Green Hydrogen and Oxygen Developments in Portuguese Economy in the Context of Vehicle Refuelling Stations

Joana Alexandra Costa Faria

Thesis to obtain the Master of Science Degree in

Energy Engineering and Management

Supervisor: Dr. Rui Pedro da Costa Neto

Examination Committee

Chairperson: Prof. Edgar Caetano Fernandes
Supervisor: Dr. Rui Pedro da Costa Neto
Member of the Committee: Prof. Susana Margarida da Silva Vieira

July 2022

MEGE

Master in Energy Engineering and Management

Declaration

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

Student name (complete): Joana Alexandra Costa Faria

Final thesis title: Green Hydrogen and Oxygen Developments In Portuguese Economy in the Context of Vehicle Refuelling Stations

Date: Lisbon, 28 de junho 2022

Student signature: Joana Faria

Acknowledgments

This thesis marks the end of my life as a university student, being the ticket for the professional world.

I would most like to give a special thank you, from the bottom of my heart to my parents, Anibal Faria and Teresa Costa, my brother, Nuno Faria, and my grandparent José Costa for the patient, love, caring and huge encouragement through all these years, being the ones that were always there for me, no matter what, holding my hand whenever I was needed, and most importantly, for believing in me, even when sometimes I doubt myself.

I would like to acknowledge my dissertation supervisor Dr. Rui Pedro da Costa Neto for his insight, support, and sharing of knowledge that contributed to this Thesis.

I want to thank you also to Prof. Susana Vieira for taking me out of my comfort zone, helping me along the process, and assisting me in this great challenge that finalizes my academic life.

Last but not least, to all my friends who have shared this journey with me and who have been present in all my adversities and achievements and supported me when I needed it most, without them it would not have been the same. Thank you for being there.

To each and every one of you – Thank you.

Abstract

This dissertation aims to evaluate the total annual cost of a hydrogen supply network refilling stations, in the Portuguese context and to understand the impact on the economy.

Firstly, a selection of 100 freight transportation companies was carried out. Afterwards, it evaluated their fleets and the number of annual kilometres travelled, their need for hydrogen and their respective production and distribution costs. The companies were organized in small clusters, distributed throughout the country (decentralized production). The division between producers and consumers was performed, and finally, the allocation of hydrogen from producers to consumers was performed, obtaining a final total cost of the supply chain. So, 11 viable clusters were obtained, with a total of 32 companies, 11 of them being considered hydrogen producers with a total annual implementation cost equal to 461 646 574€, producing a total of 105 826 tons of hydrogen and 846 609 tons of by-product oxygen, which only 1.3% is able to satisfy the entire hospital oxygen consumption of Portugal. Finally, an economic balance was performed, comparing the hydrogen consumption in a year, with the diesel consumption. It was proved that hydrogen is the most advantageous fuel in the long term, obtaining a return on investment between 2/3 years, in comparison with diesel.

It is concluded that implementing a hydrogen supply chain is feasible and advantageous over normal diesel consumption. The sale of oxygen only to the hospital sector, while not harmful, does not have enough positive economic impact to be the driver for this investment.

Keywords

Green hydrogen; Oxygen; Freight transportation; Trucks; Clusters; Optimization;

Resumo

Esta dissertação visa avaliar o custo anual de uma rede de estações de reabastecimento de hidrogénio, no contexto português, e compreender o impacto na economia.

Primeiramente, foi realizada uma selecção de 100 empresas de transporte de mercadorias. Posteriormente, foi avaliada a frota e o número de quilómetros percorridos anualmente, as suas necessidades de hidrogénio e os respectivos custos de produção e distribuição. As empresas foram organizadas em pequenos grupos, distribuídos por todo o país (produção descentralizada). Foi feita a divisão entre produtores e consumidores e a respetiva atribuição de hidrogénio dos produtores aos consumidores, obtendo-se um custo total final da cadeia de abastecimento. Foram obtidos 11 clusters viáveis, com um total de 32 empresas, com 11 produtores de hidrogénio e um custo total anual de implementação igual a 461 646 574 euros, produzindo 105 826 toneladas de hidrogénio e 846 609 toneladas de oxigénio subproduto, que apenas 1,3% é capaz de satisfazer todo o consumo de oxigénio hospitalar de Portugal. Finalmente, foi realizado um balanço económico, comparando o consumo de hidrogénio num ano, com o consumo de gasóleo.

Foi provado que o hidrogénio é o combustível mais vantajoso a longo prazo, obtendo um retorno do investimento entre 2/3 anos, em comparação com o diesel. Conclui-se que a implementação de uma cadeia de abastecimento de hidrogénio é viável e vantajosa em relação ao consumo normal de diesel. A venda de oxigénio ao sector hospitalar, embora não prejudicial, não é suficiente para ser o motor deste investimento.

Palavras Chave

Hidrogénio verde; Oxigénio; Transporte de mercadorias; Camiões; Aglomerados; Optimização;

Contents

1 Introduction **2**

1.1 Context . . . 3

2 Hydrogen Production **6**

2.1 Hydrogen Production Processes . . . 7

2.2 Steam Methane Reforming . . . 8

2.3 Water Electrolysis . . . 9

2.3.1 Main technologies available . . . 10

2.3.2 Water electrolysis requirements . . . 12

2.3.3 Water Purification . . . 13

3 Road Transportation **15**

3.1 Hydrogen: a good fuel? . . . 16

3.2 Transportation sector in Europe . . . 18

3.2.1 Road freight transportation . . . 20

4 Portugal Context **24**

4.1 Portugal energy sector and hydrogen economy . . . 25

4.2 Portuguese transportation sector . . . 27

4.3 Water and energy in Portugal . . . 31

4.3.1 Availability of water resources in Portugal . . . 31

4.3.2 Energy and electricity in Portugal . . . 33

4.4 Oxygen applications and Portuguese context . . . 34

5 Hydrogen Supply Chain in Portugal - Model Formulation **37**

5.1 Objectives . . . 38

5.2 Assumptions and Restrictions . . . 38

5.3 Model Formulation - Hydrogen Supply Chain . . . 40

5.3.1 Objective Function . . . 40

5.3.2 Transportation Companies - Producers and Consumers . . . 40

5.3.3 Oxygen demand - Hospitals . . . 49

5.3.4 Hydrogen production cost . . . 49
5.3.5 Water supply cost . . . 52
5.3.6 Hydrogen transportation cost . . . 53

6 Results and Discussion **55**
6.1 Results . . . 56
6.1.1 Geographical Assessment . . . 56
6.1.2 Supply chain - Economic analysis . . . 64
6.2 Discussion . . . 69
6.2.1 Net Present Value . . . 72
6.2.2 Internal Rate of Return and Payback . . . 75

7 Conclusions **78**

Bibliography **80**

8 Appendix **89**
8.1 Table 1 . . . 90
8.2 Table 2 . . . 93
8.3 Table 3 . . . 97
8.4 Table 4 . . . 99

List of Figures

2.1 Hydrogen production processes. 7
2.2 Hydrogen categorisation. 8
2.3 Steam Methane Reforming flow diagram. 9
2.4 Water electrolysis technologies. 11

3.1 Hydrogen Fuel Cell Vehicle (HFCV) representation. 16
3.2 Comparison between hydrogen and battery storage price, evolution/perspectives. Comparison between hydrogen and battery gravimetric density. 17
3.3 Hydrogen enables Europe Energy Transition in several sectors. 18
3.4 Transport sector CO_2 emissions by mode in the Sustainable Development Scenario, 2000-2030. 19
3.5 Hyundai fuel cell truck. Hyundai H2 Xcient. 22

4.1 Portuguese fossil fuel consumption by type in 2019. 28
4.2 Hydrogen production prediction in Portuguese context. 30
4.3 Evolution of contribution of each method to hydrogen production. 30
4.4 Portugal water treatment stations display in the country. 32

5.1 Portuguese freight companies display. Companies analysed. 41
5.2 Producers and consumers display. Freight companies considered in the analysis. 45
5.3 Clustering process. Clusters with a minimum of 2 elements and with a maximum distance of 50 kilometres.**(Left)** Respective clusters centroids.**(Right)** 47
5.4 Overlap of the map with the display of the freight Portuguese companies and the clusters map. 48
5.5 Atmospheric Alkaline Electrolyser. Nel Hydrogen. 51

6.1 Clustering method. 56 companies arranged into 19 clusters. Portugal map overlay **(on the right)** 57

6.2 Total number of clusters formed in each scenario. 58
6.3 Number of companies excluded from the clustering process due to don't fit in the restrictions imposed. 58
6.4 Clustering process. Minimum elements equal to 2 and maximum distance equal to 50km.**(Left)** Minimum elements equal to 5 and maximum distance equal to 20km.**(Right)** 59
6.5 Clustering process. Minimum elements equal to 2 and maximum distance equal to 50km.**(Left)** Minimum elements equal to 2 and maximum distance equal to 20km.**(Right)** 60
6.6 Clustering process. Minimum elements equal to 3 and maximum distance equal to 50km.**(Left)** Minimum elements equal to 3 and maximum distance equal to 20km.**(Right)** 61
6.7 Clustering process. Minimum elements equal to 4 and maximum distance equal to 50km.**(Left)** Minimum elements equal to 4 and maximum distance equal to 20km.**(Right)** 62
6.8 Number of clusters that are able to satisfy their hydrogen demand per scenario. 62
6.9 Clustering process. Minimum elements equal to 5 and maximum distance equal to 50km.**(Left)** Minimum elements equal to 5 and maximum distance equal to 20km.**(Right)** 63
6.11 Total cost of implementation of hydrogen supply chain for the different scenarios. 68
6.10 Total amount of oxygen produced as by-product in kilograms per each scenario. 68
6.12 Best sites for refuelling stations. 70
6.13 NPV of the project along 10 years, no oxygen selling. 73
6.14 NPV of the project along 10 years, with oxygen selling at 0.80€/kg. 74
6.15 NPV of the project for 10 years, considering and not considering the oxygen selling. . . . 74
6.16 Internal Rate of Return (IRR), considering and not considering the oxygen selling. 75
6.17 Payback time, considering and not considering the oxygen selling. 76

List of Tables

2.1 Electrolysis technologies characteristics. 11
2.2 Water treatment technologies available. 13

4.1 How can green hydrogen positively contribute to Portugal. 26

5.1 Data representation. Portuguese freight companies. 42
5.2 Hydrogen heavy duty fuel cell vehicles brands characteristics. 43
5.3 Companies characteristics. Representation of the data used in the study. 43
5.4 Summary of the applied restrictions and the obtained results. 48
5.5 Representation of the matrix of distance between one company to others. 54

6.1 Percentage of clusters fully satisfied. 64
6.2 Transportation assignment example. Excel Solver tool. Cluster 1 from scenario of minimum of 2 elements per cluster with 50km maximum distance. 65
6.3 Characteristics of scenarios [2,50] (left) and [2,20] (right). 66
6.4 Characteristics of scenarios [3,50] (left) and [3,20] (right). 66
6.5 Characteristics of scenarios [4,50] (left) and [4,20] (right). 67
6.6 Characteristics of scenarios [5,50] (left) and [5,20] (right). 67
6.7 Clusters informations. 71
6.8 Costs of hydrogen implementation, diesel consumption, and fuel cell vehicles acquisition per each cluster, in a year. 72

8.1 Transportation companies data 90
8.2 Companies fleet size, annual kilometres travelled and respective coordinates (latitude and longitude) 93
8.3 Data for the network. The number of vehicles to be transformed, hydrogen demand, oxygen produced (considering the hydrogen demand), amount of water required, diesel savings, and hydrogen fuel cell trucks acquisition cost. 97

8.4 Input data HSCN. The data was converted to euros. 99

Acronyms

- Alkaline Electrolisis - [AE]
- Agência Portuguesa do Ambiente - [APA]
- Associação Portuguesa de Empresas Petrolíferas - [APETRO]
- By-Product Demand - [BP_0]
- By-Product Profit - [BP^{Profit}]
- Capital Expenditure - [CAPEX]
- Carbon Capture and Storage - [CCS]
- Carbon Dioxide - [CO_2]
- Direct Current - [DC]
- Direção Geral de Energia e Geologia - [DGEG]
- Distance - [Dist]
- Efficiency of the Electrolyser - [EFF]
- Electricity Price - [ELECTR]
- Energy Information Administration - [EIA]
- Estações de Tratamento de Águas Residuais - [ETAR]
- European Union - [EU]
- Fuel Cell Vehicle - [FCV]
- Gaseous Hydrogen Delivery Cost - [GHD_{Cost}]
- Greenhouse Gases - [GHG]

- Hydrogen Fuel Cell Electric Truck - [HFCET]
- Hydrogen Supply Chain Network - [HSCN]
- Hydrogen - [H_2]
- Heavy Duty Vehicle - [HDV]
- Horse Power - [hp]
- Hydroxile - [OH^-]
- Hydrogen Fuel Cell Vehicle - [HFCV]
- Hydrogen Production Cost - [HP^{Cost}]
- Hydrogen Transportation Cost - [HT_{Cost}]
- Hours per year - [HPY]
- Hydrogen Demand - [HD_{Cost}]
- Important Projects of Common European Interest - [IPCEI]
- International Energy Agency - [IEA]
- Internal Combustion Engine - [ICE]
- Instituto de Mobilidade e dos Transportes - [IMT]
- Intergovernmental Panel on Climate Change - [IPCC]
- Internal Rate of Return - [IRR]
- Low Carbon Liquid Fuel - [LCLF]
- Mercado Ibérico de Eleticidade - [MIBEL]
- Net Present Value - [NPV]
- Nitrogen Oxides - [NO_X]
- Organic Matter - [OM]
- Oxygen - [O_2]
- Proton Exchange Membrane - [PEM]
- Potassium Hydroxide - [KOH]

- Renewable Energy Sources - [RES]
- Roteiro para a Neutralidade Carbónica - [RNC]
- Solid Oxide Electrolysis - [SOEC]
- Steam Methane Reforming - [SMR]
- Total Annualized Cost - [TAC]
- United Kingdom - [UK]
- Unit Oxygen Selling Price - [UOSP]
- Unit price of water supply from the grid - [UWS_G]
- Water - [H_2O]
- Water Demand - [WD_T]
- Water Supply Cost - [WSC^{Cost}]

1

Introduction

Contents

1.1 Context 3

1.1 Context

The present society is consuming more and more energy and there is a continuous need to supply this demand. The traditional ways of producing energy are not being enough to produce the amount that is required in the world, so every day new solutions and new ways of energy production appear.

