrogen relative to injection into the natural gas grid.

P2M: Currently, there are already several companies and promoters with P2M projects underway or in the project phase, which demonstrates the interest already generated in the field of this value chain. Several projects are underway in Portugal involving the design, development, and implementation of H2 refuelling stations for light and heavy vehicles associated with logistics centres, industries, transport fleets, and cruise ships, based on a green H2 production plant using a solar park. The investigation of the role of H2 in the decarbonization of the national economy is

also important for this application, but in this case for the areas of long-distance mobility and long-distance heavy transport.

P2I: In P2I applications it is foreseen in Portugal the production of green ammonia and aniline for industrial purposes through the production and incorporation of green hydrogen. Another project underway is the optimization of combustion in industrial plants through the injection of locally produced hydrogen.

P2FUEL: In what concerns P2Fuel applications in Portugal the project synthetic fuel production is already in course, which consists in an industrial-scale facility that will produce synthetic aviation fuel for the aviation sector, based on GH2.

P2P: Lastly, the following projects in P2P applications are underway in Portugal:

- Hydrogen at Ribatejo Thermoelectric Power Plant: Local production of GH2, storage, and co-combustion with natural gas used in the combustion of the gas turbines of the Ribatejo combined cycle power plant.
- GH2 at Tapada do Outeiro Thermoelectric Power Plant: Local production of GH2, and co-firing with the natural gas used in the combustion of the gas turbines of the combined cycle power plant of Tapada do Outeiro.
- Hydrogen production from Offshore Energy: Development and commercialization of a modular and standardized system that aims to produce H2 by electrolysis using electricity generated from offshore energy.

2.4.3. Sines' Industrial Project

This anchor project is the one that will allow Portugal to have GH2 production on an industrial scale, acting as a catalyst, fundamental to creating a hydrogen economy in Portugal. It intends to leverage solar and wind energy since Portugal is the country that has the lowest electricity production costs from these renewables.

Sines' location presents diverse advantages (Presidência do Conselho de Ministros, 2020):

- Strategic location – on the Portuguese Atlantic coast.
- Availability of a deep water harbor.
- Infrastructures for transport and storage of GH2.
- Connection to the natural gas transport network.
- Next to an industrial zone with present and future consumers of H2.
- Land availability.
- Qualified workers – that were previously working in the coal power station that was decommissioned.
- Availability of renewable resources (wind and solar).

The goal is to have 1 GW by 2030, optimizing the cost of H2 production with a hybrid solution between solar and wind power that maximizes production hours, even though it requires a higher investment than using only a single renewable energy source.

The GH2 produced will be drained in three different ways:

- Direct injection in the NG networks.
- Distribution by tanker truck to different points of consumption (e.g., service stations with hydrogen stations and/or final consumers).
- Export via the Sines terminal – even though, initially, it is estimated that all hydrogen produced will be consumed at a national level and only later exports will be more relevant, e.g., to The Netherlands via ships.

This project will make Sines an important GH2 hub and will create the necessary conditions to develop an industrial cluster around H2 and a so-called CoLab that develops technology in this sector. Initially, in total, 1500 M€ are predicted to be invested in this project, including the areas of production of renewable energy, production of hydrogen, infrastructures for transport and distribution, and storage.

The implementation of this project will be based on strategic partnerships, whether national, European, or international, starting as a joint venture between Portuguese and Dutch companies.

This strategic partnership with the Netherlands will allow giving a European dimension to the project as a way of securing community funding and finding partners for the consortium, creating synergies between public entities and companies. Other strategic reasons for this partnership include:

- The Netherlands has developed an advanced strategy for a GH2 economy, with several projects underway.
- The Netherlands faces the challenge of producing enough H2 for the high internal demand for this gas, especially in the industry sector.
- The Netherlands wants to follow a mixed strategy, with both locally produced GH2 and imports of the remaining necessary.
- The Netherlands has an important chemical industry cluster and is neighbor to countries that also have a high demand for this gas, making the export market larger.

Sines' Industrial project, as foreseen in the EN-H2, converted to projects of consortiums of companies such as the GreenH2Atlantic or the HEVO-SUL as we'll explore next.

2.4.4. GH2 Projects underway

There are dozens of GH2 projects underway in Portugal, as companies start to realize the potential of an H2 economy. Below, we highlight some of them:

GreenH2Atlantic: Creation of a 100 MW hydrogen production hub in Sines, Portugal, composed of innovative, scalable, and fast-cycling 16 MW modules to overcome bottlenecks such as

efficiency, size, lifetime, and flexibility. This consortium of 13 companies led by EDP and Galp, plans on using hybrid renewable power plants (solar and wind). It also intends to make the transition of the former coal-fired power plant into an innovative renewable hydrogen production hub (GreenH2atlantic, n.d.).

Green Pipeline Project: Injection of GH2 into the NG network in Seixal. It will distribute a mixture of Hydrogen with NG to around 80 consumers in the residential, non-residential, and industrial sectors. Already started with the first injection of 5% on 7th March 2023, and the goal is to reach 20% in this project led by Floene (Floene, n.d.).

DHRYVE: PRF Gas Solutions has officially launched its portable hydrogen refueling station for vehicles - DRHYVE. Currently supplies heavy and light vehicles at 350bar and in the future will also supply light vehicles at 700bar. A fully automated solution that comprises hydrogen compression, control, and dispensing in a portable 6 m container. The system was installed in Cascais, Portugal, and is currently supplying two buses, also nationally manufactured by Caetano Bus, and a light car (PRF, 2021).

H2EVORA: Fusion Fuel's first solar-to-green hydrogen plant, H2Evora consists of 15 HEVO-Solar generators armed with the latest generation of Fusion Fuel's HEVO micro-electrolyzer. This was not only the first plant to create green hydrogen in Iberia, but also the first plant to produce and use green hydrogen as an energy storage medium all in one integrated facility (Fusion Fuel, n.d.).

GREENGAS: Fusion Fuel's green hydrogen produced will be directly injected into the Evora NG network to pilot hydrogen blending (Fusion fuel, n.d.).

HEVO-SUL: Comprised of 178 HEVO-Solar units, representing just under 4.3 MW of electrolyzer capacity. The plant will be able to produce up to approximately 418 tons of green hydrogen annually if using both solar and night-time functionality. The facility will be located in Sines, Portugal, where Fusion Fuel has already secured over 600 hectares of land for this and other projects. The hydrogen is expected to be used for several different applications, including injection into the NG distribution network, as an input in the production of green ammonia, as well as bottling in pressurized cylinders for industrial uses (Fusion Fuel, n.d.).

H2Rail: A project that aims to transform the diesel railcars in circulation on the Vouga Line and make "Vouguinha" the first Portuguese hydrogen train. It's led by CP and CaetanoBus and has the support of FEUP (FEUP, n.d.).

Hyperion H2 Setúbal: Installation of the Hydrogen Production Plant of Setúbal, in Poçoilos, municipality of Setúbal. As detailed in the terms of reference, the object of the Tender includes the supply of a Hydrogen Production Unit, including all the elements necessary for its correct functioning, following the supply limits mentioned in the Technical Specifications, as well as the works of construction necessary for the connection and operation of the equipment and the

management of the entire project until the Central can function (Presidência do Conselho de Ministros 2022).

2.5 Hydrogen Supply Chain and Logistics Challenges: Closing Remarks

As the final section of this chapter is reached, it is essential to consolidate our understanding of the challenges associated with the hydrogen supply chain and logistics in the context of its increasing prominence as an alternative energy carrier. Drawing on the technical aspects discussed in chapter 2.2 and the specific context of Portugal presented in chapter 2.4, this closing section provides a synthesis of the complexities and obstacles that permeate the hydrogen supply chain, from production to end-use. While reflecting on the broader context and the particularities of the Portuguese scenario, we will briefly revisit the main challenges and considerations that have been addressed throughout this work, highlighting the key takeaways for future discussions in the subsequent chapters of this thesis.

2.5.1 Production Challenges

Several are the benefits related to the production of GH₂, however, some challenges need to be taken into consideration:

- Energy efficiency: green hydrogen production, through water electrolysis, requires a significant amount of renewable electricity to power the electrolyzers since a large amount of energy is lost in the process (Vidas & Castro, 2021). This increases the cost of green hydrogen, requiring the scaling-up of renewable energy infrastructure and the optimization of electrolyzer technologies to ensure cost-effective and efficient hydrogen production. Portugal intends to overcome these challenges with the large-scale project of Sines as well as with the research and development made by CoLab.
- The intermittent nature of renewable energy sources: requires effective energy management and storage solutions to maintain a stable supply of electricity for hydrogen production (Yan et al., 2020).
- High water requirements: 9 L of H₂O per kg of H₂ produced (Soulmier et al., 2020), which may pose challenges in areas with limited water resources or high-water stress. This requires innovative ways to save H₂O while maintaining a degree of purity in the Hydrogen produced. One of the innovative ways the Portuguese government intends to implement is the use of treated residual water for electrolysis.
- Availability of land: the availability and potential of renewable energy sources can vary greatly depending on location and hence the production of GH₂. This may require additional investments in energy infrastructure so that green Hydrogen can be distributed across the country.
- High market barriers: small hydrogen producers face some challenges as initial capital costs and restrictions on market entry, for example, the minimum contract size for operating in the European Energy Exchange market is 1 GWh of power, which could be

too large at the initial stages of green hydrogen market development (Abad & Dodds, 2020).

2.5.2. Storage Challenges

Storing hydrogen poses challenges due to its low volumetric energy density. To store hydrogen effectively, it must be compressed, liquefied, or bonded to other materials. Each method has its own set of challenges (Langmi et al., 2022):

- Compressed hydrogen: requires high-pressure storage tanks, which can be expensive.
- Large-scale storage: high construction costs of engineered cavities, the local geology might not have suitable salt formations to use salt caverns, and porous media storage requires good sealing and containment.
- Liquefied hydrogen: involves cooling hydrogen to extremely low temperatures (-253°C), demanding sophisticated and energy-intensive cryogenic systems.
- Chemisorption: also presents its set of challenges namely the difficult reversibility meaning the retrieval of hydrogen from the material is not efficient. Also, there's a degradation of adsorbent materials with consecutive cycles, reducing performance.
- Physisorption: typically exhibits lower hydrogen storage capacities under ambient temperature and pressure conditions. Also, developing these materials can be expensive and complex.

2.5.3. Transportation and Distribution Challenges

When it comes to distribution challenges there are a lot of factors to have in account for GH2 supply chains:

- Centralized distribution systems: they're more vulnerable to disruptions such as equipment failure or natural disasters. It may require high infrastructure costs if there's no pipeline system already established that can be reutilized since this is the transportation mode that presents lower costs for long-distance distribution. Long-distance transport also requires energy, besides from potential leakage and dissipation of hydrogen.
- Decentralized distribution systems: there's a smaller-scale hydrogen production, which has low efficiency and is expensive per unit of hydrogen produced. Another challenge of the decentralized strategy is the complex coordination and optimization efforts to balance supply and demand.

Furthermore, each mode of transportation has its complexities and challenges associated:

- Pipeline: the main challenges here are the high initial investment, and the limited flexibility limiting the ability to adapt to changing demand or supply patterns.
- Tube trailers & Tanker trucks: both have limited capacity, and both require repeated loading and unloading of hydrogen increasing the handling requirements, which can

introduce safety risks and potential for hydrogen loss. They're also vulnerable to road congestion.

- Ship: typically, slower than other transportation modes, and can have a significant environmental impact, particularly if non-zero-emission vessels are used.
- Rail: constrained by the availability of rail networks making it less flexible compared to road transportation.

2.5.4 End-use Challenges

While hydrogen offers a versatile solution for a decarbonized future, several challenges need to be addressed to ensure its effective deployment across different sectors, namely:

Transportation: The widespread adoption of fuel cell vehicles requires a vast network of hydrogen refueling stations. Powerfuel technologies are still under development and require further research. Also, there's a need for greater public awareness and acceptance of hydrogen fuel cell technologies to drive demand.

Industry: Green hydrogen-based ammonia and methanol production can be more expensive than using grey hydrogen, requiring policy support or technological advancements to become cost-competitive. The same applies to other industrial processes that use hydrogen as feedstock.

Energy: Converting hydrogen back into electricity through fuel cells or gas turbines results in energy losses, reducing the overall efficiency. There are limits to the percentage of hydrogen that can be blended with NG without affecting the performance and safety of existing infrastructure and equipment.

2.5.5. Conclusion

The topic of green hydrogen is complex and has many branches that one can focus on. In this contextualization chapter, the green hydrogen landscape in Europe were examined and specifically the case of Portugal was deeply covered. It's clear that the green hydrogen economy is still in its early stages and has a long way to become a widespread technology.

From production to end-use, the obstacles that must be overcome were highlighted, and it has become clear that not only technological advancements but also a coordinated effort among industry, policymakers, and other stakeholders is required.

The design and implementation of a robust and efficient GH₂ supply chain in Portugal is critical to achieving large-scale deployment, minimizing overall costs, and ensuring that the demand for this clean energy carrier is met. This includes deciding between a centralized or decentralized production, where to store the hydrogen, and how to distribute it depending on the consumers to be served.

The focus will now shift to a specific aspect of the green hydrogen supply chain: the distribution of hydrogen to refueling stations. This application holds significant potential in advancing the decarbonization of the transportation sector and achieving a more sustainable energy ecosystem.

This thesis aims to develop a model that optimizes the transport and distribution of green hydrogen to refueling stations, considering the technical, economic, and logistical factors involved. Understanding these factors will be essential in creating an effective model that can drive the successful integration of green hydrogen into Portugal's energy infrastructure, thereby promoting a sustainable hydrogen-powered transportation future.

3. Literature Review

As the world faces the challenges of climate change and the need for sustainable development, the transition towards low-carbon energy systems has become a critical issue. Among the potential alternatives to fossil fuels, hydrogen has emerged as a promising contender, especially in the transportation sector, where it holds immense potential for reducing greenhouse gas emissions. However, the success of hydrogen as a sustainable fuel for transportation depends on the availability of efficient and reliable infrastructure, particularly refueling stations. Surprisingly, even countries like Portugal still lack sufficient hydrogen infrastructure, forming this thesis's central focus.

In this context the purpose of this literature review is to investigate previous research related to the optimization of the hydrogen supply chain, with a focus on hydrogen distribution, the deployment of refueling station infrastructures, and the promotion of the widespread use of hydrogen vehicles. Hence, the chapter is structured as follows:

- Section 3.1 provides an overview of decision-supporting systems in the hydrogen supply chain, showing different approaches on its optimization.
- Section 3.2 delves into the optimization of hydrogen transport and distribution, analyzing literature approaches to minimize the associated costs and energy consumption.
- Section 3.3 focuses on the optimization of hydrogen refueling station locations, along with the different factors that need to be considered when determining the optimal location of these stations.
- Finally, Section 3.4 summarizes this literature review and guides future research regarding Hydrogen supply chains.

3.1. Overview of Decision-Supporting Systems Components in the Hydrogen Supply Chain

The Hydrogen Supply Chain (HSC), particularly the green hydrogen supply chain (GHSC), plays a vital role in transitioning to a sustainable energy system. It enables the production, storage, transport, and distribution of clean energy carrier, H₂. However, the GHSC faces several challenges that require attention to ensure its efficient and cost-effective operation.

One significant challenge arises from the intermittent nature of renewable energy sources used to power the electrolysis process. This variability in renewable energy availability makes it challenging to meet H₂ demand consistently. Additionally, limited infrastructure for hydrogen production, storage, and distribution increases costs and restricts availability in certain regions.

To address these challenges and improve GHSC performance, it is crucial to develop decision-supporting systems (DSS). Dagdougui (2012) classified DSS for the HSC into three categories: mathematical optimization methods, decision support systems based on geographic information systems (GIS), and assessment plans. These DSS components assist in optimizing the GHSC and facilitating the transition toward sustainable hydrogen usage.

3.1.1. Mathematical optimization models

Mathematical optimization models have been developed to strategically plan and optimize future HSCs. For example, Li et al. (2008) introduced a generic optimization-based model to plan and design future HSCs. Their model considered different combinations of potential technologies and identified the most promising pathways. Almaraz et al. (2015) created a methodological framework using multi-criteria optimization to design a five-echelon hydrogen supply chain, optimizing cost, global warming potential, and safety risk. They applied this framework to a national case study in France.

Furthermore, Li et al. (2019) conducted an extensive review of the papers that pertain to the hydrogen supply chain network design models published in scientific journals. They noticed that most literature treats this problem as a multi-echelon one taking advantage of mixed integer linear programming and is applied at a national level. These echelons include the production, storage, distribution, and different uses of H₂. Bique et al. (2019) developed a mixed integer linear program that balanced cost, safety, and environmental impact to create a three-dimensional Pareto front, enabling trade-off decisions for hydrogen infrastructure pathways. Results showed that decentralized hydrogen production plants based on water electrolysis may compete with coal-based dominant technology.

3.1.2. Geographic Information Systems

Geographic Information Systems are powerful tools that integrate spatial data with various analytical models to analyze and visualize information related to geographical locations. In the context of this research, GIS plays a role in studying hydrogen infrastructure and designing efficient supply chains.

