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

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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 paper focusses on the development and application of a model for deploying a hydrogen refueling station network. 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. The model was applied the primary Portuguese highways, considering ongoing green hydrogen production initiatives Findings 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. Insights and practical guidance for policymakers, stakeholders, and industry players in advancing the integration of green hydrogen into the Portuguese energy landscape are provided.

1. Introduction

The transition towards sustainable energy sources and the reduction of greenhouse gas (GHG) emissions have emerged as imperatives in our contemporary world. In this context, green hydrogen (GH2), 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 GH2 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. 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 GH2, and geographic considerations. By doing so, it aims to pave the way for a hydrogen fuel cell market in Portugal.

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 Portugal, a nation that already started projects towards decarbonization.

2. Contextualization

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

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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 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.

The energy transition, from fossil fuels to renewable energy, is an increasingly relevant topic and began to gain attention, especially after 2015 when the Paris agreement was signed by the United Nations. According to it, countries are required to submit Nationally Determined Contributions to reduce the emissions of GHG with the ultimate goal of limiting global warming to well below 2 degrees Celsius above pre-industrial levels.

Later, in 2019, the European Commission draws up the European Green Deal, with 3 main goals: 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 target of reducing GHG emissions by at least 55% compared to 1990 levels.

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. At the same time, the EU elaborates on the Hydrogen Strategy for a Climate-Neutral Europe, aiming to accelerate the development of clean hydrogen and, at the same time, cope with Europe's economic recovery generated by the COVID-19 crisis (European Commission, 2020).

In July 2021, the European Commission proposed a package of legislative proposals “Fit for 55” to revise and update the EU legislation. It was 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.

2.2. Understanding Hydrogen

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. When used as an energy source, hydrogen produces only water vapor as a byproduct, making it an environmentally friendly option.

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. This is because hydrogen is highly reactive and bonds with other elements.

The pursuit of hydrogen energy began way back in 1671 when it was first obtained and isolated by Robert Boyle. However, it wasn’t until 1766 that Henry Cavendish recognized it as a distinct element. 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. 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. This unsustainable technique account for 96% of current hydrogen production. Electrolysis involves 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 GH2, 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 (European Commission, 2021).

Hydrogen is a highly flammable gas that requires special 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 include (Langmi et al., 2022):

- Compressed gas storage when stored in high-pressure tanks or in large-scale cavities such as salt caverns.
- Liquid H2 storage as a cryogenic liquid at -253°C.
- Adsorption that can take the form of physisorption, when hydrogen molecules are adsorbed onto the surface of the hydrogen storage material (HSM), and chemisorption, when hydrogen molecules are chemically bonded to the HSM.

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. Both come with their own set of challenges. 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.

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. The most common H2 applications are: using it as fuel in fuel cell vehicles; using it to produce Powerfuels that can power vehicles in aviation and shipping; using it to produce ammonia, methanol and for petroleum refining; production of electronic components, flat glass, mechanical parts or alter their properties, and it enters the composition of textile fibers. It is also attractive for grid storage and a power generation backup due to its high gravimetric energy, and it is the potential replacement for natural gas systems. Other applications include using it as fuel on the space industry and it's also being studied as a therapeutic gas to treat different diseases.

2.3. Current State of Hydrogen in European Countries

By the end of 2020, it was identified as being in operation 504 H2 production sites, with a total production capacity of 11.4 MT per year. Germany, Netherlands, Poland, Italy, and France alone account for 55% of the total H2 production capacity of the EU, European Free Trade Association (EFTA), and the United Kingdom (UK).

In the European hydrogen market in 2020, 95.7% of total H2 production capacity was represented by the conventional production SMR methods. SMR with CCS (known also as "blue" hydrogen) contributed 0.5% of total hydrogen production capacity. The electrolysis process, which includes the production of H2 from electrolysis as the main product or as a by-product accounted for 3.8% (Hydrogen Europe, 2022). However, it's important to notice that most hydrogen obtained by electrolysis was not from renewable energy.

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, followed by the ammonia industry with 29% (IRENA, 2022).

Hydrogen produced only by water electrolysis 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 capacity by 2030 (Hydrogen Europe, 2022).

2.4. Hydrogen in Portugal

Portugal has made significant progress in building a robust GH2 ecosystem, including developing a national strategy, implementing pilot projects, and collaborating with international partners.

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.

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 GH2 is a key player.

In August 2020 Portugal approves its National Strategy for Hydrogen, EN-H2, aiming to establish Portugal as a leading player in the H2 industry, both in Europe and globally, and at the same time contributing to achieving PNEC 2030 goals (Presidência do Conselho de Ministros, 2020), including: 1,5 % to 2 % of GH2 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, etc. 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.

EN-H2 also predicts the investment on Sine's Industrial Project to 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. There are other GH2 projects ongoing in Portugal in diverse locations such as Évora, Seixal, Setúbal and Nazaré as companies start to realize the potential of an H2 economy.