Right now, renewable energies are growing and have been gaining popularity due to their lowering cost and lower impacts on the environment. Environmental awareness has been an important factor in the energy sector because people and companies started to realize that it is not possible to continue to produce the number of emissions and continue to damage the planet as we have been doing until now. There are concerns about the impacts of greenhouse gas (GHG) emissions and how that affects climate change and intensifies global warming. Carbon dioxide (CO_2) emissions are a huge concern and have been growing at the global level and in only 10 years emissions grow about 13.3% and this increase was mainly due to electricity and heat generation, transport, industry, and buildings [1].

People consume energy, daily energy, and if we think as individuals, we cannot see ourselves without face each day without consuming any of it. So, it is obvious to think that the higher the amount of people in the world, the higher is the energy consumption. This leads to one of the world's main concerns. energy consumption. The world is facing a huge energy challenge, where to supply the world's total energy demand, huge amounts of energy need to be produced, and for that, it requires several solutions and production ways. This consumption ends up having negative consequences on the climate. There is a study where there are the analyses of the relation between energy consumption and climate change, where some of the author's conclusions were that the "rise in the average and extreme temperatures increase electricity demand for cooling down temperatures in different regions of the world", "climate change has a larger impact on the peak electricity demand that on the average monthly electricity demand" and that "climate change affects the geographical pattern of renewable energy supply in the different regions of the world". So, it is possible to verify that climate change and energy consumption are very related. [2]

The energy that powers our daily lives produces three-quarters of global emissions. [3] So, it is clear the relation between energy and environment, and due to this, currently, we can verify that there is a huge ambition of society to reach the climate targets and carbon neutrality. A simple and obvious solution would be to reduce the world's energy consumption, but that is very difficult. So, what we need are clean production processes and efficient ones. Hydrogen (H_2) can have a major role in this evolution to a green society.

In 2019, the European Green Deal was presented by the European Commission. The European Green Deal is a set of policy initiatives that aim to reach zero emissions by 2050. One thing that this deal highlight is the role of hydrogen in this transition, to achieve carbon neutrality by 2050. [4]

Hydrogen will affect deeply the energy system, being a flexible energy carrier for industry and transportation, thus, reducing GHG and particle emissions. The European Green Deal sees hydrogen as one of the main keys to achieving EU climate targets and goals that will lead to decarbonisation.

So, saying this, to achieve the net-zero carbon and be able to implement the climate mitigation strategies, it is necessary to use and develop more Renewable Energy Sources (RES) with the purpose of them to supply the energy and electricity demand. There have been some efforts to produce green hydrogen using processes powered by renewable electricity, but these developments will not affect the transition towards clean electricity generation systems [4]. Right now, refineries in Europe consume about 30% of the total amount of hydrogen that is produced, being used for intermediate oil products processes, but it is expected that the consumption of oil decreases along the next years. This doesn't mean that hydrogen consumption will decline, because hydrogen will be used in new processes, and clean transportation, allowing to produce energy directly from it, and the Hydrogen Roadmap Europe report explains this. In this report, we can see the prediction of usage and consumption of hydrogen in Europe and the UK, where it is possible to see that hydrogen can be capable of supplying a good percentage of energy demand, about 24%. [5]

One thing important to highlight is that, unfortunately nowadays, there is no significant amount of hydrogen (4% only) that is been produced from renewable sources, and this is the major step forward that the world needs. Hydrogen can be produced from several processes, and depending on the process that it is being used, the amount of emissions that are released varies, being influenced by the technology and the energy source that is considered. We will see in more detail some different production processes and analyse each of them. Besides the emissions, the costs also change, which is an important decision factor for companies to think about in investing in it.

The world needs renewable hydrogen, or also called, green hydrogen, that produced through water electrolysis and using electricity from renewable sources, such as wind, solar, hydro, etc. This way it is possible to produce hydrogen with, almost, zero carbon emissions. But all this process has a cost, and in the end, the final price of hydrogen will be about $6 per kilogram [6]. However, there is a prediction that states the cost will lower down, achieving a price equal to $2.50 per kilogram until 2030, through the usage of electricity that comes from wind farms [4]. So, here it is possible to see a "window of opportunity". Maybe, we can think about regional hydrogen production, where the regions can be able to auto-sustain their energy consumption by producing their own energy through green hydrogen, where the electricity used can come directly from local Renewable Energy Sources (RES). This will take us to the next topic that is which is best? A centralized hydrogen production, with transportation of it to the locals, or a decentralized production and storage in the site?

Currently, hydrogen is mainly used for oil refineries, as mentioned before, but is also involved in ammonia and methanol production, in Europe. We also can see hydrogen being consumed by the metal industry, and all these four sectors make a total consumption of 90% of the total hydrogen produced. But today's direction is turned to convert hydrogen into electricity (Gas-to-Power). Focusing on green hydrogen and clean electricity generation, the amount of energy consumed during the hydrogen conversion into electricity depends on the type of electrolyser technology that we are using. There are three types of electrolysers, and we are going to see them in more detail further in the work, namely, alkaline electrolyser, proton exchange membrane (PEM), and solid oxide electrolysis (SOE), being their specific consumption's equal to 50-51kWh/kg, 55-58kWh/kg and 40-41kWh/kg, respectively [4].

Economic hydrogen production through electrolysis can be to take advantage of the periods of the day where there is a high production of energy with very low consumption, such as sunny weekends, windy nights, etc. The truth is, for regions where renewable energy is easily produced, means that will be sold at lower prices, and this way they will be able to compete with fossil fuel-based hydrogen production. This can be a reality by 2030. But, it is necessary to be aware that the demand and the fossil fuel consumption will not decline anytime soon, not at least 2030 [4], because some industrial sectors find it very difficult to be decarbonised. So, the European policies see the refineries as a "window of opportunity", that will enable the growth of the hydrogen economy, its production, its technology, and turn the energy markets more mature, and finally achieve economies of scale. Only in a long-term perspective, the hydrogen demand is expected to grow.

Europe has no fossil fuels in its constituent countries and because of this it is limited and dependent on fossil fuel imports. Taking into account the energy crisis in the world, high energy consumption and high energy production generate large carbon dioxide emissions. These emissions are taxed and are currently around 80€/ton of CO_2 emitted [7]. Over the years, the use of natural gas has reduced emissions, and had the advantage of being a cheaper fuel, however, it is still a fossil fuel and continues to have associated emissions. In the year 2021 the cost associated with natural gas has already been found to be 7 times greater, [8] than in the previous year. It is therefore clear that Europe needs to find new alternatives that are more viable, sustainable and economical, enabling Europe to be more self-sufficient and energy independent.

2

Hydrogen Production

Contents

2.1 Hydrogen Production Processes 7

2.2 Steam Methane Reforming 8

2.3 Water Electrolysis 9

2.1 Hydrogen Production Processes

As mentioned, green hydrogen is a very important energy vector and can do easy replace the use of fossil fuels. Hydrogen can be obtained through renewable sources, electrolysis of water, steam methane reforming (SMR), gasification (coal, biomass), pyrolysis, among other technologies, what we called green hydrogen can only be produced from clean sources, with low or zero GHG emissions and low environmental impacts, such as renewable sources and from water electrolysis. For the H_2 economy to be able to develop and continue to grow, it is important to have economically viable H_2 production, so the type of feedstock and the technology that is used, are the main factors that influence the economic viability of H_2 production. In figure 2.1 are summarized all processes of hydrogen production.

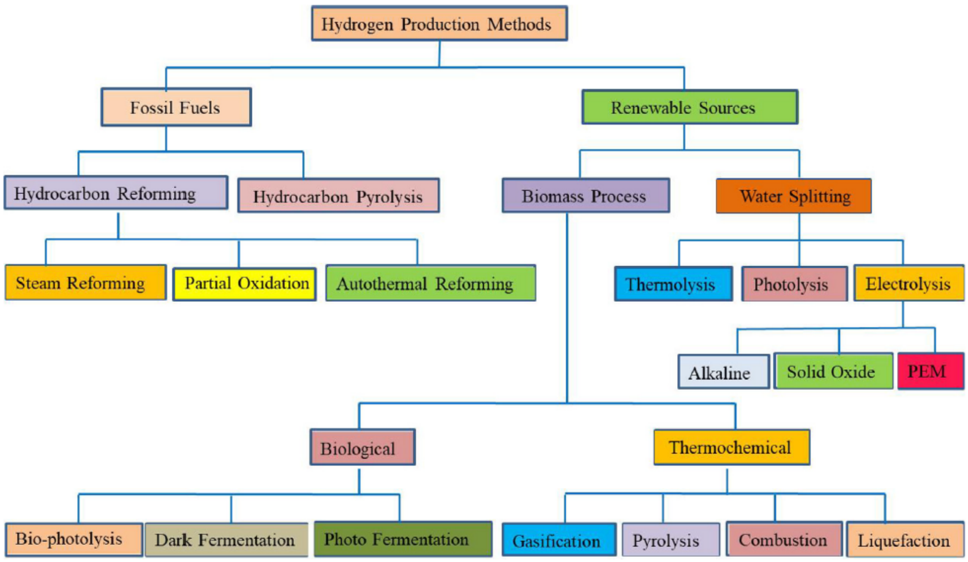

Figure 2.1: Hydrogen production processes. [9]

It is possible to separate H_2 production into two, namely, production from carbon sources and renewable sources, but we can distinguish three types of hydrogen, grey, blue, and green, and they can be simply described in figure 2.2. “Grey hydrogen” corresponds to the one that is produced by carbon sources (eg. fossil fuels), the blue is produced in a similar way that the “grey” but has Carbon Capture and Storage (CCS) technologies, that enable the reduction of CO_2 emissions, meaning lower environmental consequences, and finally, the green, produced from renewables [10].

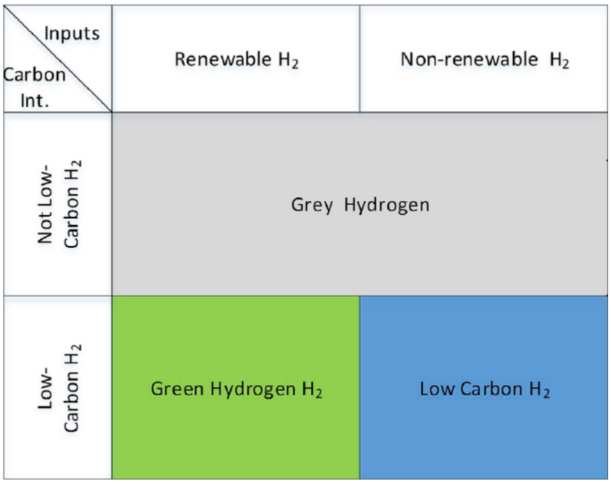

Figure 2.2: Hydrogen categorisation. [11]

Hydrogen can be extracted through different forms of energy, such as thermal, electrical, photonic, and biochemical [12], where the first two can use different types of renewable energies or even nuclear energy, the photonic use solar radiation, and the biochemical use organic matter as a source of energy. Is it possible to see, nowadays several processes that can produce hydrogen, but in this work, I will only focus on the ones that are more used, with higher efficiency. According to EIA, the most common processes in the world right now are steam methane reforming and water electrolysis [13], one method that used carbon sources, producing this way only grey or maybe blue hydrogen, and it is the most used process (being done in refineries) and the other that can use energy from renewable sources, producing the green hydrogen.

2.2 Steam Methane Reforming

As said previously, the current H_2 in the world is produced mainly from carbon sources [14] such as natural gas, coal, or even oil. By using methane, H_2 is produced through a process called Steam Methane Reforming (SMR), which is a mature and traditional production process that occurs at high temperatures (about 800-900ºC) [10], where the methane (a main component of the natural gas) reacts with steam, with a presence of a catalyst, producing the hydrogen and carbon monoxide (CO). From the 60's, this was the cheapest process to produce hydrogen, specially due to the low cost of methane, until the last year. After this reaction, another called Water-Gas Shift reaction occurs, where the CO produced from SMR reacts with steam, producing carbon dioxide (CO_2) and more H_2. The chemical reactions are:

Methane Reforming: $CH_4 + H_2O \rightarrow CO + 3H_2$

Water-Gas Shift Reaction: $CO + H_2O \rightarrow CO_2 + H_2$

After these two reactions, a third separation occurs, called Pressure Swing Adsorption (PSA) that will purify the hydrogen that was produced from the two first reactions. The "blue hydrogen", is mainly focused on the combinations of SMR with CCS [10].The process can be easily describe as in flow diagram in figure 2.3.