In the realm of GIS, Johnson et al. (2008) integrated spatial information with a techno-economic model to analyze hydrogen infrastructure in Ohio, showing that regional aggregation of infrastructure reduces costs compared to city-level distribution. Hence, results showed that the favored pathway was centralized production with pipeline distribution. Mah et al. (2022) presented a GIS-based optimization framework for designing a photovoltaic-based hydrogen-electricity supply chain, enabling optimal infrastructure locations to meet fuel and electricity demands.

3.1.3. Assessment plans

Assessment plans are a type of optimization technique that can help understand the behavior and dynamics of the HSC without creating a full mathematical model. Rather than predicting the exact cost or performance of the hydrogen infrastructure, assessment plans aim to explore different scenarios and identify promising strategies for introducing a hydrogen economy. For instance, Farrell et al. (2003) review various strategies for the introduction of hydrogen as a transportation fuel. The authors suggested that the cost of introducing hydrogen can be minimized by adopting a mode of transportation that utilizes a small number of large vehicles operating within a limited geographic area.

Integrating these DSS components is crucial, as demonstrated by Robles et al. (2020), who combined optimization models with assessment plans to evaluate the market penetration of hydrogen fuel cell vehicles. They assessed the best hydrogen supply chain network configuration, conducted a Social Cost-Benefit Analysis, and evaluated the potential benefits and costs of transitioning to hydrogen fuel cell vehicles.

3.1.4. Final notes on DSS in HSC

It's important to state that many literature articles, particularly the ones published before the 2015 Paris Agreement, consider other options for Hydrogen deployment other than green hydrogen which goes against the scope of this thesis. However, the models themselves could still be applied with slight changes in parameters, especially at the level of production. Such is the case of the work developed by Konda et al. (2011) where a multi-period optimization framework based on a techno-economic analysis is used to design spatially explicit and time-evolutionary H₂ supply networks. They reach the conclusion that the transition towards a large-scale H₂ supply infrastructure is economically viable but considering hydrogen production methods other than electrolysis.

In conclusion, this section has provided an overview of DSS in the HSC, showcasing various models and tools aimed at improving efficiency and cost-effectiveness. However, it's important to acknowledge that there are limitations and potential drawbacks to these tools. One limitation is that many of the models developed under these tools assume certain parameters or scenarios, which may not accurately reflect the real-world conditions of the HSC. Additionally, some of the models focus on specific regions or countries, which may not apply to other areas. Furthermore, while multi-criteria optimization techniques offer a way to balance multiple objectives, such as cost and environmental impact, it can be challenging to determine the weighting of each objective and to ensure that all relevant factors are being considered.

While the focus has been on comprehending the HSC, this literature review continues in the subsequent section, where the attention will shift to the topic of hydrogen transport and distribution. Strategies and approaches dedicated to minimizing costs, optimizing energy consumption, and ensuring seamless delivery of this green energy carrier will be investigated.

3.2. Optimization of Hydrogen transport and distribution

Hydrogen transport and distribution play a crucial role in the overall hydrogen supply chain, impacting the cost, efficiency, and sustainability of delivering hydrogen to end-users. Optimizing these processes is essential to ensure that hydrogen is delivered in an efficient, cost-effective, and sustainable manner.

Nevertheless, optimizing hydrogen transport and distribution is not without its challenges and constraints. Factors such as different pressure levels, trip distances, and hydrogen demand can make it difficult to find the most effective methods of transporting and storing hydrogen from one site to another.

Despite the importance of hydrogen transport and distribution, there is a lack of research that focuses solely on optimizing these processes. Typically, transport and distribution are integrated with other aspects of the supply chain and optimized as a whole. This can be seen in the articles mentioned in section 3.1.

Nonetheless, Lahnaoui et al. (2017) have shed light on this specific area by developing a model that identifies the optimal combination of compressed gas trucks at different pressure levels for cost-effective hydrogen transport across varying distances and flow demands. Their findings emphasize the importance of achieving economies of scale through greater hydrogen demand, leading to reduced transport costs.

Continuing their work, Lahnaoui et al. (2018) applied their model to North Rhine-Westphalia, Germany, considering two future demand scenarios. The results indicated that in 2050, hydrogen transport predominantly occurred at high-pressure levels – 500 and 540 bar - between storage nodes and distribution hubs, while the 2030 scenario involved transport at lower pressure levels – 250 and 350 bar.

Further supporting this research, Lahnaoui et al. (2021) conducted a study to determine the optimal transport infrastructure for various scenarios in France and Germany. Their findings reaffirmed the advantages of compressed hydrogen gas at high-pressure levels, around 500 bar, while also suggesting the potential use of liquid organic hydrogen carriers for cost-effective transport and storage in the early stages of hydrogen fuel adoption.

So far, the models presented focused on finding the best transportation method for H₂. After making this choice the problem becomes finding the more efficient way to deliver the H₂. This can be performed through the solution of vehicle routing problems (VRP), which find the most efficient routes for a fleet of vehicles to service a set of customers while minimizing travel costs or maximizing resource utilization (Laporte, 1992). Finding this optimal set of routes for the vehicles to visit all the demand points is usually subject to constraints such as vehicle capacity, time windows, and road network connectivity (Bräysy et al., 2001).

Cardoso (2009) states that VRP can be considered a merger between two well-known operations research problems: the Travelling Salesman Problem (TSP) and the Bin Packing Problem (BPP). The TSP seeks the shortest possible route that a traveling salesman can take to visit a set of cities exactly once and then return to the starting city. The origin of this problem, as stated by Dantzig et al. (1954) is somewhat obscure since this problem has been studied for many years ago, however, Dantzig credits the first explorers of this linear programming problem to Robinson (1949), Koopmans (1949), Heller (1953) and Kuhn (1955). It is a simple VRP problem since only one vehicle is considered to visit all the demand points of the network. The BPP seeks how to pack a set of items of various sizes into the minimum number of fixed-size bins, such that the total size of items in each bin does not exceed the bin capacity. It can be a 2-dimensional problem where only the height and width of items are considered (Lodi et al., 2002) or three-dimensional if the depth parameter of items is added (Lodi et al., 2002).

Sehr et al. (2022) used the VRP to solve optimize the mobile delivery system called the Mobile Modular H2 Port, which is essentially an H2 delivery system on a car trailer that can carry hydrogen and deliver it to local consumers. After comparing the performance of several solving procedures, they used the branch-price-and-cut algorithm to obtain an exact solution to this VRP.

VRP problems typically assume fixed supply and demand points, allowing for efficient planning and minimizing distances traveled. By utilizing VRP models, it becomes possible to identify optimal routes for distributing hydrogen to various consumption points, including HRSs.

To truly harness the potential of hydrogen in decarbonizing countries like Portugal, it is vital to prioritize its use in the transportation industry, particularly by introducing hydrogen-powered heavy-duty vehicles. This step holds great promise for reducing emissions and promoting sustainability.

Unfortunately, the current state of HRS infrastructure in Portugal is inadequate, with only a single station available in Cascais, which fuels an urban bus. This scarcity highlights the need for a comprehensive strategy that goes beyond mere distribution planning. Before focusing on the optimization of hydrogen distribution routes, it is crucial to first determine the most efficient locations to deploy HRSs. This aspect will be the primary focus of the upcoming section in this literature review.

3.3. Optimization of hydrogen refueling station location

One of the key challenges in the development of hydrogen-based transportation infrastructure is the "chicken and egg" vicious cycle, which refers to the conundrum of whether to build HRSs first to encourage the adoption of hydrogen-powered vehicles, or to wait for the widespread use of hydrogen vehicles before investing in the necessary infrastructure. This problem is particularly relevant in the context of optimizing refueling station locations, as decisions made in this regard can significantly impact the adoption rate of hydrogen-powered transportation.

The location of refueling stations is also critical for minimizing the distances that hydrogen needs to be transported while fulfilling demand, which has a direct impact on the overall efficiency of the hydrogen supply chain. By encouraging the use of hydrogen vehicles and reducing greenhouse gas emissions, a well-planned network of refueling stations can have significant environmental benefits. Additionally, an efficient network can also stimulate the growth of the hydrogen market, attracting investment, fostering innovation, and promoting the expansion of hydrogen-powered transportation options, including public transit, freight, and personal vehicles.

Fortunately, researchers have been working on resolving this issue for over two decades, developing models that tackle this problem from various angles and considering their objectives. Lin et al. (2020) conducted a review that investigates the existing research efforts and realized a comprehensive overview of these works on hydrogen station location models. They addressed hydrogen stations' location through the use of two main types of models according to the number of objectives: single and the multi-objective models, illustrated in Figure 7.

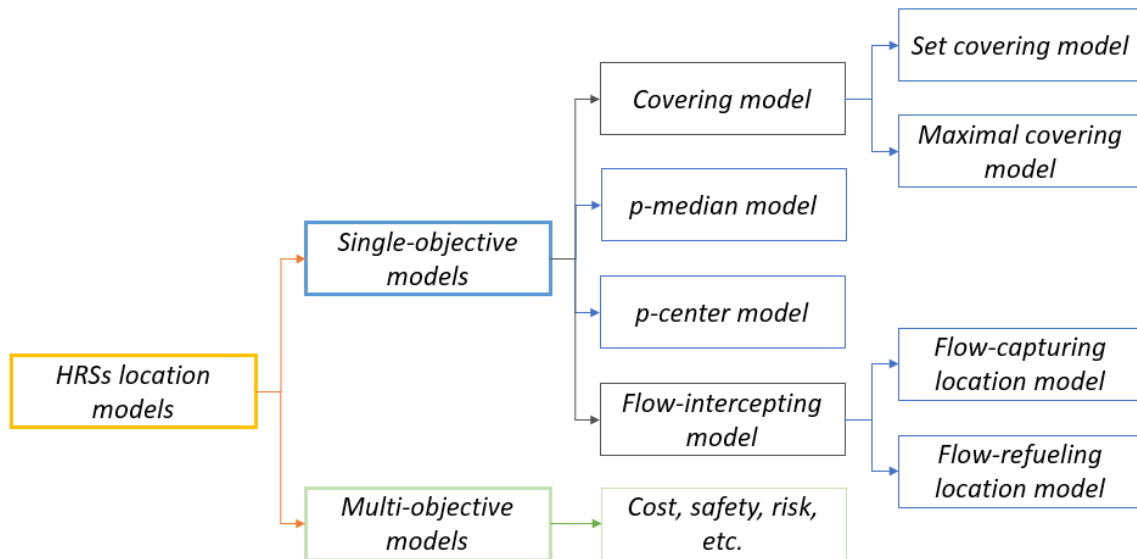


Figure 7: HRSs Location models (adapted from Li et al. (2020))

3.3.1 - Single objective models

Single-objective models for HRSs location optimization focus on optimizing a single criterion, such as cost or accessibility.

Set covering model:

The set covering model focuses on minimizing the number of stations subject to every demand point having to be covered by a station. Kang and Recker (2015) developed a set covering model for HRSs locations in the Irvine community. They incorporated the routine selection of each driver and simplified the case by assuming that a specific vehicle driver only refuels once a day. The experimental results demonstrated a reduction in the converging time of the solution, indicating improved effectiveness of the model.

Maximal covering location model:

The model was initially presented by Church and ReVelle (1974). It aims to maximize the demand coverage for a given number of refueling stations. To determine the demand for a specific location in the network, various factors such as population, income, family size, and vehicle ownership are considered. Frade et al. (2011) conducted a study on the optimal site location for electric vehicle charging stations in Avenidas Novas, Lisbon, Portugal, utilizing the maximal covering model. The findings of this study suggest that this approach can provide valuable insights for the future planning of electric vehicle charging stations.

P-median model:

Developed by Hakimi (1964), the objective is to reduce the distance between a point and a station with demand as weight. Each demand point is served by only one station, and it is considered to be a “min-sum” problem. Nicholas et al. (2004) integrated the p-median model with geographic information system technology to select potential sites for a hydrogen station in Sacramento

County, California. Their proposed model incorporated driving time as a factor for evaluating travel costs. The simulation results indicated that a strategic placement of a few refueling stations could be sufficient to meet the needs of a large number of prospective hydrogen vehicle users.

P-center model:

More recently developed by Elloumi et al. (2004) the p-center model aims to minimize the maximum distance between a given point or node and the nearest refueling station that covers it. This results in a "min-max" problem, where the goal is to reduce the largest distance between any location and its corresponding station, ensuring that all points are adequately covered. It is not directly dependent on demand calculations, hence, this approach is well-suited for locating emergency facilities, where service accessibility to the demand points is the primary concern.

Flow-capturing location model (FCLM):

This model uses traffic flow as a measure of demand, which is calculated dynamically. As a result, the problem of covering demand points is transformed into the problem of capturing traffic flow. Specifically, the goal is to maximize the flow captured between each origin-destination pair.

Riemann et al. (2015) devised a model for identifying the best locations to install wireless charging facilities for electric vehicles (EVs) out of a set of potential sites, to maximize the captured traffic flow across the network. Their approach incorporated the stochastic user equilibrium principle, which accounts for the routing preferences of EV drivers. By considering these factors, their model can efficiently identify the optimal solution on a global scale.

Flow-refueling location model (FRLM):

The previously described FCLM does not account for the scenario where drivers may need to refuel their vehicles more than once during a long journey. To address this limitation, Kuby and Lim (2005) proposed an improved model known as the Fixed Refueling Location Model (FRLM). The FRLM aims to maximize the refueled traffic flow by taking into consideration additional factors such as the average driving speed and the maximum driving range. Later Kuby et al. (2009) used this model to investigate strategies for rolling out an initial refueling infrastructure in Florida. The results indicated that an effective approach to rolling out an initial refueling infrastructure is to first create groups of refueling stations in key urban areas. Afterward, additional stations, called bridging stations, would be built to connect these urban areas, facilitating travel between them.

3.3.2. Multi-objective models

The multi-objective models involve several goals that affect the hydrogen station location. These goals include minimizing economic cost, maximizing utilization rate, and safety risk, etc., which are represented in the objective function with an associated weight coefficient.

An example of the use of a multi-objective model is presented by Sabio et al. (2012). These authors examined the environmental implications of constructing a hydrogen station network in Spain. Their approach involved minimizing the most critical life cycle assessment impacts, thereby

optimizing various environmental factors that significantly affect the supply chains. The study demonstrated that their framework is effective in considering multiple environmental factors.

3.3.3. Others

When conducting this literature review, it was noticeable that most Hydrogen Refueling stations' location models derive from one of the previously presented ones. However, some authors developed some slight deviations that are worth mentioning. This is the case of Schwoon (2007) who proposed a technique to determine the locations of hydrogen refueling stations using agent-based trip modeling and GIS-supported spatial modeling. The study assumes that the likelihood of consumers considering fuel cell vehicles increases with greater exposure to hydrogen refueling opportunities. The study concludes that the placement of hydrogen stations should consider the "Don't worry distance" of individuals.

Another interesting work was the one performed by Dagdougui et al. (2012) that created a mathematical model where the main decision is the selection of green HRSs that are powered by previously fixed production nodes based on distance and population density criteria. This study differentiates from previous ones since it also includes as an objective the control and management of the hydrogen and electric flows that are sent to the GHRs. He et al. (2017) developed a mathematical model for siting hydrogen refueling stations along a hydrogen-energy expressway, considering the life cycle cost of hydrogen energy. The model incorporates constraints such as the supply radius of hydrogen stations, the productivity of hydrogen sources, and geographic information while ensuring hydrogen supply reliability and meeting annual planning load requirements.

Furthermore, Li et al. (2018) developed an integrated optimization model which combines the generalized Bass diffusion model and FCLM to investigate the correlation between the sales of hydrogen fuel cell vehicles and the number of refueling stations. The proposed model can effectively break the "Chicken and Egg" dilemma and balance the interests of all parties.

Based on the assumption that refueling demand is higher in regions where driving is more frequent, Lin et al. (2008) created a novel model. This model aims to minimize refueling time and is applicable to optimize the deployment of refueling stations in Southern California, utilizing only data on the spatial distribution of vehicle miles traveled. The proposed approach takes into account the preference of individuals to minimize the time spent for refueling, leading to more efficient deployment of refueling stations.

Bersani et al. (2009) presented an innovative model for planning a network of service stations of a given company within a competitive framework. The author developed a variant of a multiple-facility location problem and applied it to a territory in northern Italy. He concluded that, although there are many uncertainties in what concerns the hydrogen future economy, the decision support model developed can be an important in determining optimal placements of service stations.

Most articles in the literature optimize the location of refueling stations without actually considering the costs of distributing the hydrogen from production plants to end users. Shamsi et al. (2021)

challenged this and developed a mathematical methodology for the primary deployment of a HSC including H₂ production plants and HRSs along highways. These refueling stations are meant to serve a market of heavy-duty hydrogen vehicles. After applying the model to the Highway Corridor in Ontario, the results show that hydrogen production and delivery cost can reduce from \$22.7/kg H₂ in a 0.1% market share scenario to \$14.7/kg H₂ in a 1% market share scenario.