The design and implementation of a robust and efficient GH2 supply chain in Portugal is critical to achieving large-scale GH2 projects 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.

3. Literature Review

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 challenge arises from the intermittent nature of renewable energy sources used to power the electrolysis process. This variability in its availability makes it challenging to meet H2 demand consistently. Also, limited infrastructure for H2 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.

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.

Geographic Information Systems are powerful tools that integrate spatial data with various analytical models to analyze and visualize information related to geographical locations. 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.

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) reviewed 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.

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 H2 transport and distribution is not without its challenges. 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.

Lahnaoui and colleagues (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.

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 is a vehicle routing problem, which are problems that deal with finding the most efficient routes for a fleet of vehicles to service a set of customers while minimizing travel costs or maximizing resource utilization (Laporte G., 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.

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.

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.

Single objective models:

- Set covering model, which 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.
- Maximal covering location model, initially presented by Church and ReVelle (1974). It aims to maximize the demand coverage for a given number of refueling stations.
- P-median model, developed by Hakimi (1964), where the objective is to reduce the distance between a point and a station with demand as weight.
- Flow-capturing location model (FCLM), which uses traffic flow as a measure of demand, which is calculated dynamically. 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.
- The Flow-refueling location model (FRLM), since previously described FCLM does not account for the scenario where drivers may need to refuel their vehicles more than once during a long journey. Kuby and Lim (2005) proposed an improved model FRLM.

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.

Others: some authors developed some slight deviations from these models presented, 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. 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.

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

4. Model

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 use of existing green hydrogen production sites. 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.

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*1000*50/10 = 50 kg of hydrogen per day.

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. Therefore, this is the transport mode that this generic model considers.

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. A generic output of the model is illustrated in Figure 1.

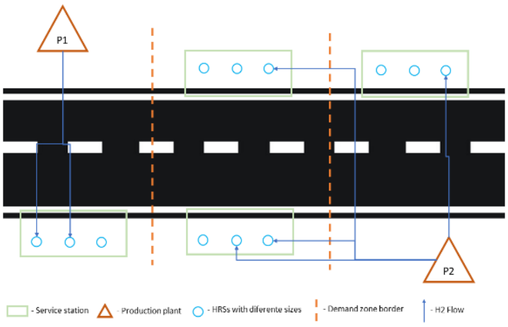

Figure 1: Generic Model Output

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, 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. This chain of operations in the H2 supply chain is depicted in Figure 2.

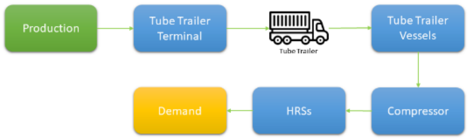

Figure 2: HSC chain of operations

4.1. *Sets*

- Set P: represents the available green hydrogen production sites, which serve as the sources for supplying hydrogen to the HRSs.
- Set L: encompasses the potential locations for the HRSs. These will ideally 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.
- Set Q: represents the available capacities of the HRSs.

4.2. *Parameters*

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

$ProdCap_i$: production capacity of plant *i* (kg/month)

CC: Capital cost of a HRS (€/month)

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

GP: gas price of tube trailer's fuel (€/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/month)

d_k: hydrogen demand at zone k (kg/month)

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

4.3. Variables

Integer variables:

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

Z_{jqk} **:** H2 delivered from station of size q at location j to demand zone k (kg/month). 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.

4.4. Objective Function

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. The factor A is computed by dividing the gas 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.

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

$$C_{ij} = A * dist_{ij} + OC \quad (2)$$

$$A = \frac{GP * 2}{FE\_TT} \quad (3)$$

4.5. Constraints

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

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

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.

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

Energy 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.

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

Energy 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.

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

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:

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

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

5. Case Study: data collection and treatment

5.1. Case Study Description

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. It is intended to promote the emergence of a H2 economy in Portugal, with a specific focus on the utilization of hydrogen-powered heavy-duty vehicles.

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.

Note that this case study will focus exclusively on the main Portuguese highways. These 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 3.

Figure 3: Brisa's highways (retrieved from Brisa's website)

5.2. Data collection and treatment

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.

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

Service Stations: Service stations will act as possible locations to build HRSs. Currently Portuguese highways are well equipped with several service stations. Highways concessioned to Brisa, with information publicly available about service stations located there are the ones used. Note that each location corresponds to two service stations, one for each direction of the highway.

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. Bing Maps API was used to retrieve the distance between an origin-destination coordinates pair.

Demand forecast: 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. 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. For the fuel efficiency the truck considered is the one developed by Hyundai, the XCIENT Fuel Cell. The fuel efficiency of buses is around 9.76 km per kg of H2.

Market Penetration: 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.

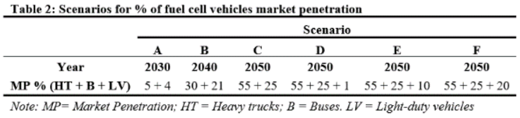

Table 2: Scenarios for % of fuel cell vehicles market penetration

	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

HRSs Data: 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. In order to normalize the capital costs, a lifespan of 20 years is considered. Therefore, the normalized capital cost becomes of approximately 7042€/month.