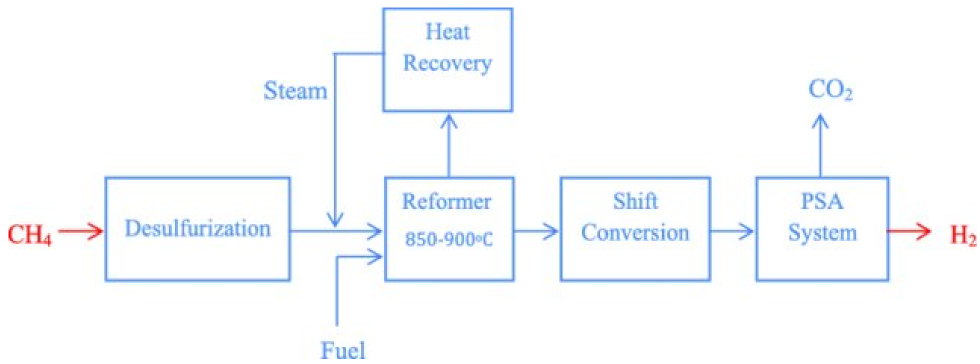

Figure 2.3: Steam Methane Reforming flow diagram. [15]

From all methods that use fossil fuels as sources, SMR is the one that has lower CO_2 emissions [14], and combining this process with CCS has a huge advantage. SMR has a very high efficiency, until 83% [14], which turns this process very attractive and it is economically feasible. But it has its disadvantages, such as the CO_2 emissions and the continuous need for natural gas (which is a limitation in terms of feedstock). It is important to mention that the major influence of SMR for H_2 production is the price of natural gas, (99€/MWh, [8]). The price of fossil fuels is never stable, they change with the demand, with productivity, and so on. Over the years, natural gas has become very popular due to the fact of emitting lower amounts of CO_2 with its usage hydrogen can be produced also by decomposing water, using different types of processes, being one water electrolysis. This process is the one that produces H_2 with a very high percentage of purity (almost 100%), it is a mature process and technology, with relatively high efficiency, 65-85% [14].

2.3 Water Electrolysis

The reason why water electrolysis is considered such a capable hydrogen producer is due to the fact of producing this energy carrier through renewable energy (using solar, wind, among other green energies sources) and using clean feedstock (H_2O) [9]. But, this is only true when we are talking about green hydrogen. The origin of the electricity that feeds the reaction influences the type of hydrogen that is being produced. Only electricity produced from renewable sources can generate green hydrogen.

The concept is simple, it consists of the separation of the molecule of water (H_2O) into hydrogen and oxygen (O_2), with no CO_2 emissions or any GHG emissions, as it will be possible to see further in this work, and it occurs due to the movement of the electrons. This process is fed by DC and this current will provide a positive and a negative charge in the electrodes, being the negative called cathode and the positive called anode.

Water electrolysis can be defined by the source of electricity that uses (fossil fuels, wind, solar, nuclear, etc) but also by the type of electrolyte that is being used, being the most known ones the Proton Exchange Membrane (PEM), Alkaline (AE) and solid oxide (SOEC).

2.3.1 Main technologies available

Currently, there are three main technologies available in the market, each of them with their technical and economical characteristics but with the same final purpose, decompose water into H_2 and O_2. These technologies, as mentioned above, are: Alkaline Electrolysis (AE), Proton Exchange Membrane (PEM), and Solid Oxide Electrolysis Cells (SOEC), and the efficiencies can vary between 60% to 90%, depending on the technology that it is being considered and the load factor of it. [16]

- **Alkaline Electrolysis (AE)**: the most mature technology of the three of them, being used since the 1920s. This method consists of using two electrolytes inside an alkaline aqueous solution, usually with a high concentration (30%w/w) of potassium hydroxide (KOH). The chemical reaction occurs at the electrode surface. On the cathode, the H_2 molecule splits into H_2 and OH^-. The hydroxyl will be attracted by the anode, since it is a negative ion, and will react and form water and oxygen. The process can be visualized in figure 2.4, on the left. This process has a lower capital cost, mainly due to the fact of not using precious materials (which occurs with anionic exchange membrane and the electrodes are made of nickel alloys) [16].

- **Proton Exchange Membrane (PEM)**: is not as mature as AE and, in opposition of it, PEM uses pure water and also uses a solid polymer between the electrolytes, the membrane. This technology occupies 2,5 less space than alkaline electrolysers, which can be attractive for regions with high popular density. The main disadvantages are related to the catalysts used, because they are made from precious materials such as platinum, ruthenium and iridium, which turns this method much more expensive and with the fact of its lifetime being shorter than AE [16]. Its representation can be found in figure 2.4, in the middle.

- **Solid Oxide Electrolysis Cells (SOEC)**: was introduced in 1980 [9]. It is not available in the market yet but there are good expectations about it. This technology uses electrolytes made with ceramic material, has a efficiency higher that 81%, works at high temperatures, and can work in reverse mode, in the same way as a fuel cell converting hydrogen into electricity [16]. The limitations of this technology are: durability of the cells, only atmospheric pressure operation, and leakage issues.Its representation can be found in figure 2.4, on the right.

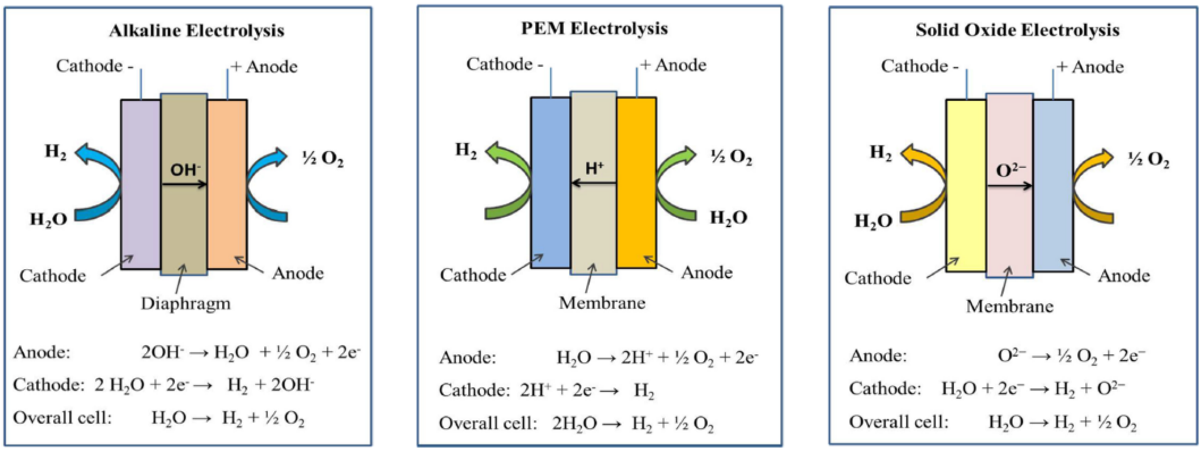

Figure 2.4: Water electrolysis technologies. [9]

Some characteristics of the previous electrolysers mentioned can be found in table 2.1, and the perspective of the evolution of those, in 10 years (meaning 2030) and as in long-term, assuming that they will be in a stage of maturity.

Table 2.1: Electrolysis technologies characteristics. [16] [17]

	AE Electrolyser			PEM Electrolyser			SOEC Electrolyser		
Electrolyte [17]	Aq. Potassium hydroxide (20-40 wt% KOH)			Polymer membrane (ex: Nafion)			Yttria stabilized Zirconia (YSZ)		
Cathode [17]	Ni, Ni-Mo alloys			Pt, Pt-Pd alloys			Ni/YSZ		
Anode [17]	Ni, Ni-Co alloys			RuO_2, IrO_2			LMS/YSZ		
Timeline	**Today**	**2030**	**Long term**	**Today**	**2030**	**Long term**	**Today**	**2030**	**Long term**
Electrical Efficiency (%) [16]	63–70	65–71	70–80	56–60	63–68	67–74	74–81	77–84	77–90
Operating Pressure (bar) [16]	1–30	—-	—-	30–80	—-	—-	1	—-	—-
Operating Temperature (ºC) [16]	60–80	—-	—-	50–80	—-	—-	650 -1000	—-	—-
Stack lifetime (operating hours) [16]	60000--90000	90000--100000	100000--150000	30000--60000	60000--90000	100000--150000	10000--30000	40000--60000	75000--100000
CAPEX (USD/kWe) [16]	500-1400	400-850	200-700	1100-1800	650-1500	200-900	2800-5600	800-2800	500-1000
Maturity	Mature	—-	—-	Commercial	—-	—-	Not even on the market	—-	—-

The production rate at which the oxygen and hydrogen are formed depends on the electric current that feeds the reaction, which is dependent on the voltage and the conductivity. A problem in this process is that water is not a very conductive environment, so to increase the current of the process, it is necessary to increase either the voltage or the conductivity. In terms of efficiency, it is much more efficient to increase the conductivity of the environment, and for that usually, it is included an electrolyte, in salt form, which works as a charge carrier. This process was expensive some years ago, and adding to this is has slow response times and starter procedures and there are some safety concerns. For hydrogen to compete with fossil fuels and batteries, it needs to decline its productions costs to make it more attractive. About 4% of the hydrogen produced in the world is done through electrolysis [18], being the remaining amount produced mainly by SMR, because until last year the methane was very low cost, 17 €/MWh, but currently (December 2021) the cost rise to 99€/MWh [8].

The cost of producing hydrogen from water electrolysis takes into consideration several aspects that are also affected by the type of technology that is going to be used. Some of them are efficiency, CAPEX, operation hours, electricity costs.

2.3.2 Water electrolysis requirements

It requires a considerable amount of energy to separate the molecule of water into hydrogen and oxygen, it is an endothermic process that consumes more energy than releases. So, this means that water electrolysis is not directly associated with green hydrogen because it depends on the type of electricity that is consumed. If the electricity that this process is consuming is produced from fossil fuels, there will be emissions of CO_2 associated, not directly from the hydrogen production, the reaction itself, but from the energy that is required for it. This is a very important factor to take into consideration.

To sustain the electrolysis process it is necessary to provide electricity. A simple way of doing this is to connect directly the technology to the energy grid. But, this way, it is not possible to guarantee that we are using 100% renewable energies, consequently, it is not possible to guarantee that the hydrogen that is being produced is 100% green. A solution for this case is to have a contract with the energy/-electricity supplier where it is agreed that we only give, to the productions site, energy that comes from renewable sources and charge an amount for that contract. Another alternative can be to negotiate with a local/regional energy producer (only with renewable sources) and use the local energy production to feed the electrolysis.

Besides the electricity, it is necessary to obtain the main component purified for the electrolysis. This component is water. For electrolysis is not possible to use any type of water available, we need 100% pure water to feed this process, free from impurities such as salts, particles, other elements (chloride, calcium, magnesium, etc). The question is how we obtain this water. It is possible to use seawater but is necessary to pass that water through a process called desalination, where salty water is transformed into “fresh” and purified water, prepared to be used in electrolysis. Another solution is to use water directly from the grid, but again here we also need to purify it, using the same method as before, desalination by reverse osmosis [19].

2.3.3 Water Purification

About desalination, there are two main methods, one being the thermal desalination, the called traditional technologies, like Multistage Flash Distillation (MSF), Multi Effect Distillation (MED), Vapor Compression Distillation (VCD), Thermovapor Compression (TVC), Membrane Distillation (MD) and the other being membrane techniques, that are modern technologies, such as reverse osmosis (RO), Electrodialysis/Electrodialysis Reversal (ED/EDR), Nanofiltration (NF), Mechanical Vapor Compression (MVC).

Table 2.2: Water treatment technologies available. [20]

Desalination Technology	Water type	Energy consumption (kWh/m3)	Thermal energy (kWh/m3)	Operation temperature (℃)
MSF	Seawater, Brackish water	2.5–3.5	12	90–110
MED	Seawater, Brackish water	1.5–2.5	6	70
TVC	Seawater, Brackish water	1.6–1.8	14.6	63–70
MD	Seawater, Brackish water	0.6–1.8	54–350	80
RO	Seawater, Brackish water	3.5–5	–	Ambient
ED	Brackish water	1.5–4	–	Ambient
NF	Brackish water	2.54–3.35	–	Ambient
MVC	Seawater, Brackish water	7–12	–	–

Table 2.2, shows some characteristics of some of the technologies previously mentioned. The water type presented in the table 2.2 is referred to as the feedwater that is possible to use with the respective technology. Thermal desalination is the most ancient process, and its concept is very simple, where the water is heated up until it reaches its vapor phase, captures this vapor, and transforms it into freshwater. This method tries to copy the effect of the sun.

In opposition to the thermal process, the membrane does not use heat to purify the water, it is used a membrane that will work as a filter, the water will pass through the membrane, under a pressure. When the water passes through that membrane, the molecules of salt, particles, and other contaminants are forced to be separated from the water and will not pass through the membrane. The method is an expensive one, due to its energy consumption [19]. The efficiency of the second technology, the modern methods, depends on the type of membrane that is being used, the operational parameters and mainly the water properties [21]. To prolong the quality of the membrane in reverse osmosis technology, it is necessary to pre-treat the water that feeds the process, being filtration, chemical coagulation, softener, and acidification (to regulate the pH) some of the pre-treatment processes [21]. Due to the developments of membrane technology, these methods are being preferred and replacing thermal ones. Between all of them, RO is the one with higher desalination installed capacity [20], with the total lower energy consumption per cubic metre water treated.