In summary, optimizing the location and operation of hydrogen refueling stations is a complex task that requires the integration of multiple factors, including infrastructure costs, vehicle demand, and transportation networks. While optimization models have been developed to address this challenge, there are still several practical issues that need to be overcome for their effective implementation. For instance, the availability of accurate and up-to-date data on hydrogen demand and transportation patterns is essential for the models to provide reliable results. Furthermore, the involvement and cooperation of various stakeholders, including government bodies, vehicle manufacturers, and energy companies, is crucial for ensuring the successful deployment and operation of these stations. Overall, while the development of optimization models for hydrogen refueling stations represents a promising direction for promoting the adoption of hydrogen fuel cell vehicles, their practical implementation requires significant effort and collaboration among various stakeholders.

3.4 Conclusion and Future Research

The existence of DSS is crucial for the success of the GHSC as it can address the challenges it faces and ensure its efficient and cost-effective operation. It provided an overview of various DSS to deal with the HSC. These include mathematical optimization methods, decision support systems based on GIS, and assessment plans. The use of optimization techniques was identified as the most effective to define the allocation of resources, minimize energy waste, reduce environmental impact, and improve the overall efficiency of the GHSC. The examples provided demonstrate that optimization can be applied at the national level balancing multiple objectives such as cost, safety, global warming potential, and environmental impact.

Within HSC, optimizing hydrogen transport and distribution is critical to ensuring that hydrogen is delivered in a cost-effective, efficient, and sustainable manner. The literature review reveals that compressed hydrogen gas at a high-pressure level of around 500 bar is generally the best option for transporting hydrogen. However, substituting compressed gas at low to medium pressure levels with liquid organic hydrogen carriers may reduce transport and storage costs at an early stage of hydrogen fuel adoption. It was also shown that the vehicle routing problem is used to find the most efficient routes for a fleet of vehicles to service a set of customers while minimizing travel costs or maximizing resource utilization.

The location of HRSs is a critical factor that impacts the adoption rate of hydrogen-powered transportation, the overall efficiency of the hydrogen supply chain, and the environmental benefits of using hydrogen. Researchers have been working on resolving the "chicken and egg" problem for over two decades and have developed several models that tackle this issue from different

angles. These models include the set covering model, the maximal covering location model, the p-median model, the p-center model, the flow-capturing location model, and the flow-refueling location model. Recently other innovative models consider the distribution of hydrogen from production sites to these new refueling stations' locations when choosing them.

By strategically planning the deployment of HRSs, it becomes possible to establish an infrastructure that effectively supports the utilization of H₂ in the transportation sector. This, in turn, will accelerate the decarbonization efforts and pave the way for a greener future. Through a combination of optimized distribution routes and a well-designed network of HRSs, the potential of hydrogen as a clean energy source can be fully realized.

Future research regarding the HSC can investigate the integration of optimization methods with artificial intelligence and machine learning techniques to enhance the performance and accuracy of the models. Additionally, research can be conducted to explore the potential of emerging technologies, such as blockchain in optimizing the HSC.

Since H₂ is in the early stage of its large-scale implementation as an energy carrier in most countries, there's a lack of research focusing only on its transport and distribution. Given the variety of pressures that hydrogen can be distributed at, future research could focus on testing which transportation and distribution modes as good suits better for different cases.

In what concerns HRSs location most models developed to ignore the distribution costs of hydrogen from production plants to the refueling stations chosen, focusing only on fulfilling demand, and future research should focus on merging the two. Also, it is essential to validate the effectiveness of these models through case studies in various geographical locations and under different scenarios. Another avenue for future research is the development of new models that integrate machine learning, big data analytics, and artificial intelligence techniques to predict the demand for hydrogen refueling stations and optimize their location. Additionally, it would be beneficial to conduct a comparative analysis of the various models and evaluate their strengths and weaknesses in different contexts.

Given the literature gaps previously identified, in the upcoming chapter of this thesis, an optimization model that aims to optimize the initial HRSs deployment is developed. This model will consider two crucial factors: the availability of hydrogen production sites and the transportation cost associated with distributing hydrogen. By considering these variables, the optimal locations for HRSs can be strategically determined, ensuring efficient access to hydrogen fuel while minimizing transportation costs. This endeavor will contribute to the broader goal of establishing a well-designed and cost-effective infrastructure to support the utilization of hydrogen in the transportation sector, facilitating the transition toward a greener future.

4. Problem Characteristics and Mathematical Formulation

So far, the present work developed the contextualization of H₂, explaining how and why it is becoming increasingly relevant in Europe's energy mix, including the Portuguese one where several funds are being invested in this clean energy carrier. A literature review on optimization models of hydrogen supply chain and more precisely optimization of hydrogen refueling stations' location was also presented, where it was identified a lack of case studies applying these optimization models in the Portuguese region.

Portugal currently has only one HRS, hence, the country hasn't overcome the "chicken and egg" barrier explained in the previous chapter. More HRSs must be built promoting the use of fuel-cell vehicles, however, it must be a feasible investment and a strategic choice of where to build these HRSs is necessary to overcome this dilemma.

The present chapter displays an optimization model developed to locate HRSs. The primary objective of the model is to identify the most strategic HRSs locations for an initial rollout of heavy-duty H₂ vehicles while also estimating the associated costs.

The model developed extended the work of Shamsi et al. (2020) by introducing key modifications. Unlike their model, which considered the possibility of building electrolyzers at new locations, this model considers the opening of green hydrogen production sites considering the existing projected ones. This modification reflects the unique characteristics of the Portuguese context, where several green H₂ production projects are already underway, and this work aims to capitalize on these existing infrastructures. Also, while Shamsi et al. (2020) model focuses on environmental and social benefits, the model developed focuses mainly on the economic aspects introducing key modifications to the objective function and new constraints that were considered crucial to this model's goal.

This chapter is structured as follows:

- Section 4.1 provides a comprehensive overview of the model's structure, outlining the H₂ pathway from production to HRSs, helping readers to understand the scope and significance of the model.
- Section 4.2 presents the mathematical formulation of the optimization model, including the relevant sets, variables, and parameters, as well as the objective function and constraints. This section describes the model's underlying logic and demonstrates how it accounts for various factors that impact HRSs' location decisions.
- Section 4.3 is a concise summary of the chapter.

4.1. Model Characterization

To keep investments at a minimum level while meeting the demand, i.e., building a cost-effective HRSs network, several important questions need to be addressed:

- What will be the demand?

- How is hydrogen being distributed from production plants to the HRSs?
- Is there enough production to fulfill demand? Which plants should be used?

4.1.1. Demand estimation

The first question is crucial since HRSs must be built and have enough capacity to fulfill the demand of a given zone. However, it is challenging since in the case of hydrogen-moved vehicles demand is a forecast intimately related to fuel availability. Most countries still have a very little market for fuel cell vehicles, both light and heavy-duty, making it hard to predict how demand will evolve throughout the years, depending also on policies and incentives applied by local governments.

For this model, demand is estimated based on important considerations. First, after choosing the road network to which this model will be applied, it is divided into smaller demand zones (e.g. an 800 km road network is divided into 50 km bits). The number of vehicles that cross these smaller chunks of the road must be measured, if possible, with the distinction between light and heavy-duty ones. Then, it is assumed a certain level of market penetration for fuel cell vehicles, and demand is estimated using the average fuel economy. This means that, for example, if 1000 heavy trucks are moving in a certain 50 km zone per day, if there's a 1% level of market penetration, and if the average fuel economy is 10 km per kg of hydrogen, then the demand in that 50 km zone would be $0,01 \cdot 1000 \cdot 50 / 10 = 50$ kg of hydrogen per day.

4.1.2 Hydrogen distribution mode

The second question revolves around the transportation of hydrogen from production plants to the HRSs. Extensive research by Lahnaoui et al. (2021) indicates that transporting hydrogen at a pressure of 500 or 540 bar is the optimal choice among various compressed hydrogen options. While pipelines are the most cost-effective for long-distance distribution and offer safety and reliability, tube trailers are chosen as the preferred mode of transport in this model. Tube trailers provide flexibility, allowing hydrogen delivery to locations without existing pipeline infrastructure or requiring substantial investments in large-scale hydrogen storage facilities. Moreover, tube trailers are already used for grey hydrogen transportation. Therefore, this is the transport mode that this generic model considers.

4.1.3. HRSs and Production Site Selection

With the transportation mode chosen, the model now decides where these tube trailers get the hydrogen from and where they deliver it. Thus, the model first chooses where to open the production plants, out of the existing possibilities. Then it decides in which service stations' locations HRSs should be open, and of what size. Moreover, the model decides how much hydrogen goes from each production plant to each HRS, considering the demand in the zone in which it is located. In practice, all these decisions are made simultaneously. The generic output of the model is illustrated in Figure 8.

One production plant might serve multiple HRSs in multiple locations, there might be multiple service stations within each demand zone and each HRS serves only the demand zone in which it is located.

Also, note that for this generic model, only one HRSs of each capacity can be opened in each service station. If, for example, there's 3 different HRSs capacities the model can choose to open, at most, 3 HRSs per service station, one of each capacity. This is of course dependent on local policies and can be easily adapted.

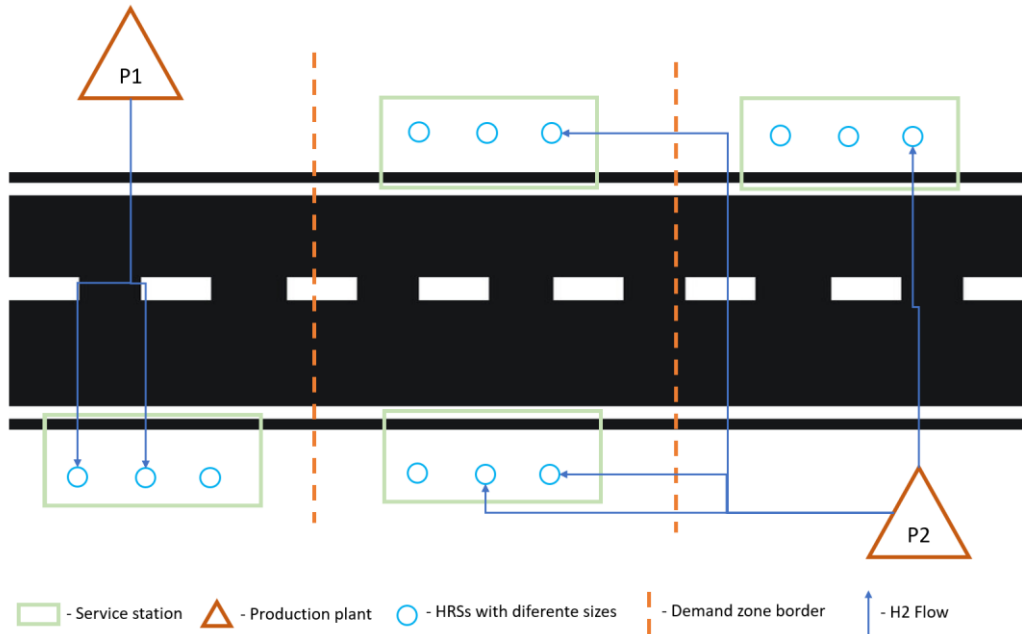


Figure 8: Generic output of the optimization model

When it comes to the production sites where hydrogen is to be picked, of all possibilities, the locations chosen should create the lowest cost combinations when considering both the production costs and the costs of distributing hydrogen from those sites to the HRSs. Also, their production capacity should be considered since, if they don't have enough hydrogen to fill trucks, even if they are closer to some HRSs, it may be cheaper to fulfill demand from further production sites. The same principle is applied when deciding where to open HRSs and their capacities, considering the cost combinations including HRSs' capital costs, yet making sure the demand of a given demand zone is fulfilled.

4.1.4. HRSs Supply chain

After being produced at low pressure, H₂ needs to be compressed so it can be more efficiently transported in tube trailers, more specifically compressed to around 500-540 bar. When trucks arrive at the service station, hydrogen needs to be dispensed and further compressed to around 700 bar. HRSs typically have 2 pressure levels, 700 bar (H₇₀) and 350 bar (H₃₅), which is the old standard. Most current methods use the H₇₀ (Genovese et al., 2023), so, for simplification purposes, that's the pressure that will be used when applying this model, assuming buffer storage

where cylinders above ground are kept constantly at that pressure (Sadi & Deymi-Dashtebayaz, 2019). This chain of operations in the H₂ supply chain is depicted in Figure 9.

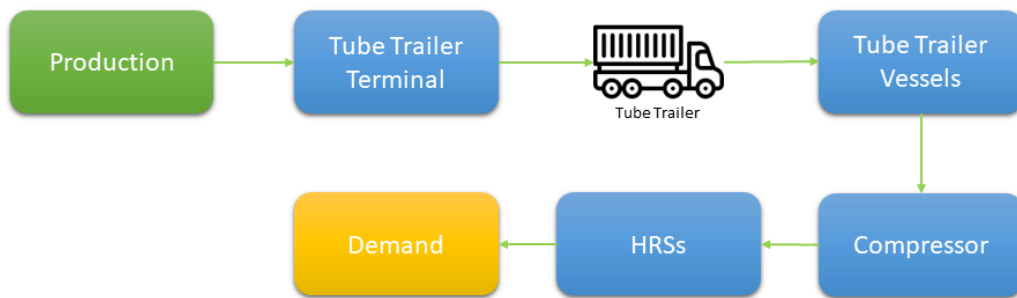


Figure 9: GH₂ supply chain modeled

All these processes of loading up the tube trailers, dispensing the hydrogen, and storing it at the HRSs have associated operational costs, which will impact the objective function. Also, there are different possible sizes, i.e., storage capacities, for the implemented HRS in each service station. The model is built so that there's the possibility of having up to one of each kind in the same service station but does not allow having multiple stations of the same size simultaneously.

Hence, the objective of this model is to find the right combination of production plants to be used and HRSs to be opened so that an initial rollout of hydrogen refueling infrastructure takes place, with the minimum costs possible considering production, distribution, and capital costs. It is meant to be applied once, for a given road network that has no infrastructure and allows a transition to a hydrogen-moved transportation industry.

4.2. Mathematical Formulation

This section provides a detailed explanation of the model's underlying mathematics, enabling a thorough understanding of its structure, logic, and ability to incorporate diverse factors that impact HRS location planning. First, the sets, parameters, and variables are defined, then the objective function and constraints are presented and explained.

4.2.1. Sets

Sets play a crucial role in defining spatial dimensions and constraints of the problem. The model developed uses the following sets:

- Set P represents the available green hydrogen production sites, which serve as the sources for supplying hydrogen to the HRSs. Each has unique characteristics including location, capacity, and production costs per kg of H₂.
- Set L encompasses the potential locations for the HRSs. Ideally these will be existing service station locations on the road network.

- Set K includes the zones in which the road network in the case study is divided. These zones help better identify demand, hence choosing the best HRSs locations.
- Finally, set Q represents the available capacities of the HRSs.

4.2.2. Parameters

This section introduces the parameters used in the optimization model, which are vital for quantifying costs, capacities, distances, and demands within the problem domain. The following parameters are considered:

PC_i : Production Cost of plant i (€/kg)

$ProdCap_i$: production capacity of plant i (kg/time unit)

CC : Capital cost of a HRS (€/time unit)

$dist_{ij}$: distance between plant i and service station j (km)

FP : tube trailer's fuel price (€/l)

FE_{TT} : tube trailer's fuel economy (km/l)

TTC : tube trailer's capacity (kg)

$StCap_q$: capacity of a refueling of size q (kg/time unit)

d_k : hydrogen demand at zone k (kg/time unit)

OC : operational costs of distributing hydrogen to a HRS (€/roundtrip)

4.2.3. Variables

This section introduces the variables utilized in the model, which are essential for capturing the decision-making and allocation aspects of the problem. The following variables are considered:

Integer variables:

X_{ijq} : H2 delivered from plant i to HRS of size q at location j (kg/time unit). Quantifies the supply of hydrogen from a production site to the respective HRS per time unit.

Z_{jqk} : H2 delivered from station of size q at location j to demand zone k (kg/ time unit). Quantifies how much hydrogen of a certain demand zone is fulfilled by the respective HRS. Notice that demand of a demand zone is only fulfilled by HRS included in that zone.

Binary variables:

δ_i : takes a value of one if plant i is being used and zero otherwise. This binary variable determines whether a particular production site is selected and utilized as part of the optimization process.

ω_{jq} : takes a value of one if a HRS of size q is built at location j , and zero otherwise. This binary variable indicates the decision to establish a HRS at a specific location and size, considering the various options available.

4.2.4. Objective function

The objective function in the optimization model is designed to minimize the total costs associated with the developed hydrogen supply chain. It consists of three distinct terms, each representing a specific cost component within the system, represented monthly.

The first term of the objective function represents the cost of producing hydrogen at each production plant i , contingent on its utilization. This term captures the expenses incurred in generating the hydrogen that leaves each plant to supply HRSs.

The second term illustrates the capital costs associated with constructing a HRS at a specific location j and size q if the decision is made to establish the station.