Tube trailers data: they typically utilize diesel as their primary fuel source. At the time this section is written, diesel costs around 1,684 €/liter on a Portuguese highway. 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. The capacities used for this study correspond to the ones used by Shamsi (2021)

Furthermore, Shamsi et al. 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.

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.

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. 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.

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. 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.

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.

6. Results and discussion

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. 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.

Table 3 shows which production plants are opened for each scenario and figure 4 shows the network of all entities for scenario A.

Table 3: Production Plants in use per scenario

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

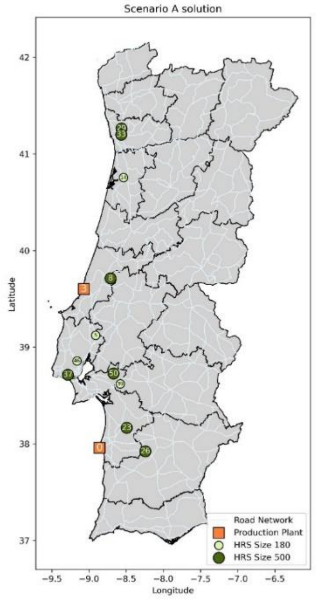

Figure 4: Scenario A network visualization

One could already expect the model 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 2 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 2 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 balancing the cheaper production costs of plant 0 and the cheaper transportation costs from plant 3. A similar thing happens in service station 14, which is much closer to Nazaré production plant but also receives hydrogen from Sines' plant.

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.

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.

Figure 5 shows a per kilogram representation of the trends for each parcel of the costs function for every scenario.

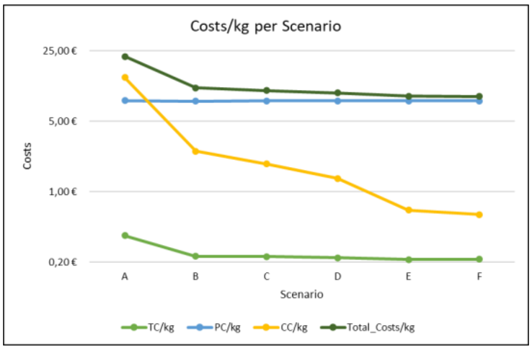

Figure 5: Costs per kg

The first insight that pops up from observing the cost trends is that the total costs gradually get closer to the production costs (PC) as demand grows. This happens because transportation costs (TC) rapidly go to as low as 0.23€ per kg of H2 distributed and capital costs (CC) 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

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.

Results showed 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. 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. A sensitivity analysis was performed to investigate the effects of varying production costs and gas prices 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.

<u>Gas price</u>: as demand grows between scenarios, so does the impact of a change in the gas 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 roundtrips, it's natural that the transportation costs cause a higher impact on the total costs generated. Nevertheless, this impact remains relatively low so changes in gas prices shouldn't be a big concern when developing a HRSs infrastructure.

<u>Production cost</u>: similar insights and conclusions can be drawn from this table as the ones from the gas 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.

6.4. Main Findings and Managerial key insights

Summarizing the main findings:

- Cost-effective production plants are prioritized over transportation costs at certain demand levels.
- Increasing demand leads to lower hydrogen prices, driving fuel cell vehicle adoption entering in a positive feedback loop.
- Findings were reinforced by testing with reversed production cost order.
- Gas price fluctuations have minimal impact in the designed network;
- Production costs greatly affect HRS network expenses.

The main managerial insights and related practical implications for policymakers, industry stakeholders, and investors interested in advancing hydrogen infrastructure are:

- For the initial refueling station investments, stakeholders should consider Scenario D, where fuel cell heavy trucks, buses and cars have a 55, 25 and 1 percent market penetration. This scenario addresses more demand for the same initial investment.
- Policymakers are urged to promote fuel cell vehicles and infrastructure development.
- Focus should be on reducing production costs via scale economies and technology research.

7. Conclusions and Future Research

The main objective of this work was to develop an optimization model to identify the optimal locations for HRSs, that could be applied to the Portuguese highways considering only the use of green hydrogen. This goes in line with the hydrogen strategy for a Climate-Neutral Europe and the Portuguese objective to decarbonize the transportation sector.

The work developed contributed to accelerate and facilitate the progress towards this goal by maximizing the benefits from an investment in HRSs.

Results confirmed previous literature findings where it was concluded that achieving economies of scale is of huge importance in order to reduce transportation costs. In fact, as demand grows, costs of deploying and maintaining a HRSs network converge to production costs.

On the Portuguese case 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.

Future work should focus on enhancing the model application and considering more information including all country highways, their traffic and parameters associated with the model. Future research should also explore 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.

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. In Portugal, efforts should be made to leverage this country unique position and advantage point regarding clean energies.

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