3

Road Transportation

Contents

3.1 Hydrogen: a good fuel? 16
3.2 Transportation sector in Europe 18

3.1 Hydrogen: a good fuel?

In the current days, the word hydrogen has been more and more associated with the energy sector and the transportation sector. But, along with this, hydrogen has become a reality in those sectors, which is more impressive. The truth is, "hydrogen application for transportation has a long history" [22]. In 1807 hydrogen was used as fuel in an internal combustion engine (ICE), mixed with oxygen, in the car, being the first internal combustion-powered automobile, invented by Francoise Isaac de Rivaz.

As mentioned previously, environmental awareness has been increasing over the years, and the concerns related to global warming, greenhouse gas emissions, lack of resources, and so on, is making society look for new ways of producing energy and alternative fuels, to maintaining a sustainable way of living, and the usage of the hydrogen plays a key role.

Hydrogen has a much higher yield per unit of mass when compared to any other fuel and it has a higher ignition temperature than gasoline. Due to its low density, hydrogen dissipates in the air, in opposition to traditional fuels such as diesel and gasoline, which in terms of safety concerns is good and better. However, the lack of studies and experience of hydrogen systems, it is difficult to determine how risky can be hydrogen under certain conditions. With that in mind, some efforts are being done and projects are being conducted to bring hydrogen technologies to usage and understand their performance. In Europe that is not any different [22].

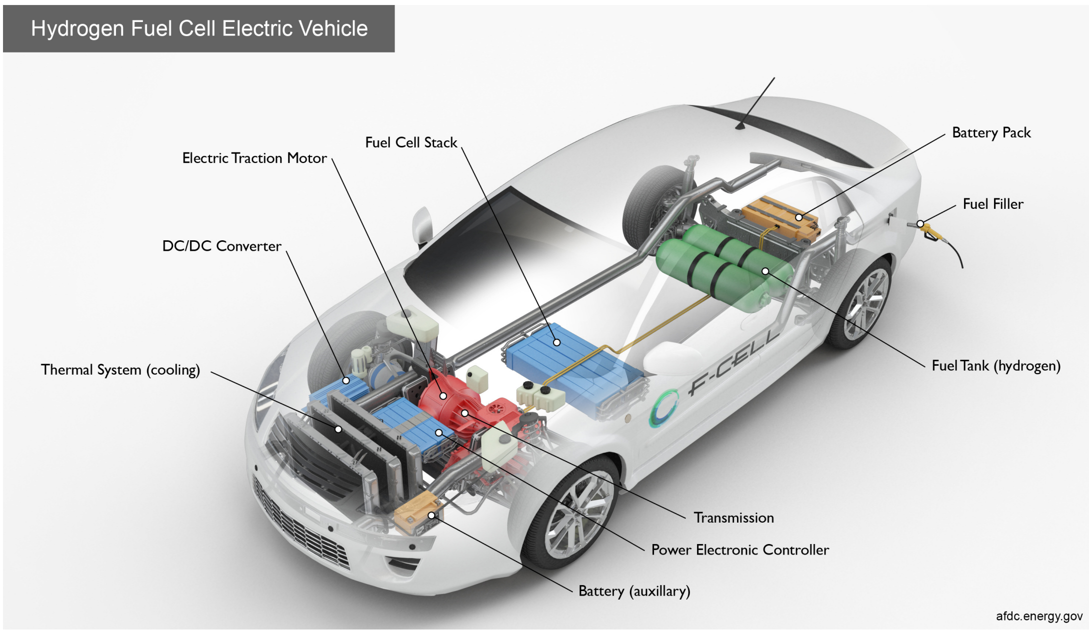

Figure 3.1: Hydrogen Fuel Cell Vehicle (HFCV) representation. [23]

It is possible to think about hydrogen mixed with traditional fuels (petroleum-derived fuels) in internal combustion engines (ICE) [24]. This way it would be possible to decrease the prejudicial emissions because hydrogen does not emit greenhouse gases after combustion (it is necessary to be careful with high temperatures though, due to NOx emissions). Besides this, hydrogen can be stored, used, and sustainable in different areas [25]. But, despite the direct usage of hydrogen as fuel in internal combustion engines is a possibility, if it is mixed with other fuels, society would still be dependent on fossil fuels and several constraints and risks would appear such as back ignition, early ignition, knock formation, that are not desirable. All of them are undesirable ignitions that can damage the engine and are dangerous. [24]. Besides using hydrogen in ICE with lower conversion efficiency (lower than 25%), it is possible to use it in fuel cell vehicles (FCV) with higher conversion efficiency (50%), called Hydrogen Fuel Cells Vehicles (HFCV), represented in figure 3.1.

Hydrogen fuel cell vehicles use hydrogen as fuel to produce energy, electricity, that will power the motor. These vehicles are electric, but instead of having a huge battery that stores the electricity and needs to be recharged, has a fuel tank that will store the hydrogen and has a fuel cell that will the reverse reaction of electrolysis, producing energy and water from hydrogen and oxygen. Hydrogen has an energy content equal to 33,33kWh per kilogram (lower heating value), being between the fuels the one with the highest value.

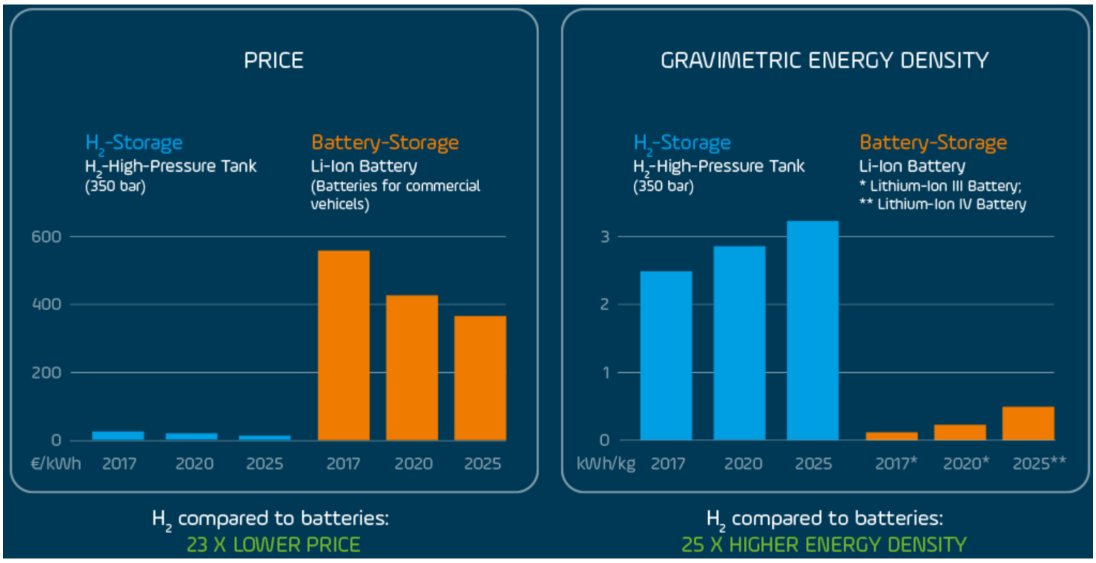

Figure 3.2: Comparison between hydrogen and battery storage price, evolution/perspectives. Comparison between hydrogen and battery gravimetric density. [26]

About the storage, hydrogen storage is very efficient, being even better than batteries, despite being an immature/innovative concept. With the increase of hydrogen economy and its sales, "it will be possible to produce hydrogen storage systems that are disproportionately more cost-effective than battery storage systems" [26], as it is possible to see in the graph of figure 3.2. Compared with today's lithium-batteries vehicles' gravimetric energy storage density equal to 100 Wh/kg, hydrogen storage offers storage 18 times higher. One of the main reasons for hydrogen storage being much lower than batteries is the lower costs of the materials that compose the tank where the hydrogen is saved. Besides this, the higher prices of batteries are also related to the manufacturing and raw material costs and scarcy.

Hydrogen has been a very important element along with the Energy Transition in Europe, an important energy vector that will help to achieve truly the carbon-neutral targets established to 2050. The truth is that, nowadays, there is still a limited market for hydrogen, and lack of refiling stations but Europe detains the conditions to rise the market interest on this element and has all the means to be cost-competitive renewable low carbon hydrogen [27] and enable to allow the energy transition in several sectors as can be seen in figure 3.3, such as industry, transportation, heating and power for buildings, and so on. The mobility based on hydrogen as a fuel has, in the present days, two major challenges that are the cost-competitive of hydrogen fuel cells and the infrastructures to produce, distribute, and also to refuel [28]. At an European level, Germany, UK, France, and European Nordic countries are strong supporters of the development of the hydrogen economy [29]

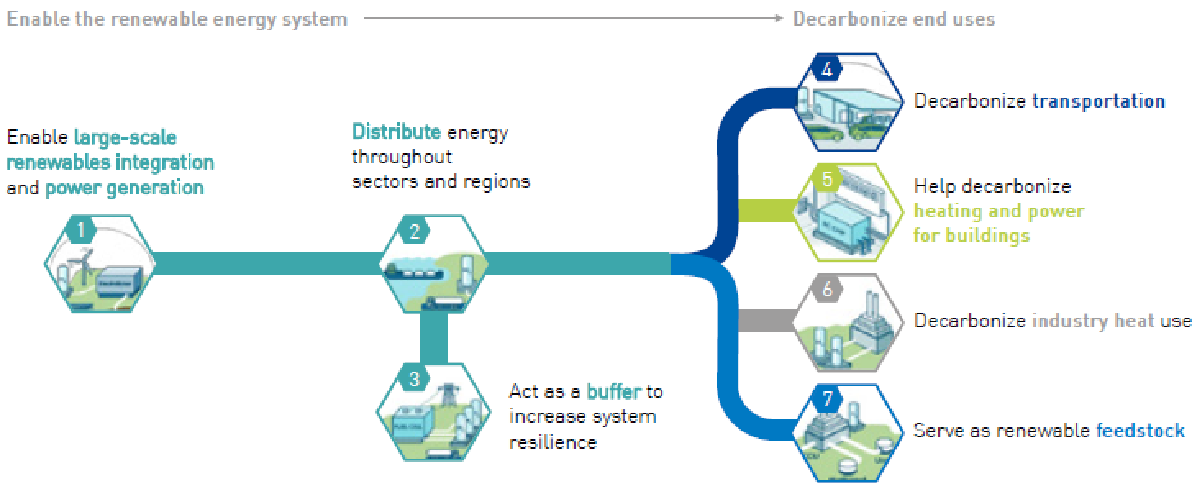

Figure 3.3: Hydrogen enables Europe Energy Transition in several sectors. [5]

3.2 Transportation sector in Europe

The transportation sector is one of the sectors the most contribute to GHG emissions. The European Commission stated that the current European transport sector annually releases almost 25% of the total greenhouse gas emissions, and inside this sector, is road transportation that has the higher influence, accounting for around 70% of GHG emissions. [30]

In figure 3.4 it is possible to verify the growth of the CO_2 emissions from the transport sector since 2000 and the predictions of the evolution of those emissions until 2030. The transportation sector is composed of shipping, aviation, road (where we can discriminate into passenger and freight), and it is easy to see that the subsector that has the highest share is road transportation, namely passenger transportation, being followed by freight road transportation.

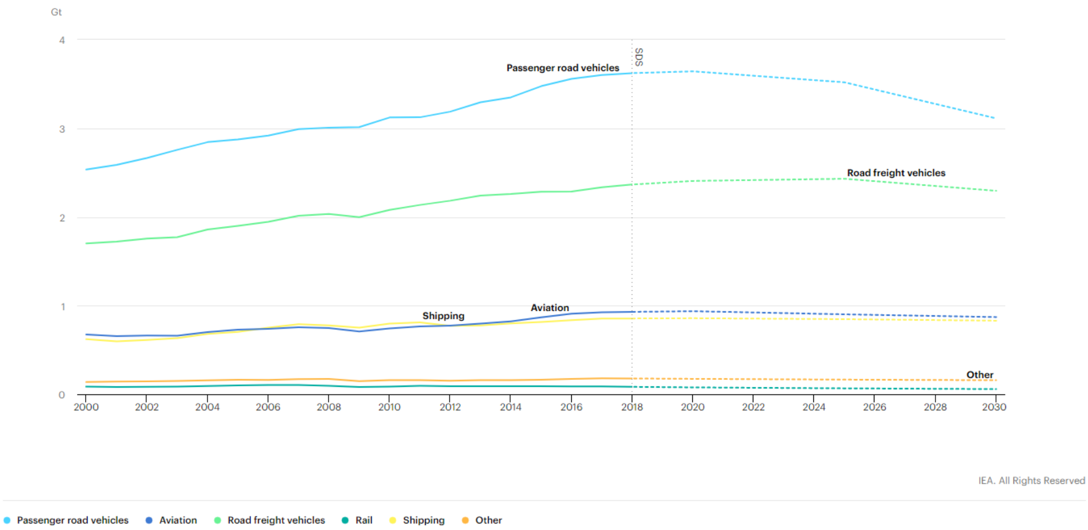

Figure 3.4: Transport sector CO_2 emissions by mode in the Sustainable Development Scenario, 2000-2030. [31]

IEA reports that "Global transport emissions increased by less than 0.5% in 2019 (compared with 1.9% annually since 2000) owing to efficiency improvements, electrification and greater use of biofuels" [32]. But even with this victory, road transportation is still a major contributor for the emissions, accounting for almost 75% of total CO_2 emissions of the transports sector.

One of the main elements of the low-emission mobility strategy of the European Commission is moving society towards zero-emission vehicles, meaning that the improvement of efficiency of internal combustion engines will help but will not be enough to decrease the carbon emissions of road transportation, so to achieve a future with a green and clean transportation sector, in all categories (road, aviation, shipping, etc), it is required to alternative vehicles fuelled by biofuels, electricity, and hydrogen. [33].