The final term represents the cost of distributing hydrogen from a production plant i to a station j , considering the roundtrip journeys made by the transportation system. This cost per roundtrip (2) is calculated based on the distance traveled, multiplied by a factor denoted as A (3), and adding the operational costs per roundtrip. Factor A is computed by dividing the fuel price by the fuel economy and then multiplying it by 2, as each roundtrip requires accounting for twice the distance between a production plant and the designated HRS.

The number of roundtrips is calculated by dividing the total hydrogen distributed from plant i to station j divided by the tube trailer capacity and rounding that number up to the nearest integer. By multiplying the number of roundtrips with the cost per roundtrip we get the total distribution costs.

$$\text{Min } Z = \sum_i \sum_j \sum_q X_{ijq} * PC_i * \delta_i + \sum_j \sum_q CC * \omega_{jq} + \sum_i \sum_j C_{ij} * \left[\frac{1}{TTC} * \sum_q X_{ijq} \right] \quad (1)$$

$$C_{ij} = A * \text{dist}_{ij} + OC \quad (2)$$

$$A = \frac{FP * 2}{FE_{TT}} \quad (3)$$

4.2.5. Constraints

The present section focuses on the constraints integrated into the optimization model, which play a critical role in ensuring the feasibility and integrity of the proposed solution. These constraints establish limitations and conditions that must be satisfied within the hydrogen supply chain network, providing essential guidelines for the decision-making process.

Plant capacity: ensures that the quantity of hydrogen delivered from any production plant does not exceed its designated production capacity. This constraint aligns the production and delivery

processes, ensuring that the supply chain operates within the capacity limitations of each production site.

$$\sum_j \sum_q X_{ijq} \leq ProdCap_i * \delta_i \quad \forall i \in P \quad (4)$$

Station capacity: ensures that the quantity of hydrogen supplied by a HRS of size q on a location j does not exceed its designated storage capacity. By incorporating this constraint, the model ensures that the operational capabilities of each HRS are respected, promoting efficient utilization of storage resources.

$$\sum_k Z_{jqk} \leq StCap_q * \omega_{jq} \quad \forall j \in L, \quad q \in Q \quad (5)$$

Material balance: ensures that the hydrogen inflow to a service station located at j is equal to or greater than the hydrogen outflow from that location. Thus, the model guarantees that the hydrogen availability at a given service station aligns with the demand, preventing any shortage or excess of hydrogen.

$$\sum_i X_{ijq} \geq \sum_k Z_{jqk} \quad \forall j \in L, \quad q \in Q \quad (6)$$

Demand: ensures that all the quantity of hydrogen leaving stations that serve demand zone k is equal to the specific demand of that zone. It guarantees that the hydrogen supply to each demand zone aligns precisely with the required amount for refueling purposes.

$$\sum_j \sum_q Z_{jqk} = d_k \quad \forall k \in K \quad (7)$$

Plant activation: ensures that a production plant is open only if it is being used.

$$\sum_j \sum_q X_{ijq} \geq \delta_i \quad \forall i \in P \quad (8)$$

Non-negativity constraint:

$$X_{ijq} \geq 0 \quad \forall i \in P, \quad j \in L, \quad q \in Q \quad (9)$$

$$Z_{jqk} \geq 0 \quad \forall j \in L, \quad q \in Q, \quad k \in K \quad (10)$$

4.3. Conclusion

The model developed is an extension of the work developed by Shamsi et al. (2020) with key modifications. It provides a solid generic basis for deploying a hydrogen refueling stations network in any given scenario.

Some assumptions were made such as the inexistence of fixed production costs and no costs associated with the acquisition of tube trailers, with the use of tolls and other taxes. Also, the assumption that only one HRS of each capacity can be built per service station, meaning that can be as many HRSs in a service station as different types of HRSs. This is, of course, an assumption dependent on local policies.

In reality, scenarios can be more complex, for example if a transportation company is outsourced, they might have their own rates and costs calculator. Hence, these changes can introduce new sets, parameters or even variables that result in new constraints or in a different objective function.

With the model developed in this chapter one already has a head start to deploy a HRS network in any scenario. It has the potential to be adapted in multiple regions and road networks, where the network designer needs to only do slight changes to adapt it.

5. Case study: data collection and treatment

This chapter presents a case study that applies the optimization model developed in Chapter 4 to address the specific context of hydrogen transport and distribution in Portugal. The primary objective of this case study is to establish an initial network of Hydrogen Refueling Stations along the main Portuguese highways, with a strategic focus on accommodating hydrogen-powered heavy-duty vehicles. By doing so, this infrastructure development aims to lay the foundation for a thriving hydrogen economy in Portugal while contributing to sustainable transportation solutions and reducing greenhouse gas emissions within the industrial context.

The chapter is structured as follows:

- Section 5.1. provides an overview of the case study, detailing the objectives and scope of the analysis.
- Section 5.2. delves into the data collection process, sources, and methodology employed in this study.
- In Section 5.3. the limitations of the data used and any constraints that might influence the applicability of the findings are discussed.
- Section 5.4 is a concise summary of the chapter.

5.1. Case Study Description

In this section, a case study that applies the optimization model developed in Chapter 4 to the context of Portugal is presented. The primary objective of this case study is to identify suitable locations for the construction of HRSs along the main Portuguese highways. Additionally, the model will determine the optimal GH₂ production sites, out of the projected ones, for transporting hydrogen to these HRSs, as well as the routes and quantities to be transported between them. The overall aim of this study is to establish an initial network of HRSs specifically designed for the Portuguese highways, considering the absence of such infrastructure at present. This infrastructure development is intended to promote the emergence of a hydrogen economy in Portugal, with a specific focus on the utilization of hydrogen-powered heavy-duty vehicles. Therefore, HRSs need to be strategically placed to fulfill a future demand of these vehicles.

The optimization model developed in Chapter 4 provides a systematic framework for decision-making regarding the placement of HRSs. By leveraging relevant factors such as existing service stations, existing GH₂ production sites, and potential demand, the model will generate recommendations on the optimal locations for HRSs deployment. These recommendations will be critical in establishing a well-distributed network that caters to the needs of hydrogen-powered heavy-duty vehicles across the Portuguese highway system. Additionally, the model enables the estimation of the costs associated with this initial HRS deployment.

To estimate the future demand for hydrogen fuel, a percentage for market penetration of hydrogen-powered heavy-duty vehicles will be considered. This approach allows to project the potential market share and identify the required number of HRSs to meet the future demand

effectively. By integrating these projections into the optimization model, the number and strategic placement of HRSs needed to serve the targeted market can be addressed.

It is important to note that this case study will focus exclusively on the main Portuguese highways. These highways, forming the backbone of the country's transportation infrastructure, provide a strategic starting point for the establishment of an initial HRS network. By concentrating our efforts on these key transportation arteries, the impact of the hydrogen economy on long-haul transportation can be maximized and effectively serve a wide range of regions and destinations.

Portuguese highways are operated under a concession system, where private entities are granted the responsibility to manage and maintain these crucial road networks. One prominent company involved in this concession model is Brisa, which plays a significant role in the management and operation of several major highways in Portugal. To facilitate data collection and treatment this case study will exclusively focus on highways that are either fully or partially concessioned to Brisa, since they happen to be the main Portuguese highways that can be seen in Figure 10⁶.

In conclusion, this case study represents a pivotal step in the development of a hydrogen economy in Portugal. By applying the optimization model to determine the optimal locations for HRSs, the foundation for a comprehensive hydrogen infrastructure network can be achieved. Through the promotion of hydrogen-powered heavy-duty vehicles, it is possible to drive sustainable transportation solutions and contribute to the reduction of greenhouse gas emissions within the Portuguese industrial context.



Figure 10: Portuguese highways concessioned to Brisa

⁶ Figure retrieved from Brisa's website (Brisa, n.d.).

5.2. Data collection and treatment

This section presents the data that will be applied in the model and therefore used to solve this case study. The data collected encompasses a diverse range of sources. While more technical data about the HRSs and tube trailers come from scientific articles, other data such as the traffic in Portuguese highways and capacities of the various production plants were collected through available online reports and in the H2 projects' websites. Also, to ensure accuracy, informal verification was conducted with professionals working in the hydrogen industry wherever possible.

5.2.1 Characterization of Production Sites and Service Station Locations

In this section, it's provided a comprehensive characterization of the potential production sites and service station locations to be considered in the establishment of the hydrogen infrastructure network for the Portuguese highways.

5.2.1.1. Production Sites

Since the ultimate goal of this work is to contribute to the decarbonization of Portugal, only green hydrogen will be considered when applying the model.

Currently, GH2 production projects in Portugal are still in development. Even though they are not completed, these will be the production sites considered for the model. These production sites vary in terms of their geographical location, production capacity, and associated costs. It is essential to evaluate these factors to determine the optimal combination of production sites that can meet the projected demand for hydrogen fuel. Notice that there's a high concentration around the center and south region of Portugal and a lack of production projects in the north region.

Table 1 summarizes the characteristics of each GH2 production site.

Table 1: Production sites characteristics

Location	Power Capacity (MW)	Production Capacity (H2 kg/day)	Cost (€/kg)
Sines	100	50000	8
Évora	0.42	165	12
Setúbal	12	3240	11
Nazaré	40	20000	10

Note: Values were retrieved and estimated based on: Hydrogen and Fuel Cell Technologies Office (2018); Fusion Fuel Green plc (2023); Santos (2022); Nazaré Valley (n.d.); Ambiente Online (n.d.)

The case study will be approached on a monthly basis. To convert the daily production capacity into a monthly equivalent, a 30-day month will be considered.

5.2.1.2. Service stations

Service stations will act as possible locations to build HRSs. Currently Portuguese highways are well equipped with several service stations. Next, it is presented Table 2 with the highways considered for this case study and their respective service stations. These are the highways concessioned to Brisa, with information publicly available about service stations located there.

Note that each location corresponds to two service stations, one for each direction of the highway (Brisa, n.d.).

Table 2: Service Station Locations per Highway

Highway Name	Service Station Location
A1	Aveiras
	Santarém
	Leiria
	Pombal
	Mealhada
	Antuã
	Gaia
A2	Seixal
	Palmela
	Alcácer do Sal
	Grândola
	Aljustrel
A3	Serviço de Almodôvar
	Coronado-Trofa
A4	Barcelos
	Águas Santas
A5	Penafiel
	Oeiras
A6	Vendas Novas
	Montemor-o-Novo
	Estremoz
A9	Crel Sul
	Crel Norte
A13	Salvaterra
	Montijo

To compute transportation costs, which are a crucial part of the model's objective function, it is essential to know the distances between these production and consumption locations. Appendix A has the complete detailed list of service stations and production sites with their coordinates and a location excel code associated. This code was used to simplify the process of creating a distance matrix through an automated process using excel VBA. The first module creates a function that uses Bing Maps API (Microsoft Corporation, n.d.) to retrieve the distance between an origin-destination coordinates pair. Then, a second module creates a Macro to automatically run through all the matrix cells and get the distances between all points. The reader can see the distance matrix in appendix B.

5.2.2. Demand Forecast

The demand estimation process of this model is intimately related to three crucial factors: the number of vehicles that currently cross the highways, the predicted percentage of market penetration of Hydrogen fueled heavy-duty vehicles and the fuel economy of such vehicles.

Regarding the number of vehicles that cross the highways, there's publicly available data containing the total number of vehicles that cross each section of each highway on a monthly basis (IMT, 2023). To better address future hydrogen needs, and since we have detailed information, the case-study highways were arbitrarily divided into demand zones that were similar in extension and in the number of service stations incorporated within those zones. Note that the number of vehicles used will be a monthly average of the total vehicles that crossed each part of the highways, from January 2022 until March 2023.

Since this work primary interest is in the number of heavy-duty vehicles, the percentage of trucks and buses that were in circulation in 2021 (0,079% and 0,297% respectively) is applied to the total number of vehicles (Pordata, 2022). In Appendix C, one can see in a more detailed manner how the demand zones are organized, that is, which sections of highway belong to each zone. Table 3 summarizes the monthly vehicles, the extension and service stations included in each demand zone. Please remember that most of the time a service station location actually represents 2 service stations, one for each direction of the highway. Also, note that the extension is an approximate estimate of the real extension since the data was not clear about the coordinates of each highway section limits.

Table 3: Demand zones with respective number of heavy-duty vehicles in circulation

Highway	Demand Zone	Average Monthly No. of Vehicles (HT & B)	Extension (km)	Included Service Stations Location
A1	D1	602 & 2273	90	Aveiras; Santarém
	D2	170 & 641	115	Leiria; Pombal; Mealhada
	D3	639 & 2413	90	Antuã; Gaia
A2	D4	336 & 1268	110	Seixal; Palmela; Alcácer do Sal; Grândola
	D5	45 & 170	125	Aljustrel; Almodôvar
A3	D6	444 & 1677	112	Coronado-Trofa; Barcelos
A4	D7	617 & 2331	50	Águas Santas; Penafiel
A5	D8	793 & 2995	25	Oeiras
A6	D9	72 & 271	158	Vendas-Novas; Montemor-o-novo; Estremoz
A9	D10	160 & 605	35	Crel-Norte
A13	D11	29 & 109	80	Salvaterra; Montijo

Note: HT = Heavy trucks; B = Buses.

For the fuel efficiency the truck considered is the one developed by Hyundai, the XCIENT Fuel Cell. This is the reference truck considered for fuel economy since it is the only heavy-duty fuel cell electric model with a proven record of real-world application. It was deployed in several countries such as Switzerland, Germany, Israel, Korea and New Zealand, and has successfully accumulated over 4 million miles so far (Hyundai Motor Group, 2023). This heavy-duty truck has a storage capacity of 31 kg of hydrogen and a tested maximum range of 400km per charge. Therefore, the fuel efficiency used for the calculations is 12.90 km/kg.

The fuel efficiency of buses is around 9.76 km per kg of H₂, according to Pederzoli et al. (2022). These fuel cell buses are already in operation in many European countries. Examples of that are the CaetanoBus buses, part of Toyota Caetano Portugal, that provide public transport in France, Germany, Italy and Spain (Toyota Europe, 2023).

When it comes to the market penetration percentage of hydrogen heavy-duty vehicles, several studies appoint to different directions that vary widely. Two studies that are concise in these predictions are the one done by Wang A. et al. (2021), which considers three scenarios, and the one done by Heid B. et al. (2017).

Even though this work is focused mainly on heavy-duty transportation, it is possible that some light-duty fuel cell vehicles penetrate the market as well. These vehicles have a tough competitor, the EVs market, and might not even have adoption in Portugal at all. As so, three separate scenarios for 2050 will be considered for the case that light-duty fuel cell vehicles have a market penetration of 1%, 10% or 20%, so that the HRSs network can also account for their needs. Notice that, for light-duty vehicles, a fuel efficiency of 181,81km/kg will be used (Toyota Newsroom, 2021). Also, light duty vehicles correspond to 79,43% of total vehicles in Portugal (Pordata, 2022).

Table 4 presents these scenarios that will be used to estimate different demands for each demand zone:

Table 4: Scenarios for % of fuel cell vehicles market penetration

	Scenario					
	A	B	C	D	E	F
Year	2030	2040	2050	2050	2050	2050
MP % (HT + B + LV)	5 + 4	30 + 21	55 + 25	55 + 25 + 1	55 + 25 + 10	55 + 25 + 20

Note: MP= Market Penetration; HT = Heavy trucks; B = Buses. LV = Light-duty vehicles

Finally, the demand can be estimated using the following equation:

$$\begin{aligned}
 & \text{Demand per demand zone (H}_2 \text{ kg/month)} \\
 & = \frac{\text{Monthly No. of vehicles} * \% \text{ of market penetration} * \text{Demand zone extension (km)}}{\text{Fuel efficiency (km / H}_2 \text{ kg)}} \quad (11)
 \end{aligned}$$

This results in the following monthly demand for each scenario:

Table 5: Monthly Hydrogen demand for each demand zone per scenario

Demand Zone	Scenario					
	A	B	C	D	E	F
	Demand (kg/month)					
D1	1048	5661	7549	10559	37641	67733
D2	378	2039	2720	3804	13560	24400
D3	1113	6011	8017	11212	39972	71926
D4	715	3859	5146	7198	25661	46175
D5	109	590	786	1100	3921	7055
D6	963	5198	6932	9695	34562	62192
D7	597	3225	4301	6016	21447	38593
D8	384	2072	2764	3865	13780	24796
D9	219	1183	1578	2207	7868	14158
D10	108	586	781	1093	3896	7010
D11	45	242	322	451	1606	2890
Total	5679	30667	40897	57198	203913	366930

Note: HT = Heavy trucks; B = Buses. LV = Light-duty vehicles. Demands were computed using fuel efficiency values of 12.9, 9.76 and 181.82 km per kg for each vehicle category respectively.

5.2.3. HRSs data

When deploying a network of HRSs, there are costs associated with the construction of the stations themselves, the capital costs. The sizes of HRSs considered for this model are 180kg, 350kg and 500kg.