Hydrogen Fuel Cell Vehicles (HFCV) are particularly interesting and have been gaining popularity because is a good solution to bet on due to its zero-emissions (NOx, particular matter, carbon dioxide, and monoxide, etc), it is suitable for long distances, which is good for freight transportation. However, the penetration of HFCV is still low in the market. [33]

3.2.1 Road freight transportation

The road freight network is a very important sector and has a major influence on the economics of the world and it has been growing through the years, as in developing countries as in developed ones, but the increase of this sector is more pronounced in the first ones. The main driver of this growth is the industrial and consumer goods demand that has been rising. [34]

Some factors can be related to the increasing of freight transportation's such as globalisation of production activities, rapid industrialisation, urbanisation, and all of this is associated with uneven distribution of raw materials, geographically speaking. Other factors can also be mentioned such as fuel prices, population density, and infrastructure, availability, and quality. [34]. Due to this, the road good transportation has a huge influence on the oil demand and on the oil primary energy consumption, which means that if one increases, the other will too.

The transportation sector is the sector that most contributes to greenhouse gas emissions, namely road transportation, being the freight transportation's second bigger emitter, following passenger transportation. It is possible to conclude that by decarbonising this sector, which is dominated by traditional fuels (such diesel, gasoline, natural gas), the positive impact that would have on the planet. But there is not enough attention to the subsector, because society is focused on road passenger transportation, and the lack of attention on road freight transport can become a problem. [34]

The question here is how are we going to improve this sector to decrease GHG emissions and consequently achieve also the carbon neutrality target. The electrification of the transports must happen, and for the interest of this work, specifically the electrification of heavy-duty trucks. European Commission admitted that "Despite some improvements in fuel consumption efficiency in recent years, these emissions are still rising, mainly due to increasing road freight traffic" [35]. Fossil fuel-powered trucks have a tremendous impact on emissions and air pollution. So, to reduce those and improve the truck's efficiency, electric vehicles technologies are necessary, like battery or fuel cell vehicles. The first emission target settled by the European Commission was established in 2019 with the view to reduce the emissions from heavy-duty trucks for 2025 and 2030 [35]. This Regulation promotes zero and low emissions vehicles and aims to achieve a reduction of 15% of CO_2 emissions by 2025 and 30% by 2030.

There are two major advantages of using electric vehicles in general, the motor power efficiency is higher (>85%), due to the fact the heat loss is much lower (compared with ICE, <25%), and there are no direct emissions on-road. Currently, the main electric technologies are battery-electric and hydrogen fuel cells that are available for trucks [6].

Comparing those two technologies, the battery-electric is a little more efficient (about 90%) at 20ºC than the fuel cell (around 50%, between -20ºC and 70ºC), and the costs of producing the hydrogen, sustainably, are still expensive, being cheaper to use electricity directly. However, the costs of hydrogen production are expected to decline through economy of scale. The advantage of using hydrogen fuel cells is that it is possible to guarantee the green origin of the hydrogen, and with electricity that is not possible, because the battery is fed directly from the grid, that is composed by the energy mix, it doesn't have only renewable sources, and to produce hydrogen it is possible to establish contracts that guarantee the all electricity that feds the electrolysis comes from renewable sources. Another advantage of using hydrogen fuel cell trucks is refuelling. Heavy Fuel Cell Electric Trucks (HFCET) have a refuelling process very similar to the traditional fuels like diesel and gasoline, and rapidly can fill the tank in a matter of 5 minutes, and the truck will be ready again to travel. With batteries that is not possible. With batteries, it is necessary to stop for several hours to guarantee that the battery is fully recharged and to avoid the premature degradation, and supercharge is not advised because decreases the number of life cycles. This means that the usage time of that battery will be reduced and will not be operational for the number of years that was supposed. Another disadvantage of battery electric vehicles is what to do to the battery when its life cycles end.

Decarbonising the transportation sector, namely road freight transportation, is not an easy process to do. This is related to heavy loads, which account for more than one-third of global energy demand and GHG emissions and the truth is that the freight activity is to increase to double by 2050 due to the rise of the energy demand [36].

The introduction of battery and fuel cell electric vehicles will help, with no doubt, to mitigate carbon emissions, particle matter emissions, NOx emissions, and other pollutants. Comparing light, medium, and heavy-duty freight transport, battery vehicles can easily manage the travels for the first two mentioned before, but for heavy freight transportation, that are long-haul transportation's, with high utilization and power-consuming, battery-electric vehicles will not be enough or fast charge efficient, so hydrogen fuel cell will be more suitable [37]. Focusing on heavy-duty vehicles (HDV's), fuel cell electric vehicles are a better choice compared to battery vehicles since these vehicles have higher power and range requirements [38], specifically for heavy duty vehicles, like taxis, Ubers, forklifts and mining and construction vehicles. Unfortunately, there are some barriers to the growth of fuel cell trucks and their commercialization, being them the initially high costs, the lack of infrastructures (refuelling stations for example), and the low lifetime, however, hydrogen economies of scale, technological developments, and right control rules for vehicle operations are boosters of the hydrogen economy and allow to improve its system durability [38]. Although today's hydrogen fuel cells have a lifespan of 32000 hours, assuming 3 hours operation per day, the vehicle would have a lifespan of 30 years.

There are some hydrogen fuel cell electric trucks on-road today but are a very small number compared with what is needed to mitigate the current effects of the emissions and to achieve 2050's targets. An example of fuel cell trucks can be seen in figure **??**, a truck produced by Hyundai, model H2 Xcient. This particular brand is composed of a 190-kilowatt (258-hp) hydrogen fuel cell system with two 95-kilowatt fuel cell stacks connected in parallel. Its 7 hydrogen tanks with a storage capacity of 35 kilograms of hydrogen should enable a range of more than 400 kilometres [39].

Figure 3.5: Hyundai fuel cell truck. Hyundai H2 Xcient. [39]

However, there are few studies available about the feasibility of hydrogen fuel cell trucks, in their wide variety of truck classes, and it is important to understand if the performance of these vehicles are good enough to replace internal combustion engines (ICE) trucks that are been used today [40], and if will enable to change the road transportation sector as society aims. This sector is very important for the global economy is what allows the buying and selling of products, the change of goods at a national and international level, the occurrence of imports and exports, so this sector can't stop or become less efficient or more expensive.

At the present, a hydrogen fuel cell uses high compressed gas storage tanks (350 or 700 bar), a battery, a fuel cell stack, and a battery pack for regenerative braking. One constraint of using fuel cell technology is the volume of the tank to store the hydrogen because the amount of hydrogen that is required to travel the same distance as an ICE vehicle is greater than gasoline or diesel, which means that the hydrogen tank requires to be bigger. This factor will affect even more the aerodynamics and the weight of the vehicle, which affects fuel consumption. So, the truck's design is very important, affecting the performance of hydrogen fuel cell trucks.

A study was conducted, for hydrogen fuel cell trucks, with the purpose of understanding which class or classes of trucks were suitable or indicated to be adapted to fuel cell technology [40]. This study showed that not all trucks will be acceptable hydrogen fuel cell vehicles, not even considering the most favourable assumptions. Classes of trucks with smaller dimensions would not be able to store the amount of fuel (hydrogen) that would be required for maintaining the performance of ICE trucks, it would be necessary to change the design of the truck to be worthy.

In opposition, larger trucks have enough space to store the amount of hydrogen necessary, without changing their design. But this doesn't mean that hydrogen fuel cell technology is not feasible for trucks. The study also shows that hydrogen fuel cell trucks are feasible and viable as zero-emission vehicles and, with some changes in the design in some classes, this option can meet the performance requirements of freight transportation.

A hydrogen fuel cell truck is possible and a suitable option but it is important to look for its components and size them and adapt the components to the performance that we need. In terms of components, it is necessary to look after the baseline of the vehicle, its weight, its cargo mass, acceleration performance (peak power output and gear ratios), motor, battery, fuel cell stack, onboard hydrogen storage and also consider the replacement of certain elements such as engine and fuel tank by a motor, fuel cell and hydrogen storage tank, and the removal of others like gearbox and torque converter [41].

4

Portugal Context

Contents

4.1 Portugal energy sector and hydrogen economy 25

4.2 Portuguese transportation sector 27

4.3 Water and energy in Portugal 31

4.4 Oxygen applications and Portuguese context 34

4.1 Portugal energy sector and hydrogen economy

Portugal has been reducing its fossil fuel consumption, and consequently, its fossil fuel imports. The reduction has been compensated with the increasing share of renewable energies [42]. Portugal has become a pioneer in green hydrogen by setting public policies, a national hydrogen strategy and helping to promote the hydrogen value chain, specifically promoting its production, storage, usage, and transportation/supply.

Nowadays, Portuguese society is starting to realize the advantages of introducing hydrogen in the energy sector. Hydrogen is a good energy carrier, that can be produced from a wide range of sources and used in several different ways. Adding to this, besides the reduction of fossil fuel dependency, there will be an improvement in the flexibility of the energy system (eg. energy storage at different scales), and there will be a better and higher energy mix.

But the real deal here is green hydrogen in Portugal. The European Union's senior official states, Christian Weinberger, states that believe that Portugal is capable of producing clean hydrogen at low costs. Christian also mentions that Portugal has a very good position to be competitive in the market, stating "For a country like Portugal, with great potential for producing green hydrogen at competitive prices, mixing it with other gases in the distribution networks represents efficient, low-cost solutions for the society, which could contribute to the hydrogen value chain as the production increases and logistics and distribution networks are being built". [43]

Portugal assumed the goal of being carbon neutral in 2050 [44] and to follow that objective, it started by closing the coal-fired power station. Portugal also states that hydrogen has a huge influence in decarbonisation, and aims to start to produce green hydrogen on an industrial scale, mainly due to its strategic advantages, such as the well-equipped deep-water harbour in Sines, solar energy (Portugal has a good sun exposition) at low prices (comparing with the world), available land that will allow implementing hydrogen production sites and a good natural gas network supply (using this grid will decrease the cost of hydrogen supply). It's clear that Portugal wants and will invest in the hydrogen economy and it will be very soon.

Decentralising production is one of the priorities. Instead of just having a huge central of hydrogen production and then the distribution would occur to all the country (called centralizing production), Portugal intends to have several hydrogen production sites, not limiting its production to Sines (the old coal-fired station), allowing a better production distribution to all territory. Sines has also its value because Portugal wants to develop a large production centre in the old refinery, and it has been preparing to move

Table 4.1: How can green hydrogen positively contribute to Portugal. [47]

	In summary
H_2	Reduces the imports and the energetic dependency Helps achieve the Energetic National goals Promotes innovation, research and developments Industry decarbonisation. Promotes new usages for natural gas grid and infrastructure. Transportation sector decarbonisation. Allows to Portugal to be an European green H_2 producer and export energy. Provides energetic security.

forward with a worldwide reference project, in partnership with the Netherlands. This partnership will have the participation of several private investors, through the application to IPCEI (Important Projects of Common European Interest) [45]. A centralized production will indeed produce greater amounts of hydrogen and the production cost would be lower, but the costs of the hydrogen will be higher due to the hydrogen distribution. Decentralized production produces lower amounts of hydrogen but the costs of distribution are lower. A decentralized production will be good also for the Portuguese economy. This will allow to make new investments in the interior of the country, develop the local economy, generate more jobs and opportunities to those locations that have been affected by emigration due to the lack of opportunities, these locations that started to be abandoned, will "gain life again" [46].

Right now, Portugal presents impressive conditions to produce green hydrogen on account of its geographic location, its renewable sources that have available (wind, solar, hydro), its capacity of producing renewable energy, already being capable of producing electricity with a very market competitive price (low production costs), with a mean value equal to 20,33€/kWh, ranging between 14,76€/kWh and 31,16€/kWh [47]. Some of the advantages of producing green hydrogen in Portugal are related to helping to decrease the decarbonisation costs, incentives and helping to implement the electrification strategy, helps to decrease also the energy dependency from external sources, promoting economic growth and creating jobs. Portugal intends to finance and to support projects that will contribute to achieving the target of decarbonisation by 2050, and will allow direct some of the European funds for that purpose, having committed to allocate 30% of the overall spending budget to climate action, which is 577 billion euros, including the energy transition [47]. Table 4.1 shows several contributions of green hydrogen for Portugal.

According to the approved National Plan of Hydrogen, [47] one of the short-term actions is to develop a mechanism that will help to develop hydrogen production and make sure that will be financial resources available in European funds to support renewable gases production. Another great advantage of Portugal is its natural gas infrastructure. The grid is still recent and modern, and its usage will allow to the distribution of green hydrogen through the offshore pipes. It is less expensive and enables to cover a greater territorial area. The combination of hydrogen with natural gas can be easily transported to a point where there is a need for energy. The particular case of refuelling stations is no exception. In order to supply a refuelling station through the natural gas grid, it would be necessary two things, a membrane, and a compressor. The membrane will allow the separation of the hydrogen and the natural gas, selecting the first from the grid and extracting it. Can be also called an electrochemical hydrogen separator. The membrane is a separation and purification technology and increases the range and potential of hydrogen as a more sustainable vector of fuel and energy, becoming an economic solution and ready to operate connecting to the existing natural gas network, and maintaining the purity of both gases, allows the selectivity of supply (natural gas or hydrogen) [48]. Then, after the hydrogen is collected, it is stored and for that, it is necessary to compress it. This compression can vary between 350 to 1000 bar. Being stored this way, it can easily refuel hydrogen vehicles, namely hydrogen fuel cell vehicles.