According to Koleva & Melaina (2021), the capital costs associated with HRSs are estimated to be on average approximately 1.69 million euros. These costs vary widely depending on the construction company, and on the prices of the components. For this study it will be considered the 1.69 million euros of investment for all the HRSs irrespective of their size, since in practice price variations should be very dim between these capacities, validated by professionals in the industry. In order to normalize the capital costs, a lifespan of 20 years is considered (Zhang et al., 2020). Therefore, the normalized capital cost becomes approximately 7042€/month.

One might argue that bigger HRSs allow a faster return on investment, with hydrogen having the price of around 15€/kg in France in 2022 (glpautogas, n.d.). However, the focus of this model is not to achieve profitability but to reduce initial investment on the initial HRSs network rollout.

This way, the normalized capital costs will not serve as a basis for comparing economic viability of different HRS capacities. They will rather serve the purpose of “punishing” the model for choosing to open a HRS, minimizing the initial investment required to fulfill the future forecasted demand.

5.2.4. Tube trailer data

Tube trailers play a crucial role in the transportation of hydrogen, offering a reliable and efficient means of delivery, being the transportation mode considered in the model. This section provides an overview of the key characteristics and parameters associated with tube trailers used for

hydrogen transport at approximately 500 bar. These data will serve as a baseline to essentially estimate the costs associated with the transportation of hydrogen from production plants to refueling stations.

Tube trailers typically utilize diesel as their primary fuel source. The use of diesel enables seamless integration of tube trailers into the existing logistics framework, ensuring smooth distribution throughout the hydrogen supply chain. At the time this section is written, diesel costs around 1,684 €/liter on a Portuguese highway (DGE, n.d.).

The fuel efficiency of tube trailers is an essential factor to consider, as it directly impacts the operational costs and environmental footprint of hydrogen transportation. For the purpose of this study, the fuel efficiency of tube trailers is estimated to be 10.5 mpg which is equivalent to 22.4 l/100km (Tayarani & Ramji, 2022).

To accurately assess the hydrogen operational costs, the HDSAM 3.0 (Hydrogen Delivery Scenario Analysis Model) developed by the Argonne National Laboratory in 2006 is utilized (Argonne National Laboratory, n.d.). The capacities used for this study correspond to the ones used by Shamsi (2021) and can be seen on Table 6 as well as the total operations cost per roundtrip. By leveraging the HDSAM 3.0, a more accurate assessment of the operational costs can be achieved, ensuring the optimization model's reliability.

Table 6: Operational costs per roundtrip per HRS capacity.

Dispensing Rate (kg H2 per day)	180	350	500
Compressed Gas H2 Terminal			
Compressor	2,11 €	2,11 €	2,11 €
Storage	0,57 €	0,57 €	0,57 €
Remainder	0,45 €	0,45 €	0,45 €
Compressed H2 Truck			
Capital Cost	2,96 €	2,25 €	1,90 €
Other O&M	0,29 €	0,35 €	0,33 €
Dispensing at Refueling Station			
Compressor	2,01 €	1,63 €	1,34 €
Storage	0,45 €	0,46 €	0,32 €
Dispenser	0,41 €	0,42 €	0,29 €
Refrigeration	0,47 €	0,47 €	0,35 €
Electrical	0,22 €	0,12 €	0,09 €
Controls/Other	0,73 €	0,42 €	0,30 €
Total	10,68 €	9,25 €	8,04 €

Nevertheless, the way the optimization model is built uses only one value for the operational costs and an average of the three values will be used as the fixed operational costs per roundtrip.

Furthermore, Shamsi et al. (2021) considered a tube trailer transportation capacity of 1042 kg. This value is consistent with the findings of Reddi et al. (2018), who reported that tube trailers can

transport up to 1100 kg of hydrogen at a pressure of 500 bar. Therefore, this study will also consider the value of the former for the tube trailers capacity to transport hydrogen.

By incorporating these up-to-date tube trailer data parameters, the optimization model will be able to effectively estimate hydrogen distribution costs using a 500 bar tube trailer.

5.3. Assumptions and limitations

Throughout this chapter, some assumptions had to be made regarding the data that will be used to run the optimization model. It is important to recognize that these assumptions, while integral to this work, may introduce certain constraints when applying the model's findings in real-world scenarios. This section identifies these possible constraints, outlining the reasons for using these assumptions while proposing ways to overcome them.

Different service stations within the Portuguese highways have different fuel providers. The first assumption that needs to be made is that there is no competition between these players, so that all service stations can be considered as possible locations to place HRSs. The government should push towards policies that ensure cooperation between these entities so that all can benefit from an emerging H2 economy.

Additionally, it's worth noting that the conversion rate for currency stands at 1€ to 0.89\$ (as of July 15th, 2023). This was the rate used to convert public available costs in US dollars.

In what concerns hydrogen production, in alignment with the objectives of this study, the focus has been exclusively on green hydrogen production facilities. Presently, these facilities either remain in the construction phase or exist solely as conceptual projects awaiting implementation. Consequently, the monthly hydrogen output values are derived from the projected production capacities and are supplemented with data sourced from similar projects worldwide. Furthermore, this H2 output as well as its costs are dependent on the available green electricity generated and its price. Despite the inherent volatility of these parameters, for the sake of computational simplicity, they are treated as fixed when executing the optimization model.

Additionally, it's assumed that all hydrogen produced can be allocated to the HRSs network, so that this model has no restrictions in terms of capacity available to promote fuel cell vehicles.

Regarding demand, notice how it uses a percentage of each type of vehicle to calculate the correspondent number of vehicles in that category. That percentage might not be accurate since it represents the fraction of vehicles in all Portugal and not specifically the fraction of vehicles that are in the highways. For example, if 1% of all Portuguese vehicles are trucks, it doesn't mean that 1% of the vehicles in the highways are trucks as well. The lack of public available information makes this assumption necessary. If companies that have the concession of the highway are open to share this information, the results of the model can be more accurate.

Transportation costs do not consider the cost of tolls. Also, due to the lack of precise location data for production plants, a city center approximation was taken as the reference point for calculating distances between these plants and the service stations.

It's important to note that several companies were reached out with the request to provide data that could enhance the credibility of this study. Unfortunately, due to the confidential nature of much of this information, these companies were unable to disclose it.

5.4. Conclusion

In this chapter the case study developed for this master thesis as well as the data used to run the model were presented. Even though data was gathered from multiple international fonts, it will give a good approximation of the total costs related with deploying a HRS infrastructure in Portugal, specially thanks to the informal communication with experts working on the hydrogen industry.

Notice also that this case study only uses data of highways concessioned to Brisa, aiming to test the reliability and validity of the model. With enough resources and data, the case study can be further amplified to include all Portuguese highways concessioned to multiple companies, therefore deploying HRS at a national level.

6. Results and discussion

This chapter presents the results derived from executing the optimization model established in Chapter 4, utilizing the data presented in Chapter 5. It illustrates the optimal configuration of the initial hydrogen refueling station network, designed to minimize investment expenses. Furthermore, it conducts a thorough analysis of the results and the insights that can be taken from such analysis.

The chapter is structured as follows:

- In Section 6.1 a simultaneous evaluation of results across all scenarios within the study is conducted.
- Section 6.2. introduces variations in production costs to observe the corresponding reactions of the optimization model.
- Section 6.3. introduces a sensitivity analysis to study the impact of some parameters that might be volatile in real life.
- Section 6.4. summarizes the main findings and discusses practical implications for policymakers and industry stakeholders.

6.1. Scenarios Analysis

The essence of this study's findings is intimately correlated to the examined scenarios, where the forecasted demand plays a crucial role in dictating the optimal locations and sizes for the HRSs. As such, this chapter initiates with the simultaneous analysis of the results for every scenario. In this way, one can determine which factors have the most significant influence over the costs and the network configuration. This analysis aims to shed light on the interplay between parameters and the resultant implications for an efficient H2 transport and distribution infrastructure.

6.1.1. Facilities Location

To begin the results analysis section, the facilities opened, and their respective location will be examined. This is the core objective of this master thesis optimization model, providing insights on investing capital for the initial deployment of hydrogen refueling stations. These stations are strategically positioned to simultaneously optimize investment costs and meet the forecasted hydrogen demand.

Tables 7 and Table 8 show which production plants and refueling stations are opened for each scenario respectively. Please note that the number notations for production plants and Service Stations' location refer to the python code notation. To see the location of these facilities please go to Appendix D.

Moreover, to offer readers a more tangible comprehension of the spatial distribution, Figure 11 showcases the geographical distribution of production plants and HRSs on a detailed map of Portugal.

Table 7: Production Plants in use per scenario

Production Plant	Scenario					
	A	B	C	D	E	F
Sines	✓	✓	✓	✓	✓	✓
Évora	-	-	-	-	-	-
Setúbal	-	-	-	-	-	-
Nazaré	✓	-	-	-	✓	✓

Before running the model one could already expect it to preferably choose production plants that have the cheapest hydrogen and are simultaneously closer to existing service stations in the demand zones. These are the two objective function parcels that can be “played with” since the costs of opening refueling stations are always dependent on fulfilling the demand for each zone and are somewhat “fixed”. It’s quite interesting to see how the optimization model balances these costs.

Indeed, no scenario uses other than the two cheapest stations. However, some intriguing results require further analysis.

Take scenario A, which opens both production plants in Sines and Nazaré (0 and 3 respectively). No service station in Demand zone D1 is simultaneously the closest to both hydrogen plants. Hence, the model opens service station number 5 of size 0 (s_{5_0}) balancing the cheaper production costs of plant 0 and the cheaper transportation costs from plant 3. A similar thing happens in service station 14 of size 0 (s_{14_0}), which is much closer to Nazaré production plant (3) but also receives hydrogen from Sines’ plant (0). Please refer to table 9 for hydrogen flows between production plants and hydrogen refueling stations.

Interestingly, scenarios B, C, and D only use production plant 0. Since this is the plant with the cheapest hydrogen and most production capacity, this indicates that, from a certain demand point, transportation costs become irrelevant when compared to the difference in production costs from one plant to another. This will be further investigated in the subsequent sections of this chapter. Please remember that production costs were arbitrarily chosen based on production capacities, and they are intimately related to green electricity availability and price, making them a volatile parameter in a real-case scenario.

It’s important to notice that different model runs for the same scenario might cause different HRSs sizes to open in the same service station location. This happens for the lowest demand scenarios when it is not big enough to require the highest capacity HRSs, and because all HRSs have the same capital costs the model just chooses one of the three capacities as long as it’s enough to fulfill demand.

Another insight that can be retrieved is the fact that for scenarios A, B, C, and D only 11 refueling stations are opened. This means that, for all these scenarios, only one station is necessary per

demand zone to fulfill the respective H2 needs. This corresponds to an initial investment of 18.59 million Euros.

Table 8: HRSs Opened per scenario

Variable	Scenario					
	A	B	C	D	E	F
s_4_1	-	✓	-	-	✓	✓
s_4_2	-	-	✓	✓	✓	✓
s_5_0	✓	-	-	-	-	-
s_5_2	-	-	-	-	✓	✓
s_6_2	-	-	-	-	-	✓
s_7_2	-	-	-	-	-	✓
s_8_0	-	✓	✓	✓	-	-
s_8_1	-	-	-	-	-	✓
s_8_2	✓	-	-	-	✓	✓
s_14_0	✓	-	-	-	-	-
s_14_1	-	-	-	-	✓	✓
s_14_2	-	✓	✓	✓	✓	✓
s_15_1	-	-	-	-	-	✓
s_15_2	-	-	-	-	✓	✓
s_16_1	-	-	-	-	-	✓
s_16_2	-	-	-	-	-	✓
s_23_1	-	-	-	✓	-	✓
s_23_2	✓	✓	✓	-	✓	✓
s_24_1	-	-	-	-	-	✓
s_24_2	-	-	-	-	✓	✓
s_26_1	-	✓	✓	✓	-	-
s_26_2	✓	-	-	-	✓	✓
s_29_1	-	-	-	-	✓	✓
s_29_2	✓	✓	✓	✓	✓	✓
s_30_1	-	-	-	-	-	✓
s_30_2	-	-	-	-	✓	✓
s_31_2	-	-	-	-	-	✓
s_33_1	-	✓	✓	-	✓	✓
s_33_2	✓	-	-	✓	✓	✓
s_34_2	-	-	-	-	-	✓
s_37_0	-	✓	✓	✓	-	-
s_37_1	-	-	-	-	-	✓
s_37_2	✓	-	-	-	✓	✓
s_39_0	✓	✓	✓	✓	-	-
s_39_2	-	-	-	-	✓	✓
s_46_0	✓	-	✓	-	-	-
s_46_2	-	✓	-	✓	✓	✓
s_50_2	✓	✓	✓	✓	✓	✓
Total	11	11	11	11	19	31

Note: s_4_1 corresponds to HRS of size 1 located in service station 4 in Python code notation. This is a binary variable that is 1 if this service station is being used. See the correspondent location in Appendix D.

Scenarios E and F require a larger number of HRSs since some of the demand zones have monthly H2 needs higher than the capacity of the largest HRS. Also, these 2 scenarios use once

again production plant 3 since the total demand is higher than the production capacity of plant 0. The model then goes for the second cheapest hydrogen plant, reinforcing the idea that from a certain demand point, the transportation costs are irrelevant.

Table 9: H2 flow (kg) from production plants to Hydrogen refueling stations in kg

Variable	Scenario					
	A	B	C	D	E	F
x_0_5_0	1042	0	0	0	0	0
x_0_8_0	0	2039	2720	3804	0	0
x_0_14_0	1042	0	0	0	0	0
x_0_37_0	0	2072	2764	3865	0	0
x_0_39_0	219	1183	1578	2207	0	0
x_0_46_0	108	0	781	0	0	0
x_0_4_1	0	5661	0	0	10137	10011
x_0_8_1	0	0	0	0	0	9400
x_0_14_1	0	0	0	0	10384	10500
x_0_15_1	0	0	0	0	0	10008
x_0_16_1	0	0	0	0	0	6882
x_0_23_1	0	0	0	7198	0	10500
x_0_24_1	0	0	0	0	0	10500
x_0_26_1	0	590	786	1100	0	0
x_0_29_1	0	0	0	0	10500	10008
x_0_30_1	0	0	0	0	0	10008
x_0_33_1	0	3225	4301	0	6447	10047
x_0_37_1	0	0	0	0	0	9796
x_0_4_2	0	0	7549	10559	15000	14997
x_0_5_2	0	0	0	0	12504	14588
x_0_6_2	0	0	0	0	0	14588
x_0_7_2	0	0	0	0	0	13546
x_0_8_2	378	0	0	0	13546	15000
x_0_14_2	0	6011	8017	11212	15000	14508
x_0_15_2	0	0	0	0	14588	15000
x_0_16_2	0	0	0	0	0	15000
x_0_23_2	715	3859	5146	0	14588	15000
x_0_24_2	0	0	0	0	11073	10175
x_0_26_2	109	0	0	0	3921	7055
x_0_29_2	963	5198	6932	9695	14684	15000
x_0_30_2	0	0	0	0	9378	15000
x_0_31_2	0	0	0	0	0	12176
x_0_33_2	597	0	0	6016	15000	14961
x_0_34_2	0	0	0	0	0	13546
x_0_37_2	384	0	0	0	13780	15000
x_0_39_2	0	0	0	0	7868	14158
x_0_46_2	0	586	0	1093	3896	7010
x_0_50_2	45	242	322	451	1606	2890
x_3_5_0	6	0	0	0	0	0
x_3_14_0	71	0	0	0	0	0
x_3_5_2	0	0	0	0	0	3

Table 9: (Continued from previous page)

Variable	Scenario					
	A	B	C	D	E	F
x_3_8_2	0	0	0	0	14	0
x_3_14_2	0	0	0	0	0	28
x_3_33_2	0	0	0	0	0	39

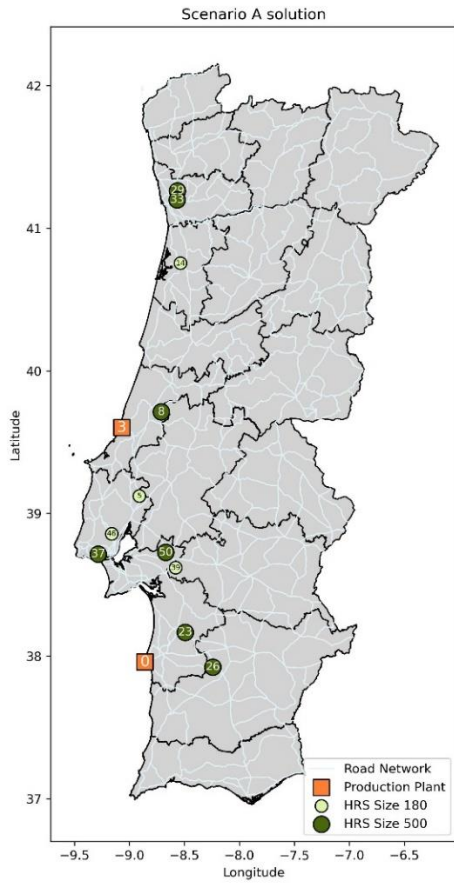
Note: x_0_4_1 corresponds to the flow from production plant 0 to HRS located in service station location 4 with a capacity of 1. See the correspondent codes in Appendix D.

The number of roundtrips for each distribution route is available in Table 10. This table highlights the interesting case of scenario A, where the model optimized the costs by using two roundtrips from different production plants to service station 5 whereas in scenarios B, C, and D it used only the production plant 0 to fulfill this service station, even though it's further away.

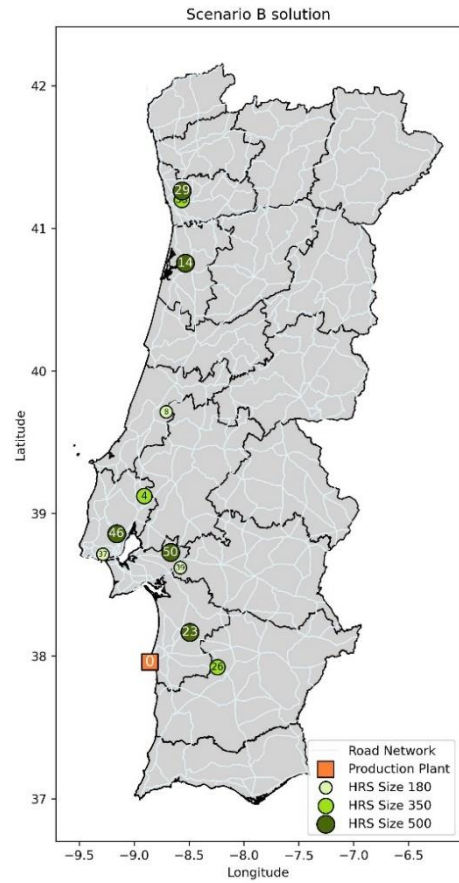
Table 10: Number of roundtrips between production plants and service stations.

Variable	Scenario					
	A	B	C	D	E	F
NR_rounded_0_4	0	6	8	11	25	24
NR_rounded_0_5	1	0	0	0	12	14
NR_rounded_0_6	0	0	0	0	0	14
NR_rounded_0_7	0	0	0	0	0	13
NR_rounded_0_8	1	2	3	4	13	24
NR_rounded_0_14	1	6	8	11	25	24
NR_rounded_0_15	0	0	0	0	14	24
NR_rounded_0_16	0	0	0	0	0	21
NR_rounded_0_23	1	4	5	7	14	25
NR_rounded_0_24	0	0	0	0	11	20
NR_rounded_0_26	1	1	1	2	4	7
NR_rounded_0_29	1	5	7	10	25	24
NR_rounded_0_30	0	0	0	0	9	24
NR_rounded_0_31	0	0	0	0	0	12
NR_rounded_0_33	1	4	5	6	21	24
NR_rounded_0_34	0	0	0	0	0	13
NR_rounded_0_37	1	2	3	4	14	24
NR_rounded_0_39	1	2	2	3	8	14
NR_rounded_0_46	1	1	1	2	4	7
NR_rounded_0_50	1	1	1	1	2	3
NR_rounded_3_5	1	0	0	0	0	1
NR_rounded_3_8	0	0	0	0	1	0
NR_rounded_3_14	1	0	0	0	0	1
NR_rounded_3_33	0	0	0	0	0	1
Total	13	34	44	61	202	358

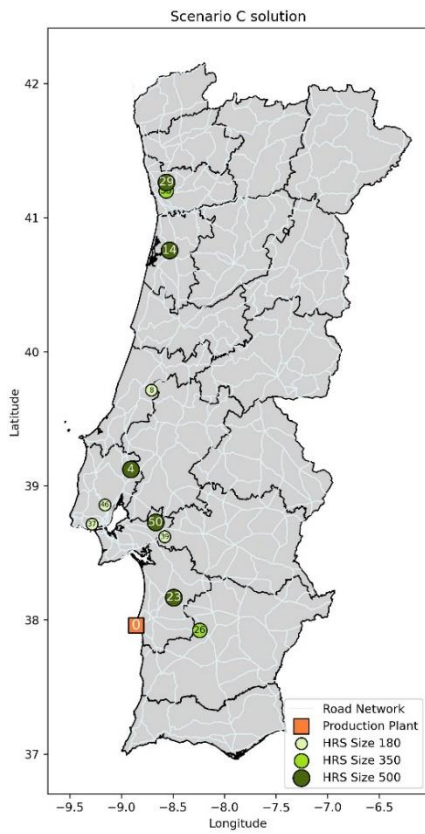
Note: NR_rounded_0_4 = Number of roundtrips value between production plant 0 and service station in location 4. See the correspondent location in Appendix D.



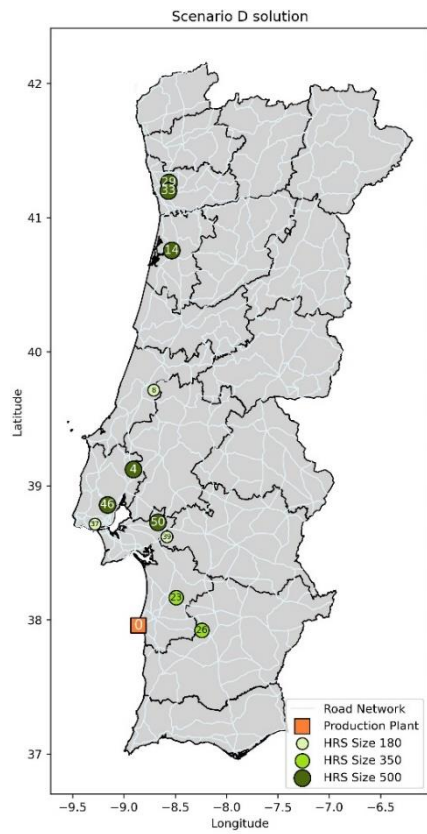
(a) Scenario A



(b) Scenario B



(d) Scenario C



(c) Scenario D

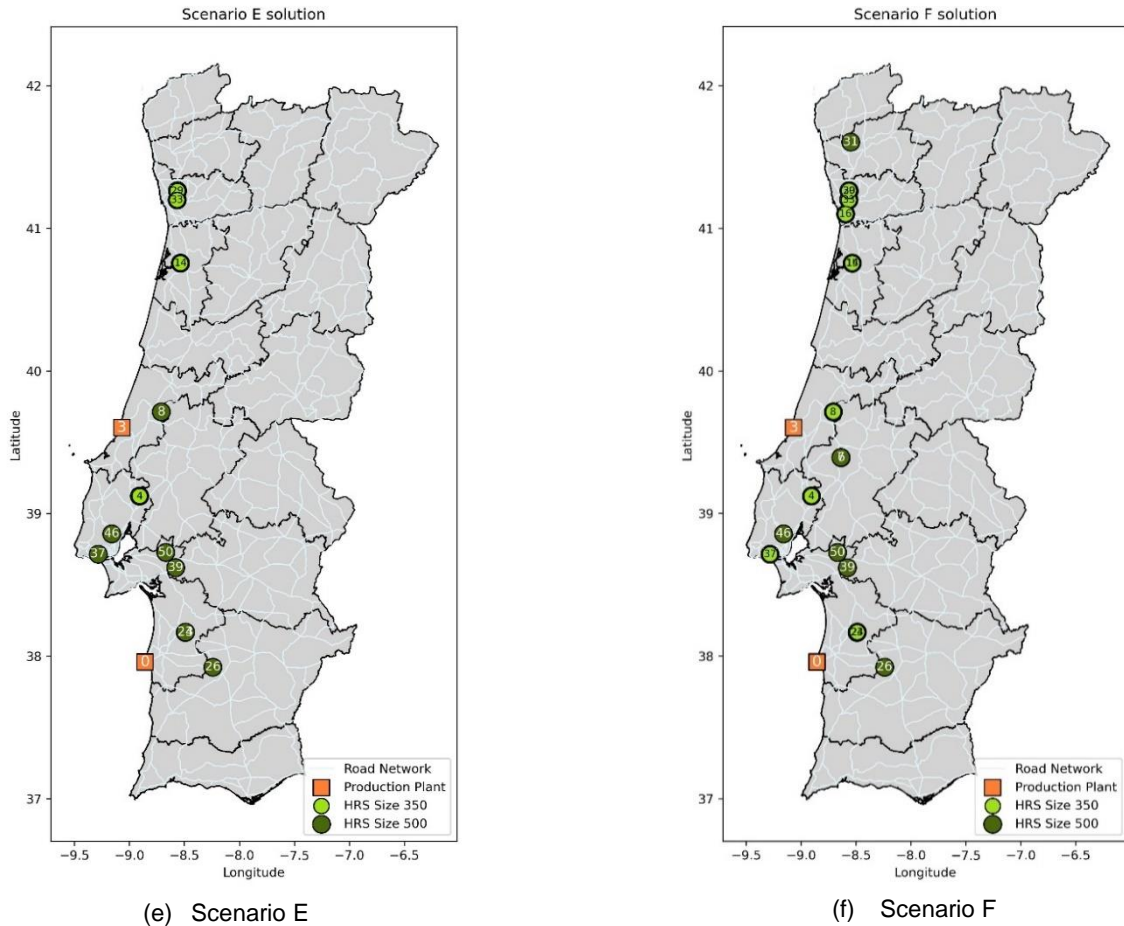


Figure 11: Geographical distribution of HRSs per scenario

6.1.2. Costs

Turning our attention to an essential aspect of this analysis, we delve into the investment costs required for the deployment of the H2 infrastructure, a crucial support for the growing fuel cell vehicle market. Table 11 has the total objective output for each scenario, with the costs minimized, and the amount corresponding to each parcel of this objective function: Production costs, HRSs capital costs, and Transportation costs.

Table 11: Objective function values

	Scenario					
	A	B	C	D	E	F
Total Demand (kg)	5679	30667	40897	57198	203913	366930
Total Costs	125 137 €	329 810 €	413 931 €	547 756 €	1 808 394 €	3 232 437 €
Production Costs	45 586 €	245 328 €	327 168 €	457 600 €	1 631 340 €	2 935 564 €
HRSs CC	77 462 €	77 462 €	77 462 €	77 462 €	133 798 €	218 302 €
Transportation Costs	2 089 €	7 020 €	9 301 €	12 694 €	43 256 €	78 571 €

To conduct a more comprehensive analysis of total costs, Table 12 provides a per kilogram representation, while Figure 12 offers a visual insight into their trends. These also include capital costs, production costs, and transportation costs. This gives the possibility to examine the

hypothesis that the model considers transportation costs irrelevant beyond a certain demand level.

Table 12: Costs per kg of demand

Scenario	TC/kg	PC/kg	CC/kg	Total Costs/kg
A	0,37 €	8,03 €	13,64 €	22,04 €
B	0,23 €	8,00 €	2,53 €	10,75 €
C	0,23 €	8,00 €	1,89 €	10,12 €
D	0,22 €	8,00 €	1,35 €	9,58 €
E	0,21 €	8,00 €	0,66 €	8,87 €
F	0,21 €	8,00 €	0,59 €	8,81 €

Note: TC = Transportation costs, PC = Production Costs, CC = Capital costs

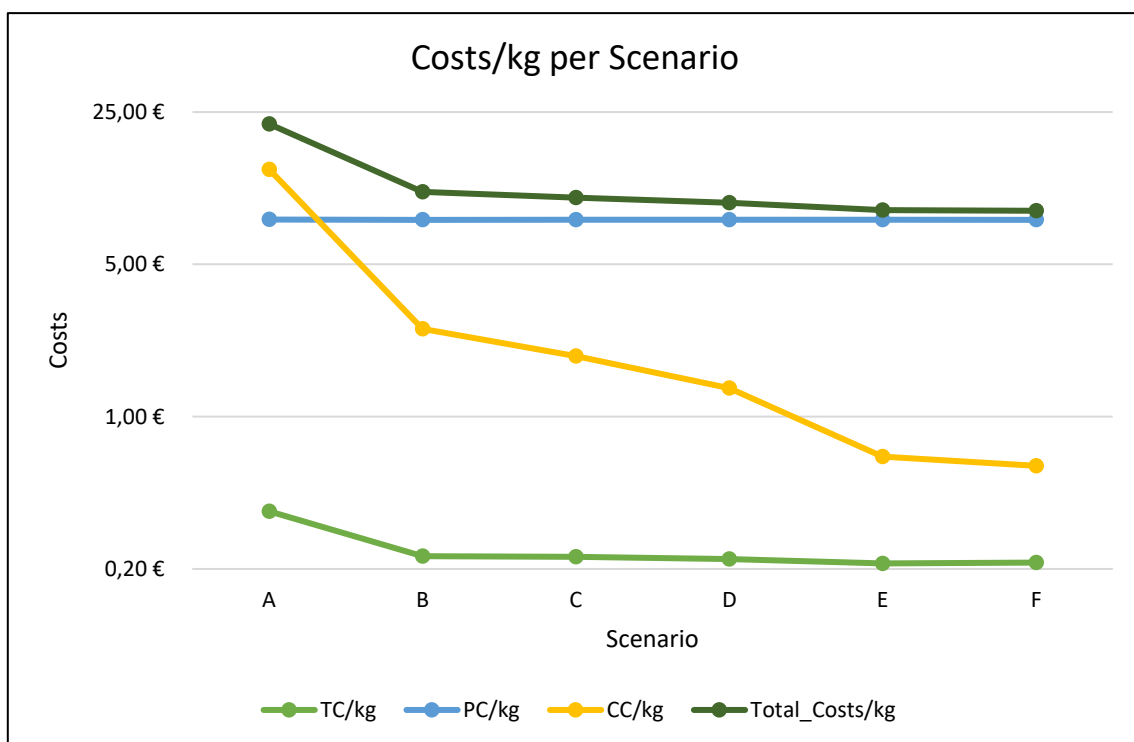


Figure 12: Costs per kg for each scenario

The first insight that pops up from observing the cost trends is that the total costs gradually get closer to the production costs as demand grows. This happens because transportation costs rapidly go to as low as 0.23€ per kg of H₂ distributed and capital costs also have a steep fall with higher demand. Higher demand allows the use of full truck loads and the use of full tanks of HRSS, making the price per kg more optimal by taking advantage of economies of scale.

For the end customer, this means that a higher market penetration of fuel cell vehicles will translate to lower hydrogen prices, which can go almost as low as the average production cost of the hydrogen being distributed.

6.2. Inversing production costs

In this section, the model was tested with the production costs in inverse order. This means that now the production costs are lower for lower production capacity plants, as opposed to what was originally arbitrarily chosen.

This procedure aims to test the model behavior when choosing between lower production costs or lower transportation costs for the cases where it's not simultaneously possible. Table 13 shows the new overall costs for this new set up and Table 14 shows the suppliers opened for each scenario.

Table 13: Costs table for inversed production costs

	Scenario					
	A	B	C	D	E	F
Total Demand (kg)	5679	30667	40897	57198	203913	366930
Total costs	126 231 €	379 480 €	483 413 €	648 847 €	2 286 424 €	4 180 842 €
Production Costs	47 021 €	296 919 €	399 120 €	562 160 €	2 131 094 €	3 924 248 €
HRSs CC	77 462 €	77 462 €	77 462 €	77 462 €	133 798 €	218 302 €
Transportation Costs	1 748 €	5 099 €	6 831 €	9 225 €	21 533 €	38 292 €

Table 14: Production plants opened per scenario for inverse production costs

Production Plant	Scenario					
	A	B	C	D	E	F
0	-	-	-	-	-	-
1	✓	✓	✓	✓	✓	✓
2	✓	✓	✓	✓	✓	✓
3	✓	✓	-	-	✓	✓

With these new parameters' values, it's natural that the total costs are higher. This happens since the lowest H2 cost production plant doesn't have enough capacity to fulfill all demand. It's once again interesting to see that for scenarios A and B the model opens production plants 1, 2, and 3 and for scenarios C and D, it only opens plants 1 and 2. It's only when plants 1 and 2 don't have enough capacity that plant 3 is used once again. Notice how, this time, plant 0 is not used in any of the scenarios.

From scenario B to scenario C, it stops using plant 3 even though it's closer to some service stations, using only the 2 cheapest production plants. This reinforces the idea that there's a demand threshold where the model chooses lower production costs even if transportation costs are higher.

6.3. Sensitivity Analysis

Sensitivity analysis is a vital tool for understanding how changes in individual variables impact overall outcomes. By systematically altering these critical variables while keeping others constant, the aim is to uncover their distinct influences on cost dynamics.

In this section, a sensitivity analysis is performed to investigate the effects of varying production costs and fuel price on the total costs within this hydrogen refueling infrastructure optimization model. These two parameters are the most volatile ones, hence are the ones that require further analysis of their impact. Production capacity is also somewhat unstable but it's big enough so that the changes wouldn't impact the most realistic scenarios A, B, and C. These are the scenarios in which this sensitivity analysis will take place.