4.2 Portuguese transportation sector

According to the Portuguese Association of Oil Companies (called APETRO, Associação Portuguesa de Empresas Petrolíferas), says that liquid fuels (gasoline, diesel, etc) are the most ”visible” fuels that are originated from petrochemical distillation and are the ones most used in the road sector. Their wide use is due to their advantages compared with other forms of energy, concerning mobility, such as easy to store, easy to transport, a good energy density and intensity. But, throughout the years, there has been an evolution in this branch related to the improvement of fuel quality with the addition of additives, that promoted the better performance of the motors. This evolution took also into consideration the effects of the fuel consumption and usage were having in the planet, so the liquid fuels were also improved in order to decline the negative impacts on the environment, helping to enhance the air quality and to be more ”sustainable” [49]. In figure 4.1 it is shown the fuel consumption of 2019 per type of fuel and it is easy to see that road diesel is the one most consumed by far. On the horizontal axis it is discriminated the different fuels used being them (from right to left) butane gas, propane gas, GPL, gasoline 95, gasoline 98, road diesel, coloured diesel, diesel for heating, petroleum products, fuel and petro coke. On the vertical axis in t≪is discriminated the total amount of fuel consumed per tons.

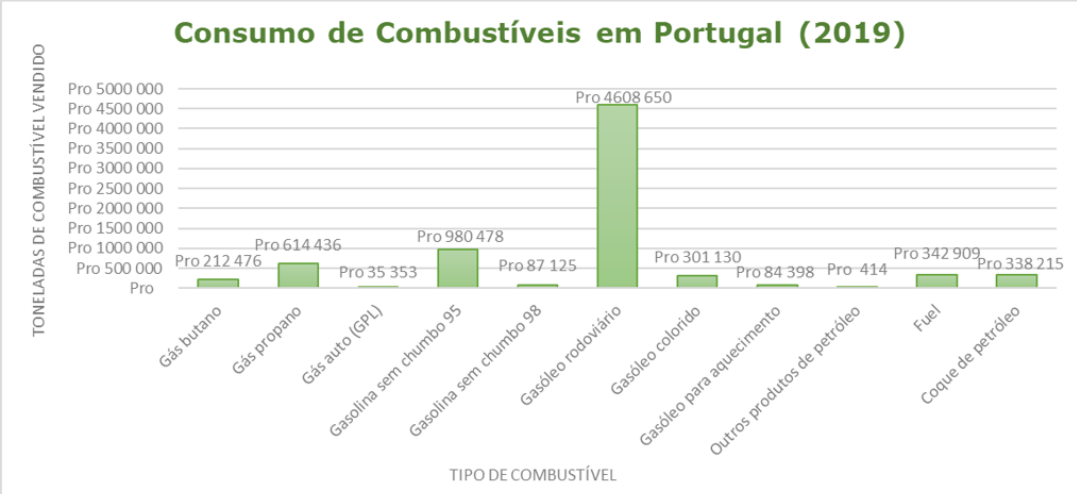

Figure 4.1: Portuguese fossil fuel consumption by type in 2019. [50]

However, the European Refinery Industry supports and shares the ambition of achieving carbon neutrality by 2050 and is investing in technology, research, and innovation to develop and to provide fuels that are capable to meet those goals. Examples of that are biofuels, from the first and second generation, like biodiesel, bioethanol, vegetable oils, biomethane, green hydrogen, and so on, or also called low carbon liquid fuels (LCLF). European Refinery Industry predicts to develop of liquid fuels with lower carbon content for all three transportation sectors (road, maritime and air) until 2050 with a capital investment of 30€-40€ billion euros and affirms that, if until 2050 150Mt of low carbon liquid fuels is produced, there would be a saving of 425Mt of carbon emissions, a value that accounts 90% and 50% of road and maritime emissions, respectively [49].

Concerning the Portuguese scenario, for the Long-Term Strategy for Carbon The neutrality of the Portuguese Economy by 2050, it is mentioned that ”Decarbonisation of the transport sector will be almost total (98% reduction in GHG emissions compared to 2005) and will be based fundamentally on strengthening the role of the public transport system and replacing current fossil fuel vehicles with a mainly electric fleet. The use of hydrogen and advanced biofuels will also play an important role in replacing current fuels” [44].

The RNC 2050 report also highlights that hydrogen is an important energy vector and also a good decarbonisation vector in road transportation, namely heavy transportation. It is even present that hydrogen will be produced by **alkaline electrolysis**, only using energy from **renewable sources**. So, all hydrogen that will be produced in Portugal will be green and will try to mitigate a little the emissions of freight transportation.

In Portugal, road transport accounts for 85.9% of the transport of goods and merchandise [51] and this is a very important sector for the Portuguese economy, due to the exportation of goods at the international level.

Transportation is fundamental to the economy and society, being crucial in terms of growth and job creation. Efficient transport systems are essential to enable European companies to compete in the global economy. The volume of exports, in 2017, totalled 39.4 million tons of goods, where the road mode that ensured the export of 39.1% of the quantity transported, being the second most used means of transport, after maritime transport. Compared to 2016, there was an increase of 2.9% in exportation's of goods [52]. In 2017, the sector of transports was responsible for more than 37% of final energy consumption in Portugal and due to that, and according to the Portuguese Directorate-General for Energy and Geology (Direção Geral de Energia e Geologia, hereafter DGEG), "this should be a priority sector in the definition of policies and measures that promote the security of supply and the diversification of the energy mix, through the use of more sustainable alternatives, with positive impacts on the reduction of oil dependence" [53].

Due to the influence of this specific transportation sector, it is easy to understand why it is necessary to act on it. New alternatives, better and more sustainable ones are needed, to reduce our carbon footprint, decreasing GHG emissions. This is a sector that cannot simply stop working, or working less, because would have a huge impact on several economical sectors in Portugal. It is necessary to transform this sector into a cleaner one but allow it to continue efficiently. For this, hydrogen fuel cell vehicles would be a good solution. Intending to give incentives and ensure stability to the energy sector in general and promote green hydrogen, Portugal developed a Hydrogen National Strategy, also called EN-H2. This plan, or strategy, proposes a set of action measures and targets for the incorporation of hydrogen in the various sectors of the economy [54]. EN-H2 assumes as main goals for 2030:

- **5% green hydrogen** in final energy consumption, **road transport** and industry;
- 15% green hydrogen injected into natural gas grid;
- **50 to 100 filling stations for hydrogen**;
- between 2 and 2.5GW of production capacity (using electrolysers).

The EN-H2 shows the evolution of hydrogen production through the years, from 2010 to 2050. In figure 4.2 it is possible to visualize that there's only available data of hydrogen production since 2015, and even in that time hydrogen was produced by SMR, to be use in refineries, in petrochemical processes to produce fuels. But a good thing that is also possible to see is the intentions of producing green hydrogen in the future, and by 2040 hydrogen will only be produced by sustainable methods, and gas reforming will not be a method used. Another interesting thing that is easily perceived is the main process that will produce green hydrogen, meaning the process that will produce hydrogen in higher amounts, is the water electrolysis, which makes sense taking into consideration the availability of water that Portugal has (sea, rivers, etc).

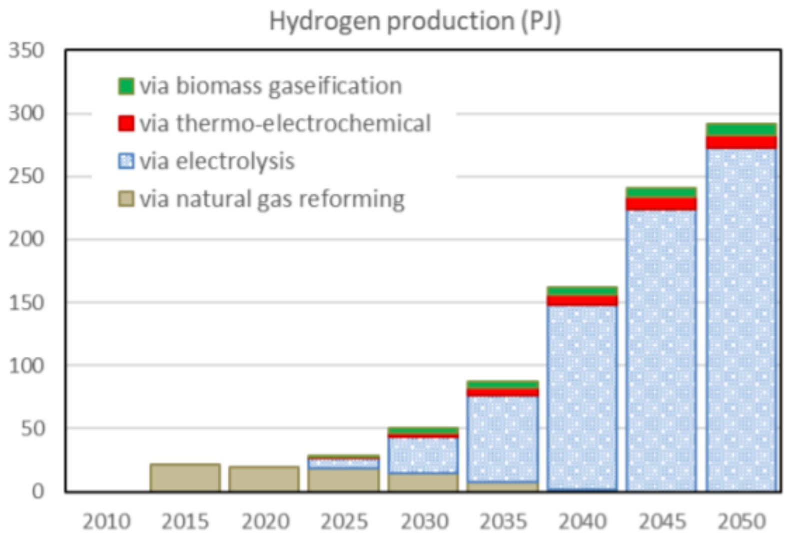

Figure 4.2: Hydrogen production prediction in Portuguese context. [55]

In the figure 4.3 there is the respective data of figure 4.2, where we can see the predictions of the amount of hydrogen that Portugal intends to produce in the future, discriminated by the process. The goal of Portugal is the remove all fossil sources of hydrogen production until 2045.

	2010	2015	2020	2025	2030	2035	2040	2045	2050
via natural gas reforming *		21.9	19.6	18.2	14.3	7.9	1.7		
via electrolysis				8.5	29.5	68.6	145.9	223.8	272.5
via thermo-electrochemical				1.11	2.95	5.8	8.7	9.5	10.4
via biomass gaseification				0.99	3.65	4.8	6.0	7.4	8.8
Total		*22*	*20*	*29*	*50*	*87*	*162*	*241*	*292*
renewable total				*11*	*36*	*79*	*161*	*241*	*292*
mix of production %									
non--biological		*100%*	*100%*	*97%*	*93%*	*94%*	*96%*	*97%*	*97%*
biological		*0%*	*0%*	*3%*	*7%*	*6%*	*4%*	*3%*	*3%*
*fossil **		*100%*	*100%*	*63%*	*28%*	*9%*	*1%*	*0%*	*0%*
renewable		*0%*	*0%*	*37%*	*72%*	*91%*	*99%*	*100%*	*100%*

(*) completely consumed within refineries

Figure 4.3: Evolution of contribution of each method to hydrogen production. [55]

4.3 Water and energy in Portugal

The production of hydrogen through electrolysis consumes water as raw material, and per each kilogram of hydrogen that is produced, it is consumed 9 litres of water, and it is only being considered the water for the stoichiometry of the reaction, which makes water consumption very relevant. Besides the water that is being consumed, it is necessary energy (electricity) to sustain this process. Depending on the technology that is being used and the source of energy that is being considered, the consumption values may vary. Electrolysers suppliers give an estimation that the average is of the order of 13.4 L of water/kg of hydrogen, which corresponds to about 400 m^3 of water/GWh of hydrogen produced. [47]

4.3.1 Availability of water resources in Portugal

There is a variety of water sources that can be used for electrolysis, such as seawater, estuaries, surface waters, groundwater, rain waters, or even treated and recycled water, and it is very important to explore the multiple options available, since freshwater is such a scarce resource, being even more at risk due to the impacts of climate change, as explained by Intergovernmental Panel on Climate Change (IPCC) [56].

Portugal is located at the point of the European continent and is a territory that is bordered by water, except for one side, making it part of a peninsula, the Iberian Peninsula. Despite the vast amount of water around its territory, it is salty, which greatly limits its use. However, besides being surrounded by this resource, Portugal also has good water resources in its interior, freshwater resources. Water resources are used at the National level in a great variety of sectors such as industrial, agricultural, domestics, public, and so on.

The Portuguese territory has good water reserves, that can be discriminated into surface reserves and groundwater reserves, but the amount of water stored is not constant throughout the year. According to the Portuguese Environmental Agency (APA - Agência Portuguesa do Ambiente) ”knowledge of water availability allows for more sustainable management of resources (...) This indicator reveals the water availability in a given year, comparing it with average values, allowing us to evaluate whether it was a wet, average or dry year” [57]. For hydrogen production, both types of waters (sea and fresh) are viable for the process, it is only necessary to resort to the use of desalination methods that will help to purify the water, turning it suitable to use. Two of those methods are thermal desalination or membrane methods, previously mention in 2.

When the subject is natural resources, it is crucial to know how to manage them and more importantly, to preserve them. Instead of using freshwater as raw material for electrolysis to produce hydrogen, it is possible to think similarly as a "circular economy" and give a second chance to the waters that are being treated in water treatment stations. With the right treatment, there is a possibility of reusing residual waters, which allows transforming the hydrogen economy even more sustainable with lower environmental impacts. Portugal has a vast number of water treatment stations dispersed per all country, as it is represented in figure 4.4.