This analysis enables the identification of scenarios sensitive to these changes and enhances decision-making by providing insights into potential cost implications under different conditions. This way, the ultimate goal of this sensitivity analysis is to provide information to future decision-makers to improve decision-making strategies in the context of sustainable energy infrastructure planning.

6.3.1. Fuel price's impact

The first parameter varied for this sensitivity analysis is the fuel price. Table 15 shows its impact on the total costs.

Table 15: Fuel price sensitivity analysis

FP Δ	Scenario	Total Costs Δ	Scenario	Total Costs Δ	Scenario	Total Costs Δ
-15%		-0,24%		-0,31%		-0,32%
-10%		-0,16%		-0,20%		-0,22%
-5%	A	-0,08%	B	-0,10%	C	-0,11%
5%		0,08%		0,10%		0,11%
10%		0,16%		0,20%		0,22%
15%		0,24%		0,31%		0,32%

Note: FP = Fuel Price

The first thing to notice is that symmetric changes in the fuel price cause symmetric changes in the overall costs. This suggests that the same routes are opened irrespective of the fuel price.

The second insight is that, as demand grows between scenarios, so does the impact of a change in the fuel price. This makes sense since the same number of refueling stations are opened, they just require more roundtrips to distribute enough hydrogen to fulfill the demand. Having the same capital costs but a higher number of round trips, it's natural that the transportation costs have a higher impact on the total costs generated. Nevertheless, this impact remains relatively low so changes in fuel price shouldn't be a big concern when developing a HRSs infrastructure.

6.3.2. Production costs' impact

The second parameter analyzed is the production costs. Table 16 shows its impact on the total costs for the same % changes used before.

Similar insights and conclusions can be drawn from this table as the ones from the fuel price fluctuations. However, this time the impact on the total cost is much higher. This was already expected from the previous analysis done in this chapter, nevertheless, it's interesting to see

that a relatively small increase in production costs will cause a significant increase in the total costs of this HRSs network.

Table 16: Production costs sensitivity analysis

PC Δ	Scenario	Total Costs Δ	Scenario	Total Costs Δ	Scenario	Total Costs Δ
-15%		-5,46%		-11,16%		-11,86%
-10%		-3,64%		-7,44%		-7,44%
-5%	A	-1,82%	B	-3,72%	C	-3,95%
5%		1,82%		3,72%		3,95%
10%		3,64%		7,44%		7,90%
15%		5,46%		11,16%		11,86%

Note: PC = Production costs

This analysis stresses the importance for network designers to find and use cheap H2 producers when developing the H2 network, more important as demand grows since total costs tend to meet production costs as seen in the previous analysis.

6.4. Conclusion

In this section, the critical insights drawn from this chapter are presented, which not only inform our understanding but also provide valuable guidance for stakeholders in the hydrogen infrastructure domain.

6.4.1. Main findings

Summarizing the findings:

- From a certain demand point, the study developed demonstrates a preference for selecting the most cost-effective production plants, even if this choice leads to increased total transportation costs. Economies of scale allow a steep reduction in the transportation costs per kilogram of H2, making them neglectable when compared to other costs per kilogram. Hence the model stops using the production plants that are closer to service stations, preferring to use the ones where production is cheaper.
- With the growth of demand, the price per kilogram of hydrogen experiences a notable decline, nearly aligning with the production cost. This price reduction fosters the adoption of fuel cell vehicles, creating a positive feedback loop.
- The robustness of these findings was reinforced through testing with production costs in reverse order, further enhancing their credibility.
- A sensitivity analysis was performed, revealing that while fluctuations in diesel fuel prices have a limited impact on total costs, variations in production costs significantly influence the monthly expenses of the hydrogen refueling station network in the three most realistic scenarios.

6.4.2. Managerial key Insights

Turning the attention to practical implications for policymakers, industry stakeholders, and investors interested in advancing hydrogen infrastructure, now some practical implications drawn

from this chapter are presented. These aim to advise each involved entity on the best practices to develop a hydrogen economy regarding the transportation sector, in the most efficient way, and could only be achieved resorting to the developed model. The model serves as an effective tool for hydrogen infrastructure network designers, offering valuable insights into cost-efficient configurations. This model serves as a solid basis for a network designer that has access to even more detailed and informed real-world data.

- Industry stakeholders and investors are advised to consider Scenario D when making initial investments in refueling stations. This scenario accounts for the maximum demand achievable with the same initial capital costs. While initial market penetration might not immediately meet expectations, this approach ensures infrastructure readiness to support potential exponential growth in fuel cell vehicles on Portuguese highways.
- The results advocate for a proactive approach by policymakers, focusing on both infrastructure development and the promotion of fuel cell vehicle usage. Greater market penetration correlates with lower costs for end consumers, emphasizing the importance of policies that foster fuel cell vehicle adoption.
- Efforts should be directed towards reducing production costs. Strategies could include the development of projects that capitalize on economies of scale, investments in electrolysis and hydrogen storage technologies research and development, and the implementation of policies that incentivize and subsidize green hydrogen production.

In conclusion, this analysis not only enriches a comprehension of hydrogen infrastructure dynamics but also provides actionable insights to shape informed decisions and strategies for a sustainable and economically viable hydrogen future in Portugal.

7. Conclusions and Future Research

This chapter summarizes the main takeaways from this Master Thesis dissertation project. It presents a recap of all chapters and the key insights that can be retrieved from this project. Furthermore, it presents limitations of the work developed as well as future research suggestions.

It is structured as follows:

- Section 7.1. presents a concise summary of what was developed throughout the Master thesis.
- Section 7.2. describes the limitations felt, mainly when applying the optimization model.
- Section 7.3. provides guidance for future research regarding the topic of HRSs network development.

7.1. Central Conclusions

The main objective of this work, to develop and apply an optimization model to identify the optimal locations for HRSs in Portuguese highways considering only the use of green hydrogen, was successfully achieved. This goes in line with the fit for 55 goals, the hydrogen strategy for a Climate-Neutral Europe, and the Portuguese objective to decarbonize the transportation sector in the country.

As described in Chapter 2, hydrogen is a clean and versatile energy carrier with a lot of potential uses, and the use of fuel cell vehicles is one of them. Portugal can follow the example of the current biggest hydrogen players in Europe by applying this model and deploying a hydrogen refueling station network, hence facilitating the adoption of this type of vehicles that use green hydrogen as fuel.

This dissertation took the Portuguese Hydrogen National Strategy, EN-H2, as the guide for its objectives and development of the case study. In fact, this document predicts that by 2030 between 50 to 100 refueling stations are built. As of now, Portugal stands far from this objective, having only deployed 1 refueling station. This dissertation can accelerate and facilitate the progress towards this goal by maximizing the benefits from an investment in HRSs across the main Portuguese highways.

The EN-H2 also describes several ongoing green hydrogen production projects. The case study developed capitalizes on these projects and uses them as possible fonts of green hydrogen to support the HRS network.

The generic model developed in Chapter 4 to solve the case study is both a GIS and a mathematical optimization model, described in depth in Chapter 3. After applying it to the case study, it was proven that it can be easily adapted to different regions and available data.

Results confirmed Lahanoui et al. (2017) findings: achieving economies of scale is of huge importance in order to reduce transportation costs. In fact, further in-depth analysis showed that,

as demand grows, the costs of deploying and maintaining a HRSs network converge to production costs.

Since Sines is the Portuguese “mega production project”, efforts should be made to achieve its completion and reducing its production costs so that H2 fuel is available at low prices and large quantities.

Simultaneously it is crucial that policy makers act in a way that promotes the wide adoption of fuel cell heavy-duty vehicles, promoting demand growth at a national level. It is crucial that the deployment of the HRSs infrastructure is associated with a high demand increase so that hydrogen prices can go as low as the production costs. This way all stakeholders can benefit from this clean energy transition.

7.2. Work limitations

The limitations felt throughout the elaboration of this work were mainly concerned with acquiring real-world data that accurately represents the Portuguese case study. This comes from the fact that most of this information is confidential, and companies are, rightly so, reluctant to share it.

This implied the simplification of some parameters such as the capital costs of building a hydrogen refueling station and the operational costs associated with the loading and unloading of tube trailers with hydrogen.

Other data that was also simplified, as previously explained in chapter 5, is the total traffic for each category of vehicles across the Portuguese highways. Since demand is estimated based on these parameters it is crucial that a real-world implementation of this model tries to increase the accuracy of this information as much as possible.

Nevertheless, the credibility of the sources used and the informal talks with experts of the hydrogen industry give a solid level of trust for the results presented. The network developed and the total costs presented should be a close approximation to a real case scenario.

In what concerns the model itself, one could argue that VRP should also be used to calculate routes and further optimizing the optimization costs. This is a possible future line of research that can be explored to expand the proposed model.

The model assumes that there can only be one station per type per service station. This assumption comes from the paper that inspired this work by Shamsi et al. (2021). Putting a limitation to the number of HRS that are built in each service station simplifies the resolution of the problem at hand, provides a more realistic case study and can be easily changed or adapted to other applications.

One limitation of the model is that it does not account for the initial investment in tube trailers within the cost function. The model assumes that if multiple roundtrips are required between the same two points, the same truck can perform these trips consecutively without considering the additional time required for each trip.

It is important to note that the model is intended for a one-time application. If there are significant fluctuations in the demand zones utilized, the model's solution may not be suitable for real-life implementation. To mitigate this limitation, as done in the present study, it is advisable to use an average annual demand to minimize the potential discrepancies between the model's output and real-world requirements.

7.3. Future Work

The generic model conceived provides a solid basis for more complex implementations. Future work should use this dissertation as a basis for a more complex implementation, one that has access to diverse information including all country highways, their traffic and parameters associated with the model. A partnership between government and private entities would be perfect to provide a real case scenario, adapting this model and providing results and insights that can support the implementation of a HRSs in the Portuguese highways network.

Future research should also focus on the best policies to implement so that there's an exponential growth in the hydrogen fuel cell heavy-duty vehicles market, being trucks or passenger buses.

Furthermore, this dissertation can serve as inspiration to develop models to deploy HRS network at the city center level, specially applied to the case of Portugal. This urban network requires different ways to estimate future demand and different policies and incentives to promote a different hydrogen fueled market, more focused on passenger transportation. The model developed in chapter 4 and papers explored in chapter 3 can be a good start for this research. The major Portuguese cities such as Lisbon and Porto should follow the example of Paris, Madrid and other big European cities where fuel cell vehicles are being implemented in a large scale.

To conclude, the use of hydrogen as a clean energy is still in the early stages of its adoption. There's a need for continuous research in technologies and policies to reduce costs associated with each stage of the hydrogen supply chain. The use of fuel cell vehicles is no different and is still in its infancy.

In Portugal, efforts should be made to leverage this country unique position and advantage point regarding clean energies. Urgent action is required to shift from fossil fuels to green energy sources, and this transition is linked to advancements in technology. Research into renewable energy sources is crucial to facilitate this critical transition. Hydrogen, as a versatile energy carrier, offers the potential to expedite this shift. Hence, it is evident that investing in hydrogen research is imperative to meet the evolving demands of our progressive society.

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Appendix A

A.1. Locations' codes and coordinates

Excel Code	Coordinates	Location description
i	37.958856301151286, -8.857204665042408	Fábrica de produção de Hidrogénio em Sines
ii	38.57301237000906, -7.9144461334057175	Fábrica de produção de Hidrogénio em Évora
iii	38.5267030126743, -8.893214894918907	Fábrica de produção de Hidrogénio em Setúbal
iv	39.60186814811712, -9.06914809276097	Fábrica de produção de Hidrogénio em Nazaré
1A	39.12246567258405, -8.908075296018845	Área de Serviço de Aveiras, sentido Lisboa-Porto
1B	39.12390752983834, -8.908611420161737	Área de Serviço de Aveiras, sentido Porto-Lisboa
2A	39.39192932822791, -8.637163000302726	Área de Serviço de Santarém, sentido Lisboa-Porto
2B	39.3934507484453, -8.640728900997388	Área de Serviço de Santarém, sentido Porto-Lisboa
3A	39.712711180392034, -8.709498450655124	Área de Serviço de Leiria, sentido Lisboa-Porto
3B	39.71244631912838, -8.711766825278088	Área de Serviço de Leiria, sentido Porto-Lisboa
4A	40.01234499528875, -8.599124296881444	Área de Serviço de Pombal, sentido Lisboa-Porto
4B	40.014456303999594, -8.601233216169597	Área de Serviço de Pombal, sentido Porto-Lisboa
5A	40.33342633471752, -8.492540823819043	Área de Serviço de Mealhada, sentido Lisboa-Porto
5B	40.33159469956702, -8.493395797485288	Área de Serviço da Mealhada, sentido Porto-Lisboa
6A	40.75606705251977, -8.534953079073412	Área de Serviço de Antuã, sentido Lisboa-Porto
6B	40.75559695388667, -8.536898418339973	Área de Serviço de Antuã, sentido Porto-Lisboa
7A	41.10142731898786, -8.597241677896044	Área de Serviço de Gaia, sentido Lisboa-Porto
7B	41.101391750299506, -8.599364412526146	Área de Serviço de Gaia, sentido Porto-Lisboa
8A	38.62323699519944, -9.1342864753174	Área de Serviço do Seixal, sentido Lisboa-Algarve
9A	38.58479682797637, -8.930294498553277	Área de Serviço de Palmela, sentido Lisboa-Algarve
9B	38.585926699861915, -8.929127004281591	Área de Serviço de Palmela, sentido Algarve-Lisboa
10A	38.51549741584524, -8.58643268707771	Área de Serviço de Alcácer do Sal, sentido Lisboa-Algarve
10B	38.51602280022585, -8.584015388346302	Área de Serviço de Alcácer do Sal, sentido Algarve-Lisboa
11A	38.16661772489678, -8.492283586292437	Área de Serviço de Grândola, sentido Lisboa-Algarve
11B	38.167764661655966, -8.490680618910892	Área de Serviço de Grândola, sentido Algarve-Lisboa
12A	37.9235733946184, -8.243839689783414	Área de Serviço de Aljustrel, sentido Lisboa-Algarve
12B	37.92383887535243, -8.24133346602292	Área de Serviço de Aljustrel, sentido Algarve-Lisboa
13A	37.53590163228451, -8.184358847084495	Área de Serviço de Almodôvar, sentido Lisboa-Algarve
13B	37.5359682351498, -8.182846999910852	Área de Serviço de Almodôvar, sentido Algarve-Lisboa
14A	41.26306956406535, -8.56297691783525	Área de Serviço da Coronado-Trofa, sentido Porto-Valença
14B	41.264135770139376, -8.564808129526869	Área de Serviço de Coronado-Trofa, sentido Valença-Porto
15A	41.60465230104594, -8.55002402932731	Área de Serviço de Barcelos, sentido Porto-Valença
15B	41.605047955161524, -8.551139357761722	Área de Serviço de Barcelos, sentido Valença-Porto
16A	41.19998378244484, -8.566530231844359	Área de Serviço de Águas Santas, sentido Porto-Amarante
16B	41.20088073675712, -8.56779400931214	Área de Serviço de Águas Santas, sentido Amarante-Porto
17A	41.23277669471957, -8.178644017194502	Área de Serviço de Penafiel, sentido Porto-Amarante
17B	41.233128324325364, -8.179308647192832	Área de Serviço de Penafiel, sentido Amarante-Porto
18A	38.714856143981805, -9.28439809745019	Área de Serviço de Oeiras, sentido Lisboa-Cascais
18B	38.71337778614847, -9.28607077690454	Área de Serviço de Oeiras, sentido Cascais-Lisboa
19A	38.620609973938976, -8.580275852144789	Área de Serviço de Vendas Novas, sentido Marateca-Caia
19B	38.62242574446779, -8.578085964627736	Área de Serviço de Vendas Novas, sentido Caia-Marateca
20A	38.61730526919787, -8.081351161707733	Área de serviço de Montemor-o-Novo, sentido Marateca-Caia
20B	38.61855525939161, -8.079332910323236	Área de serviço de Montemor-o-Novo, sentido Caia-Marateca
21A	38.799161300878914, -7.660713790058402	Área de Serviço de Estremoz, sentido Marateca-Caia
21B	38.80093182428885, -7.661175075635827	Área de Serviço de Estremoz, sentido Caia-Marateca
22A	38.859706178122266, -9.160784414520952	Área de Serviço da Crel Norte, sentido Alverca-Estádio Nacional
22B	38.85886553021418, -9.160887519325291	Área de Serviço da Crel Norte, sentido Estádio Nacional-Alverca
23A	39.054282497775155, -8.669304803499127	Área de Serviço de Salvaterra, sentido Almeirim-Marateca
23B	39.05293152741024, -8.668281539682075	Área de Serviço de Salvaterra, sentido Marateca-Almeirim
24A	38.72610653437874, -8.670780148831797	Área de Serviço do Montijo, sentido Almeirim-Marateca
24B	38.72677659447588, -8.669209980933733	Área de Serviço do Montijo, sentido Marateca-Almeirim