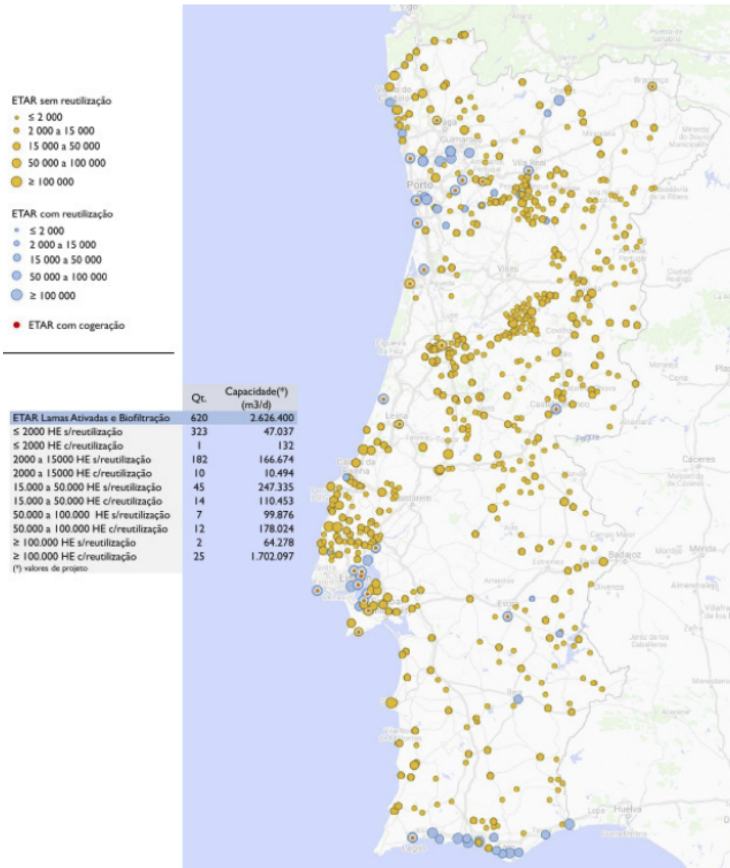

Figure 4.4: Portugal water treatment stations display in the country. [47]

In terms of numbers, Portugal accounts for 4370 treatment stations, being 2759 of the residential water treatment stations (also called ETAR - Estação de Tratamento de Águas Residuais). But the less positive part is only 30 stations from the total of 2759 stations are currently treating residential water with the final purpose of reusing it, and this only accounts for 1.2% of the total amount of residential water treated [47].

The reuse of this water helps promote the synergy between the energy sector, through electrolysis producing hydrogen, and the hydro sector, and more importantly, it can help to display the hydrogen economy along with all Portuguese territory, allowing general access to it.

It is possible to verify that water resources will not be a problem for hydrogen production via electrolysis and it is possible to green hydrogen sustainably, without using scarce resources, and even encourage reuse and recycling of materials (residual waters). This aligns with the usage of water treatment techniques, mentioned in chapter 2, namely in subsection 2.3.3, provides all tools to the implementation of green hydrogen and enables its growth.

4.3.2 Energy and electricity in Portugal

The energy in Portugal comprises energy and electricity production, consumption, and also imports. Portugal belongs to the Iberian Electricity Market (also called MIBEL) that results from the cooperation between Portugal and Spain and encourages the integration of electrical systems of both countries [58]. The electricity price of MIBEL is very competitive, and the prince from Portugal and Spain match 95% of the time. Just in Portugal, there are around 40 electricity suppliers, on the free market.

Focusing on Portugal, it is important to highlight the incorporation of renewable energy, which has been increasing, helping reduce the GHG. In the past few years, Portugal has been showing high levels of renewable incorporation from several sectors, with a value above the European average, achieving a share equal to 52,2% in 2018, assuming the 5th place of the European country with the highest share of renewables in the energy mix [47].

Portugal has been declining its dependency on energy imports and raising its domestic production. This gives a higher level of security in the energy supply. The energy targets that Portugal wants to achieve are a reduction between 45% to 55% on the emissions, increase until 35% in the energy efficiency, improve the renewable energy consumption/usage until 47%, implement until 20% renewable energy in the transportation sector and finally use improve until 15% the electrical interconnections. [47]

The transformation of the energy sector will give a better contribution to decarbonization and renewable energies have a crucial role in it. Portugal is currently less dependent on energy from abroad and more efficient. In 2009 it had an energy dependence of 81.2% and in 2019 this stood at 74.2%.

In the same year, 2019, renewable energy represented 30.6% of the gross final energy consumption (GFC) and Portugal was positioned as the 7^{th} country in the EU-28 with the highest weight of energy from Renewable Energy Sources (RES) in GFC. In 2020, the import balance of energy products was 2,914 million euros which, compared to 2019, represented a reduction of 38.6% in euros. Between 2009 and 2020, installed power for electricity generation increased by about 4 GW, mainly in power plants producing electricity from renewable sources, where photovoltaic power accounted for only 7.1% of total installed power [59].

The transport sector remains the main energy consumer, accounting for 36.1% of total final energy consumption in 2019. So, it is easy to understand the need of changing and the need of adopting new and cleaner alternatives [59].

Concerning energy and electricity, Portugal has been improving and green hydrogen will not be a drawback. To produce green hydrogen through water electrolysis it is necessary large amounts of electricity, so Portugal needs to be able to sustain this process, without needing to appeal to energy imports. Renewable energies are been increasing their shares in the energy mix, and Portugal has good conditions to improve even more the energy sector.

4.4 Oxygen applications and Portuguese context

Oxygen has several utilities and can be used in several different sectors. Oxygen is a strong oxidizing agent and easily reacts with flammable materials to release energy, under heat form, during the reaction or combustion process. This gas is one of the largest industrial gases used and its usage is related to its reactivity. Currently, the majority and the largest amounts of oxygen produced are through cryogenic distillation, providing high purity levels of oxygen. Besides this process, oxygen can be also produced through adsorption methods but the quality/purity is lower.

In terms of applications, oxygen is used in the medical sector, water treatment stations, metal refining and fabrication processes (for example steel making), in several industries such as glass, ceramic, pulp and paper, in petroleum refining, and even in pharmaceuticals processes.

- **Medical sector:** the majority of living beings require oxygen to live, so it is easy to understand the importance of this gas in healthcare. The oxygen is used to aid resuscitation, life support, to improve cardiovascular stability, in modern anesthetic techniques, helps restore tissue oxygen tension [60].
- **Water treatment stations:** to treat the residential waters, usually, it is used the open air. But, the usage of enriching the air with oxygen or pure oxygen (around 90% oxygen) helps to improve the efficiency of the aerobic treatments, improving the dissolution of oxygen in the water and avoiding the entering of nitrogen [61]. The usage of oxygen is important during the aerobic stage of water treatment and it is influenced by several factors, being one of them the temperature. If

the temperature rises (for example during summer), the aerobic bacteria used during this stage, require more oxygen to dissolve the pollutants and organic matter (OM). Oxygen allows improving the biodegradation.

- **Metal refining and fabrication:** steel making is the largest user of oxygen. The gas is used to increase the combustion temperature in order to produce combustible materials, avoiding this way coke formation (that is unwanted). Helps also to decrease the energy requirements of the process [62].
- **Petroleum industry processes:** oxygen is used for coal gasification, in large amounts, and also helps enrich the air that feeds a process called catalytic cracking, in regenerators. Oxygen enables to have a more complete reaction (combustion process) and destroy hazardous or waste materials inside the incinerators. [62].
- **Glass and ceramic:** the usage of oxygen, instead of air that has only 21% of oxygen, improves the heating and the efficiencies of the furnaces, helping reduce the NO_X gases emissions and allowing a lower fuel consumption [62].
- **Pulp and paper industry:** oxygen works as an oxidant specifically in mills, during processes such as delignification, bleaching, chemical, and wastewater treatment processes. This enables to improve product quality and energy consumption [63].

The previous applications correspond to several oxygen applications that are used worldwide. Focusing on the Portuguese context, 4 major sectors consume oxygen, being them: healthcare, glass industry, pulp and paper industry, and wastewater treatment stations. The level of purity required in the different sectors is not the same and the selling price is different considering the sector that is being applied.

Industrial oxygen, due to the larger amounts that use for several processes and applications, has a lower price compared to the oxygen that is used in hospitals or home care. For the industry purpose, oxygen selling prince in the market is around 100€/ton to 150€/ton (which gives between 0.10€ to 0.15€ per kilogram of oxygen) [64]. Concerning the medical oxygen price, it is influenced by a few such as whether the oxygen is delivered from an external supplier in cryogenic vessels or if it is produced on-site (medical facilities like hospitals). For the neighbouring country, Spain, the oxygen selling price may vary between 0.675€/kg to 6.7€/kg. The lowest price of 0.675€/kg corresponds to the liquid oxygen in bulk, for 50L barrels of oxygen the price rises to 1.342€/kg and the highest price of 6.7€/kg goes to the 10L barrels [65]. In Portugal the prices are similar. The last complete data available from Portugal is from 2020, where the total cost of the medical oxygen accounted for 10 588 103€, rising 1.7% comparatively to 2019. But, the year 2020 was a particular year due to the pandemic situation. Covid-19 is a disease that affects the respiratory systems, so this promoted the increase of oxygen consumption in this sector. Using the data from 2019, considering the total amount of oxygen that was consumed and the associated costs of it, the selling price of the oxygen is around 1€/kg. This will be explained in more detailed further in chapter 5 and chapter 6.

The sectors previously mentioned are possible Portuguese costumers to whom it would be possible to sell the oxygen, that comes as a by-product of water electrolysis. The level of purity of the oxygen produced from electrolysis is high, which enables this gas to be used in all different sectors, even in healthcare. But, the selling price is an important question to ask also is if the national market will be enough or if it would be necessary to expand to other countries.

5

Hydrogen Supply Chain in Portugal - Model Formulation

Contents

5.1 Objectives 38
5.2 Assumptions and Restrictions 38
5.3 Model Formulation - Hydrogen Supply Chain 40

5.1 Objectives

In this work, I intend to create a Hydrogen Supply Chain Network (HSCN), in a Portuguese context, to understand **where it would be more interesting to implement hydrogen production sites** in the country, namely **green hydrogen** production sites through **water electrolysis**. My case study will be **freight transportation companies** , specifically heavy-duty trucks . Being road transportation is one of the biggest emitters, it is my interest to understand the impact this sector will suffer by adopting hydrogen fuel cell technologies into their fleets and having hydrogen refuelling stations infrastructures. **One of the goals** of this work is to understand if it would be **economically attractive** or not to start to develop a green hydrogen economy in this sector. As explained previously in this work, the production of green hydrogen is still very expensive and corresponds to a very small percentage, worldwide. This is not different from Portugal's case. One key element in this study will be the oxygen that comes as a by-product of water electrolysis, and the associated **profit** of its **selling**. So, the main purpose of this work is to try to understand the impact of implementing hydrogen economy, where would be more efficient to implement hydrogen refuelling stations, who would be the **first adopters** (or which entities would make more sense to adopt this technology) and how oxygen selling can contribute to that.

In Portugal, several sectors could be oxygen consumers like pulp and glass industry, metallurgic, hospitals, and water treatment stations but to simplify the network it was decided to choose only one of them. For this study it was selected **the hospitals as the oxygen consumers**, meaning that they will be the entities to whom it will be sold. It will evaluate the oxygen consumption levels, taking into consideration national data, and analyse the amount of oxygen that is needed and the amount it will be possible to supply to them.

5.2 Assumptions and Restrictions

A non-empiric scenario will be created and the hydrogen sites will be inside the transportation companies, where they all agreed to assume a target of decarbonisation of 5%. This means that they assume a commitment to reduce about 5% of their fleet, and consequently decrease their fossil fuel consumption, in a year, replacing them with hydrogen fuel and fuel cell vehicles. The intention is not all companies have their own hydrogen refuelling station, meaning not all companies will produce hydrogen in their infrastructures because economically would not be profitable, which would be unattractive for them. So, the intention is to find strategic points/locals where would make sense to install these stations, by forming clusters of companies and to evaluate where would be feasible to produce the hydrogen fuel in order to supply it in an efficient way to all the companies in the neighbourhood, of each cluster. Further, will be possible to understand the selection criteria of producers and consumers of this work.

The purpose is to find the optimal combination of these components and to obtain the minimum cost of implementation of hydrogen supply chain, by using an **optimization method** called **Transportation Assignment**. This method is a simple optimization tool that will find the lowest combination cost of distribution of hydrogen from a producer to the consumers, from all network involved, based on the objective function 5.1 that gives the unitary cost of hydrogen (€/kg), not considering the selling of the by-product on a first analysis, because this will depend on the consumer demand too. To this optimization some restrictions are associated, that will be clarified along the work. They are:

- The amount of hydrogen corresponds to 5% of fleets transformation of each company, based on the number of kilometers traveled and mean hydrogen tank capacity.
- Companies hydrogen demand.
- Hospital's oxygen demand.
- The energy required for the water electrolysis will be supplied completely from renewable sources.
- Water consumption for the electrolysis. The water comes directly from the water grid and a reverse osmosis technology is implemented.
- The distance in kilometers between the companies. The maximum distance between the companies involved in the study, varying between 20km to 50km.
- The minimum number of elements associated to the network. For the clustering it was considering a variation between 2 and 5 elements.
- The oxygen is only being sold to hospitals, based on there total demand.
- The associated costs of transporting the hydrogen is based on the linear distance between the producer to the consumer.

After the creation of this network, an optimization formulation is solved and the output of the optimization gives:

- The optimal structure of HSCN in Portugal;
- The minimum cost of implementation;
- Which companies will be totally satisfied (and which not);

A similar study was performed for the industrial sector decarbonisation in Qatar [66]. This work intends to adopt the same idea, to the Portuguese economy, in the context of the refuelling stations and for the freight transportation sector.

5.3 Model Formulation - Hydrogen Supply Chain

5.3.1 Objective Function

The hydrogen supply chain network (HSCN) proposed function consists of the following main cost/profit components: the costs are related to hydrogen production, hydrogen transportation, and water supply. The profits considered are associated with oxygen selling. Each of these components will be described in thesis. The purpose of this work is to minimize the cost of HSCN. The equations formulated will give the cost per unit of hydrogen (€/kg H_2). The final objective function will provide the minimum Total Annualized Cost (TAC) for the supply chain:

Objective function:

$$TAC = HP^{Cost} + HT^{Cost} + WSC^{Cost} - BP^{Profit} \tag{5.1}$$

Where,

- HP^{Cost} is the hydrogen production total cost [€ / y]
- HT^{Cost} is the hydrogen transportation cost [€ / y]
- WSC^{Cost} is the water supply cost [€ / y]
- BP^{Profit} is the total oxygen sold to Hospitals [€ / y]

This equation is crucial to evaluate the unitary cost of the hydrogen in the network and it is what will allow to apply the Transportation Assignment method, allocate the hydrogen from the producers to the consumers, choosing the most cost efficient path. All of the elements present in the equation 5.1 will be describe in the following pages.