Appendix B

B.1. Distance Matrix

	i	ii	iii	iv	1A	1B	2A	2B	3A	3B	4A	4B	5A	5B	6A	6B	7A	7B	8A	8A	9A	9B	10A	10B	11A	11B	12A	12B	13A	13B	14A	14B	15A	15B	16A	16B	17A	17B	18A	18B	19A	19B	20A	20B	21A	21B	22A	22B	23A	23B	24A	24B
i	0	169	126	254	173	181	210	211	251	252	290	299	330	343	380	387	422	425	155	142	123	119	91	57	72	94	70	139	144	441	446	486	508	435	438	465	488	165	169	103	133	150	164	196	208	170	164	191	158	144	114	
ii	168	0	99	227	146	154	183	183	224	225	263	272	303	316	353	360	395	398	129	115	97	82	97	125	103	161	105	146	151	414	419	459	481	407	411	438	461	139	142	86	65	41	18	36	48	143	138	164	130	117	86	
iii	125	99	0	158	87	95	128	128	169	170	208	217	248	261	298	305	340	343	46	33	14	39	48	82	105	118	130	163	168	359	364	404	426	352	356	383	406	56	60	33	64	81	94	126	139	61	55	122	88	66	44	
iv	256	230	159	0	110	82	95	88	48	47	78	87	118	131	163	170	206	208	134	153	157	170	183	212	236	249	261	294	299	224	229	269	291	218	221	248	271	125	129	164	195	212	225	257	270	112	107	114	130	142	155	
1A	182	157	96	81	0	8	41	41	81	82	121	129	161	174	211	218	253	255	75	95	94	96	110	139	162	175	187	221	226	271	277	317	339	265	269	296	319	72	76	91	121	138	152	184	196	50	57	56	64	68	81	
1B	174	149	88	110	28	0	69	70	110	111	149	158	189	202	240	247	282	284	68	87	86	88	102	131	154	167	179	213	218	300	305	346	368	294	298	325	347	64	68	83	113	130	144	176	188	42	49	89	56	60	73	
2A	212	186	129	89	70	41	0	1	41	42	80	89	120	133	171	178	213	215	109	128	127	125	139	168	192	205	217	250	255	231	237	277	299	225	229	256	278	105	109	120	150	168	181	213	226	83	90	54	71	98	111	
2B	211	185	129	94	69	41	41	0	42	43	81	90	121	134	171	178	213	216	108	127	126	125	139	168	191	204	216	249	255	232	237	277	299	225	229	256	279	105	108	120	150	167	180	213	225	82	89	53	70	97	110	
3A	253	228	171	48	111	83	84	42	0	2	39	48	79	93	130	137	172	174	150	170	169	167	181	210	233	246	258	292	297	190	196	236	258	184	188	215	237	147	151	162	192	209	223	255	267	124	131	95	112	139	152	
3B	252	226	169	49	110	81	82	41	1	0	40	49	80	93	131	138	173	175	149	168	167	165	179	208	232	245	257	290	295	191	197	237	259	185	189	216	238	145	149	160	190	208	221	253	266	123	130	94	111	138	151	
4A	300	274	217	87	158	129	130	89	49	48	0	9	40	53	90	98	133	135	197	216	215	214	227	256	280	293	305	338	343	151	156	196	218	145	148	175	198	193	197	208	238	256	269	301	250	171	178	142	159	186	199	
4B	291	266	209	78	149	121	122	80	41	40	24	0	64	77	114	122	157	159	188	207	206	205	219	248	271	284	296	330	335	175	180	220	243	169	173	199	222	185	188	200	230	247	293	305	162	169	133	150	177	190		
5A	344	318	261	131	202	173	174	133	93	92	77	53	0	13	50	58	93	95	241	260	259	258	271	300	324	337	349	382	387	111	116	156	179	105	109	135	158	238	241	252	283	300	313	345	270	215	222	186	203	230	243	
5B	331	305	248	118	189	160	161	120	80	79	64	40	19	0	69	76	111	114	228	247	246	244	258	287	311	324	336	369	374	130	135	175	197	123	127	154	177	224	228	239	269	287	300	332	257	202	209	173	190	217	230	
6A	389	363	306	171	247	218	219	178	138	137	122	98	77	58	0	1	43	45	286	305	304	302	316	345	369	382	394	427	432	61	66	106	128	55	58	85	108	282	286	297	327	344	358	390	315	260	262	231	248	275	288	
6B	381	356	299	163	239	211	212	170	131	130	114	90	69	51	19	0	61	64	278	297	296	295	309	338	361	374	386	420	425	80	85	125	147	74	77	104	127	275	278	290	320	337	351	383	307	252	255	223	240	267	280	
7A	423	398	341	205	281	253	254	212	173	172	156	132	111	93	43	42	0	3	320	340	339	337	351	380	403	416	428	462	467	24	30	70	92	78	22	56	79	317	320	332	362	379	393	425	349	294	297	265	282	309	322	
7B	422	396	339	204	280	252	252	211	171	170	155	131	110	91	42	41	0	3	319	338	337	336	349	379	402	415	427	460	465	25	30	70	92	78	22	56	79	316	319	330	361	378	391	424	348	293	295	264	281	308	321	
8A	143	117	32	141	74	82	114	115	155	194	203	234	247	285	292	327	329	0	19	28	56	65	99	123	136	148	181	186	345	351	391	413	339	343	370	392	29	33	51	81	98	112	144	156	44	38	119	185	69	62		
9A	123	98	13	157	86	94	126	127	167	168	207	215	246	260	297	304	339	341	41	0	9	37	46	80	103	116	128	162	167	357	363	403	425	351	355	382	405	51	55	32	62	79	93	125	137	60	54	120	87	64	42	
9B	142	117	32	154	86	94	127	128	168	169	207	216	247	260	297	304	339	342	32	19	0	56	65	99	122	135	147	181	186	358	363	403	425	352	355	382	405	42	46	51	81	98	112	144	156	57	51	114	81	65	61	
10A	86	114	71	200	119	127	155	156	196	197	235	244	275	289	326	333	368	370	101	88	69	0	31	43	66	79	91	125	130	386	392	432	454	380	384	411	434	111	115	48	79	96	109	142	154	116	110	137	103	89	59	
10B	91	98	49	183	102	110	139	140	180	181	219	228	259	272	309	317	352	354	79	66	47	37	0	48	71	84	96	130	135	370	375	415	437	364	367	394	417	89	92	32	62	79	93	125	137	93	88	120	87	73	43	
11A	72	103	106	234	153	161	190	190	231	232	270	279	310	323	360	367	402	405	135	122	103	98	71	0	23	37	49	82	87	421	426	466	488	414	418	445	468	145	149	83	113	130	144	176	188	150	144	171	137	124	93	
11B	58	126	82	211	130	138	166	167	207	208	247	255	286	300	337	344	379	381	112	99	80	75	48	16	0	53	65	98	103	397	403	443	465	391	395	422	445	122	126	60	90	107	121	153	165	127	121	148	114	100	70	
12A	71	106	131	259	178	186	215	216	256	257	295	304	335	348	385	392	427	430	160	147	128	124	96	65	49	0	12	46	51	446	451	491	513	440	443	470	493	170	174	108	138	155	169	201	213	175	169	196	163	149	119	
12B	94	162	119	247	166	174	203	203	244	245	283	292	323	336	373	380	415	418	148	135	116	111	84	53	37	63	0	108	113	434	439	479	501	428	431	458	481	158	162	96	126	143	157	189	201	163	157	184	151	137	106	
13A	145	152	169	298	217	225	253	254	294	295	334	342	373	387	424	431	466	468	199	186	167	162	134	103	87	113	51	0	5	484	490	530	552	478	482	509	532	209	213	147	177	194	207	240	252	214	208	235	201	187	157	
13B	140	147	164	293	212	220	248	249	289	290	329	337	368	382	419	426	461	463	194	181	162	157	129	98	82	108	46	35	0	479	485	525	547	473	477	504	527	204	208	142	172	189	202	235	247	209	203	230	196	182	152	
14A	463	438	381																																																	

Appendix C

C.1. Demand zones

Highway	Subsection	Demand Zone	Extension (km)	Encompassed SS location
A1	Sacavém – S. João da Talha	D1	90	Aveiras; Santarém
	S. João da Talha – Stª Iria de Azóia (A1/IC2)			
	Stª Iria de Azóia (A1/IC2) – Alverca (A1/A9)			
	Alverca (A1/A9) – Vila Franca de Xira II			
	Vila Franca de Xira II – Vila Franca de Xira I			
	Vila Franca de Xira I – Castanheira do Ribatejo			
	Castanheira do Ribatejo – A1/A10			
	A1/A10 – Carregado			
	Carregado – Aveiras de Cima			
	Aveiras de Cima – Cartaxo			
	Cartaxo – Santarém			
A1	Santarém – A1/A15	D2	115	Leiria; Pombal; Mealhada
	A1/A15 – Torres Novas (A1/A23)			
	Torres Novas (A1/A23) – Fátima			
	Fátima – Leiria			
	Leiria – Pombal			
	Pombal – Soure			
	Soure – Condeixa			
	Condeixa – Coimbra Sul			
	Coimbra Sul – Coimbra Norte (A1/A14)			
	Coimbra Norte (A1/A14) – Mealhada			
	Mealhada – Aveiro Sul			
A1	Aveiro Sul – Albergaria (A1/A25)	D3	90	Antuã; Gaia
	Albergaria (A1/A25) – Estarreja			
	Estarreja – Feira			
	Feira – Espinho (A1/A41)			
	Espinho (A1/A41) – Feiteira			
	Feiteira – Carvalhos			
	Carvalhos – Jaca			
	Jaca – Santo Ovídio			
	Santo Ovídio – Coimbrões			
	Coimbrões – Canidelo			
	Canidelo – Afurada			
A2	Afurada – Arrábida	D4	110	Seixal; Palmela; Álcácer do Sal; Grândola
	Ponte 25 de Abril			
	Almada – Fogueteiro			
	Fogueteiro – Coia			
	Coia – Palmela			
	Palmela – A2/A12			
	A2/A12 – Marateca			
	Marateca – A2/A6/A13			
	A2/A6/A13 – Alcácer do Sal			
	Alcácer do Sal – Grândola Norte			
	Grândola Norte – Grândola Sul			
A2	Grândola Sul – Aljustrel	D5	125	Aljustrel; Almodôvar
	Aljustrel – Castro Verde			
	Castro Verde – Almodôvar			
	Almodôvar – S. B. Messines			
	S. B. Messines – Paderne (A22)			
A3	Porto (VCI) – EN 12	D6	112	Coronado-Trofa; Barcelos
	EN 12 – Águas Santas (A3/A4)			
	Águas Santas (A3/A4) – Maia			
	Maia – Santo Tirso			
	Santo Tirso – Famalicão			
Famalicão – Cruz				

	Cruz – Braga Sul			
	Braga Sul – Braga Poente			
	Braga Poente – EN 201			
	EN 201 – Ponte de Lima Sul			
	Ponte de Lima Sul – Ponte de Lima Norte			
	Ponte de Lima Norte – EN 303			
	EN 303 – Valença (Sul)			
	Valença (Sul) – Valença			
	Valença – Fronteira			
	Matosinhos – Sendim			
	Sendim – Guifões			
	Guifões – Custóias			
	Custóias – Via Norte			
	Via Norte – Ponte da Pedra			
	Ponte da Pedra – Águas Santas (A3/A4)			
	Águas Santas (A3/A4) – Ermesinde			
	Ermesinde – Valongo			
A4	Valongo – Campo	D7	50	Águas Santas; Penafiel
	Campo – A4/A41			
	A4/A41 – Baltar			
	Baltar – Paredes			
	Paredes – Guilhufe			
	Guilhufe – Penafiel			
	Penafiel – Castelões (A4/A11)			
	Castelões (A4/A11) – Amarante Poente			
	Amarante Poente – Amarante (Margem Esqª)			
	Amarante (Margem Esqª) – Geraldês			
	A2/A6/A13 – Vendas Novas			
	Vendas Novas – Montemor-o-Novo Poente			
	Montemor-o-Novo Poente – Montemor-o-Novo Nascente			
	Montemor-o-Novo Nascente – Évora Poente			
	Évora Poente – Évora Nascente			
A6	Évora Nascente – Estremoz	D8	158	Vendas-Novas; Montemor-o- novo; Estremoz
	Estremoz – Borba			
	Borba – Elvas Poente			
	Elvas Poente – EN246			
	EN246 – Elvas Central			
	Elvas Central – Elvas Nascente			
	Elvas Nascente – Caia			
	Caia – Fronteira do Caia			
	Estádio Nacional (A5/A9) – Queluz			
	Queluz – A9/A16			
	A9/A16 – Radial da Pontinha			
A9	Radial da Pontinha – Radial de Odivelas	D9	35	Crel-Norte
	Radial de Odivelas – A8/A9			
	A8/A9 – Bucelas (Zambujal)			
	Bucelas (Zambujal) – A9/A10			
	A9/A10 – Alverca			
	Marateca (A2/A6/A13) – Pegões			
	Pegões – Stº. Estevão			
A13	Stº. Estevão – A10/A13	D10	80	Salvaterra; Montijo
	A10/A13 – Salvaterra Magos			
	Almeirim (EN118) – Almeirim (IC10)			
	Atalaia (A13/A23) – Atalaia (EN110)			

Note: SS = Service Station

Appendix D

D.1. Locations' python codes

Python Code (PP & SS)	Coordinates
0	Fábrica de produção de Hidrogénio em Sines
1	Fábrica de produção de Hidrogénio em Évora
2	Fábrica de produção de Hidrogénio em Setúbal
3	Fábrica de produção de Hidrogénio em Nazaré
4	Área de Serviço de Aveiras, sentido Lisboa-Porto
5	Área de Serviço de Aveiras, sentido Porto-Lisboa
6	Área de Serviço de Santarém, sentido Lisboa-Porto
7	Área de Serviço de Santarém, sentido Porto-Lisboa
8	Área de Serviço de Leiria, sentido Lisboa-Porto
9	Área de Serviço de Leiria, sentido Porto-Lisboa
10	Área de Serviço de Pombal, sentido Lisboa-Porto
11	Área de Serviço de Pombal, sentido Porto-Lisboa
12	Área de Serviço de Mealhada, sentido Lisboa-Porto
13	Área de Serviço da Mealhada, sentido Porto-Lisboa
14	Área de Serviço de Antuã, sentido Lisboa-Porto
15	Área de Serviço de Antuã, sentido Porto-Lisboa
16	Área de Serviço de Gaia, sentido Lisboa-Porto
17	Área de Serviço de Gaia, sentido Porto-Lisboa
18	Área de Serviço do Seixal, sentido Lisboa-Algarve
19	Área de Serviço de Palmela, sentido Lisboa-Algarve
20	Área de Serviço de Palmela, sentido Algarve-Lisboa
21	Área de Serviço de Alcácer do Sal, sentido Lisboa-Algarve
22	Área de Serviço de Alcácer do Sal, sentido Algarve-Lisboa
23	Área de Serviço de Grândola, sentido Lisboa-Algarve
24	Área de Serviço de Grândola, sentido Algarve-Lisboa
25	Área de Serviço de Aljustrel, sentido Lisboa-Algarve
26	Área de Serviço de Aljustrel, sentido Algarve-Lisboa
27	Área de Serviço de Almodôvar, sentido Lisboa-Algarve
28	Área de Serviço de Almodôvar, sentido Algarve-Lisboa
29	Área de Serviço da Coronado-Trofa, sentido Porto-Valença
30	Área de Serviço de Coronado-Trofa, sentido Valença-Porto
31	Área de Serviço de Barcelos, sentido Porto-Valença
32	Área de Serviço de Barcelos, sentido Valença-Porto
33	Área de Serviço de Águas Santas, sentido Porto-Amarante
34	Área de Serviço de Águas Santas, sentido Amarante-Porto
35	Área de Serviço de Penafiel, sentido Porto-Amarante
36	Área de Serviço de Penafiel, sentido Amarante-Porto
37	Área de Serviço de Oeiras, sentido Lisboa-Cascais
38	Área de Serviço de Oeiras, sentido Cascais-Lisboa
39	Área de Serviço de Vendas Novas, sentido Marateca-Caia
40	Área de Serviço de Vendas Novas, sentido Caia-Marateca
41	Área de serviço de Montemor-o-Novo, sentido Marateca-Caia
42	Área de serviço de Montemor-o-Novo, sentido Caia-Marateca
43	Área de Serviço de Estremoz, sentido Marateca-Caia
44	Área de Serviço de Estremoz, sentido Caia-Marateca
45	Área de Serviço da Crel Norte, sentido Alverca-Estádio Nacional
46	Área de Serviço da Crel Norte, sentido Estádio Nacional-Alverca
47	Área de Serviço de Salvaterra, sentido Almeirim-Marateca
48	Área de Serviço de Salvaterra, sentido Marateca-Almeirim
49	Área de Serviço do Montijo, sentido Almeirim-Marateca
50	Área de Serviço do Montijo, sentido Marateca-Almeirim

Note: PP = Production Plant; SS = Service Station

D.2. Service Stations capacity python codes

Python Code (HRS Size)	HRS Capacity (kg)
0	180
1	350
2	500