5.3.2 Transportation Companies - Producers and Consumers

As mentioned previously, the case scenario of this work visualize the cost of hydrogen economy implementation in Portugal in the context of road transportation, namely freight transportation, because the transportation sector is one of the biggest GHG emitters, has a huge influence on the Portuguese economy and travels long distances.

This work intends to create a realistic scenario, that would help to understand the cost of implementing hydrogen in Portugal. For that reason, the selection of the transportation companies was made based on their ranking position, where the ranking presents Portuguese companies and is ordered according to the value of their sales, allowing to know the position that a particular company occupies nationally, region, or sectoral [67]. This ranking contains 7621 companies but only the first 100 companies were selected.

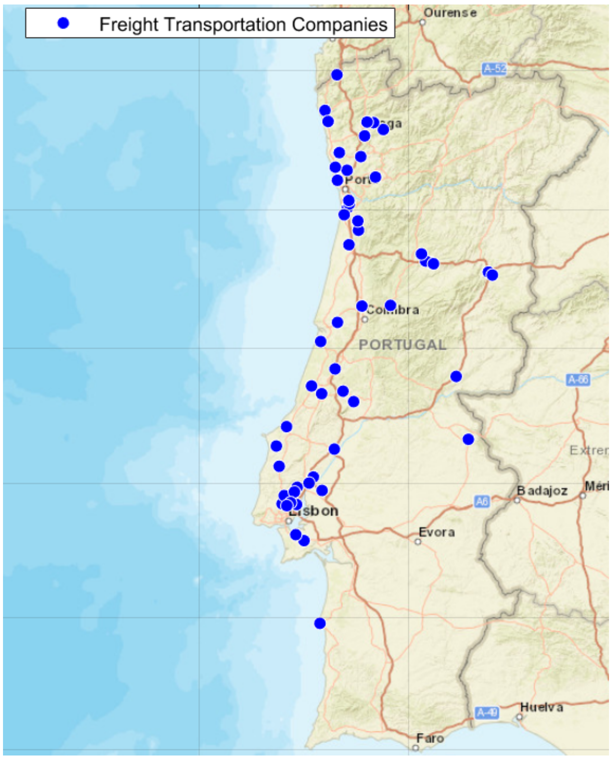

Figure 5.1: Portuguese freight companies display. Companies analysed.

The next step was to evaluate which of those companies did international transportation because this work is only interested in long distances travels because it is where heavy-duty hydrogen fuel cell trucks will have the advantage in relation to electric heavy-duty vehicles. For that, it was consulted a document of Mobility and Transportation Institute (also called IMT - Instituto de Mobilidade e dos Transportes), where I could find every freight company that is present in Portugal and discriminates the type of transportation that each company does, if national, international or both [68].

International trips require to travel longer distances and the trip itself already requires too many hours, so it is not possible to think about making a stop during this transportation to recharge the vehicle battery, which will take several hours, even if it uses supercharge. It is important to mention that using this mode of recharging the battery (supercharge), as a frequent form of recharge, throughout the time, will affect the battery system and damage it, which is not a good scenario. Heavy-duty hydrogen fuel cell is a good alternative since a fuel tank can be filled in 15 to 20 minutes, similar to internal combustion engines, like diesel.

The final selection of companies was done based on 2 factors and it was given priority to the ones with available data: the number of vehicles in the fleet and the number of kilometres travelled in a year. In table 5.1 is possible to visualize a representation of the selection of the companies, in red are the ones that are excluded because didn't fill all the parameters, didn't have data available (like the number of vehicles in the fleet) and/or because only do national transports. With this selection, the number of companies suitable for the study decreased to 56. All companies can be visualized in table 8.1, presented in the appendix.

Table 5.1: Data representation. Portuguese freight companies.

Raking	Company	County	District	National/International	Fleet Size
1	DOCTRANS - Transportes Rodoviários de Mercadorias Lda	Azambuja	Lisboa	Both	2000
2	Luís Simões - Logística Integrada, S.A	Loures	Lisboa	Both	2100
3	Lamision - Sociedade de Transportes, Lda	Azambuja	Lisboa	Both	—
4	TJA - Transportes J. Amaral, S.A	Estarreja	Aveiro	Both	800
5	LASO - Transportes	Mafra	Lisboa	Both	2000
6	Patinter - Portuguesa de Automóveis Transportadores, S.A	Mangualde	Viseu	Both	2000
7	Dachser Portugal, Sociedade Unipessoal, Lda	Vila do Conde	Porto	National	—
8	STEF Portugal - Logística e Transporte, Unipessoal, Lda	Vila Franca de Xira	Lisboa	Both	2300
9	TRANSBASE - Transporte e Logística, S.A	Alcacena	Santarém	International	—
10	Transportes Paulo Duarte, Lda	Torres Vedras	Lisboa	Both	1179
11	Transportes Florêncio &Silva, S.A	Mafra	Lisboa	Both	—
12	Transportes Broliveira, Lda	Ourém	Santarém	Both	400
13	Transportes Pascoal	Mealhada	Aveiro	Both	350
14	Dilofar - Distribuição, Transportes e Logística, Lda	Vila Franca de Xira	Lisboa	National	—
15	LUSOCARGO - Transitários	Maia	Porto	Both	—
16	XPO Transport Solutions Portugal, Lda	Vila Nova de Gaia	Porto	Both	—
17	Transmaia	Trofa	Porto	Both	435
18	ZAS - Transportes e Logística, S.A	Mafra	Lisboa	Both	—
19	Transwhite - Transportes, Unipessoal, Lda	Caldas da Rainha	Leiria	Both	170

To be able to determine the amount of hydrogen that each company needs, to agree with the 5% decarbonisation target, it was necessary to search for the average kilometres that each company does per year. With this information would be possible to know the average kilometres that each truck does for a specific company. This is very important because influences the hydrogen consumption of each truck depending on the company. Here, again, there was a lack of available data but due to the fact of having already a small number of companies for the study, instead of eliminating the ones that didn't have the information, it was used the average value of kilometres for them, taking into consideration the data from the other companies.

Table 5.2: Hydrogen heavy duty fuel cell Vehicles brands characteristics. [69], [70], [71], [72]

Type	H2 Storage Capacity (kg)	Pressure (bar)	kilometres	Fuel cell Capacity (kW)	Battery (kWh)	kg/km
Mercedes	2×40	—-	1000	300	—-	0,08
Hyundai	32,09	350	400	190	—-	0,080225
Toyota	40	700	482	226	12	0,082987552
Nikola	TBA	TBA	805-1207	TBA	250	—-

Based on some hydrogen heavy truck vehicle brands available, considering their tank capacity in kilograms (kg) and the kilometres (km) that they were capable to travel, it was calculated a hydrogen consumption factor per kilometer (kg H_2/km). With this, it was possible to determine the amount of hydrogen that it is necessary to supply to a company considering the kilometres that it does per year. Some truck brands characteristics can be seen in table 5.2.

Knowing the number of vehicles that each company's fleet, it is possible to know the number of vehicles that need to be transformed to agree with the 5% decarbonization target. If a fleet has 2000 vehicles, it needs to acquire 100 hydrogen fuel cell vehicles in its fleet. Adding the knowledge of the average kilometres, it is possible to know the total consumption of hydrogen that the company will have, using the hydrogen consumption factor that I developed. Considering still the previous example of 100 vehicles, multiplying it by the average kilometres per truck and by the hydrogen consumption factor (0.08 kg H_2/km), it is obtained the total amount, in kilograms, of hydrogen that the company requires. Table 5.3 represents a sample of the process previous explained. All data can be found in the appendix, table 8.3. On the first column, it is the raking that is related to the position of the company of the list used, the second column shows the number of vehicles that each company has followed by the number of total kilometres that the company does per year than the fourth and fifth columns is the number of vehicles that corresponds to a 5% transformation, being the fifth the rounded value, and the final three columns are the hydrogen demand, the total oxygen produced considering the demand and the total amount of water that would be required, respectively.

Table 5.3: Companies characteristics. Representation of the data used in the study.

Ranking	Fleet Size	Kilometres	5% fleet	5% fleet	Hydrogen Need (ton)	Oxygen (ton)	Water (ton)
1	2000	125000000	100	100	10000	80000	90000
2	2100	200 000 000	105	105	16000	128000	144000
4	800	80 000 000	40	40	6400	51200	57600
5	2000	50 000 000	100	100	4000	32000	36000
6	2000	125000000	100	100	10000	80000	90000
8	2300	125000000	115	115	10000	80000	90000
10	1179	45 000 000	58,95	58	3600	28800	32400

Since this technology is currently expensive, it wouldn't make sense to all companies to acquire it, **plus acquiring the fuel cell vehicles** and each of them to implement the infrastructure necessary for the production. With this in mind, it was necessary to decide which of the companies were better ones to produce hydrogen, meaning which companies should be chosen to install the infrastructure to produce and store green hydrogen through water electrolysis. Two approaches were considered and both will be described in the following.

When thinking about refuelling the vehicles, it is not possible to think about a station that is too far from the vehicle or that requires to travel long distances to refill the tank. So, for the first approach considered, it was calculated the distance between each company to the other with help of MATLAB Software, using geographic coordinates, latitude and longitude, present in table 8.2 presented in the appendix. These coordinates were obtained from Google Maps and the same company had more than one logistics centre, the position considered was or the major or the headquarters. But, only one logistics centre per company was taken into consideration. For each company was determined the average value of kilometres (the mean distance from one company to the others), and the 10 companies with the lowest mean value were selected to be the producers.

The companies selected to be hydrogen producers, or shortly called ”producers”, assume also the decarbonization target of 5%. This means that the producer will produce for itself and the others. For this work, it is assumed that producers will produce until 10% of their fleet transformation, supplying their own fleet and the remaining 5% is to supply the other companies, also called ”consumers”, that have a demand of 5% of their fleet.

In figure 5.2, it is possible to see the displacement of the companies considered, where they are differentiated by colors, which in green are that companies that are being considered as producers and in red and the companies considered as only consumers. An interesting thing to mention is that the majority of the companies are located in the north and centre of Portugal, close to the coast, and Porto and Lisbon’s districts are the ones with the highest number of companies.

Looking to figure 5.2, it is possible to see that are some companies very close to each other and, there are no producers close to those groups, for example, the case of Lisbon, Porto, and/or Braga districts. Analysing this situation, it would not be efficient to have a group of consumers without a close producer or have a producer isolated in the interior of the country. Due to this, it was decided to change the strategy of choosing the producers and consumers. Instead of taking into account the mean distance from one company to all others, the decision was to evaluate as groups. Considering all companies, clusters were formed with them and, per each cluster, there would be one producer. The clusters were determined based on the position of companies with help of MATLAB Software.

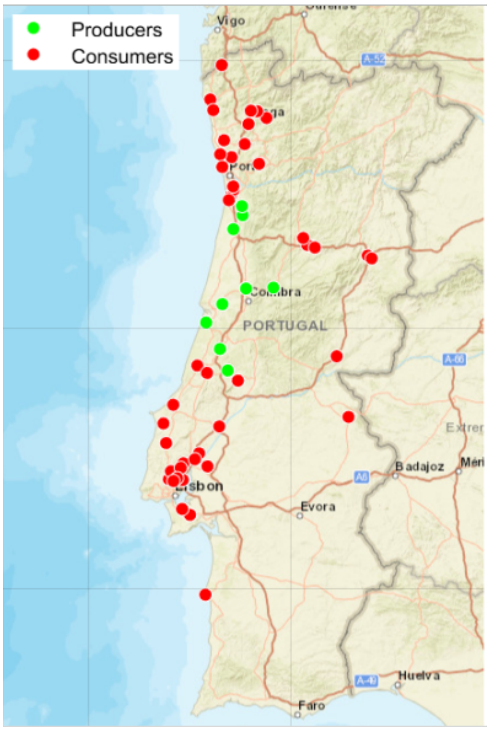

Figure 5.2: Producers and consumers display. Freight companies considered in the analysis.

With this new approach other factors require to take into consideration such as the number of clusters that will be formed (that affects the number of necessary producers), the minimum number of elements that each cluster must have (for example would not make sense to create a cluster with only one company), the maximum distance between the two furthest points in the cluster, because a cluster where the two furthest points distant from each other 100 kilometres would not be efficient for the supply chain and finally, a very important thing to take into consideration is if every company will participate on the supply chain. For a company that does not follow every requirement, it will be excluded from the clusters.

The function used in MATLAB finds clusters in a set of spatial points expressed in XY coordinates [73]. So, the geographic coordinates (latitude and longitude) of each company were transformed into Cartesian coordinates and they were displayed into an XY graphic. To obtain a more realistic result, and to be possible to work with distances and preserve the companies characteristics, it was used a simple equirectangular projection, and the data of the companies were converted into distances to Earth's referential origin, namely, Equator (Latitude) and Greenwich Meridian (Longitude), using equations 5.2 and 5.3:

$$x = L_1 \times \cos(\phi_0) \tag{5.2}$$

$$y = L_2 \tag{5.3}$$

Where:

- x is the longitude in kilometres;
- y is the latitude in kilometres;
- ϕ_0 is the longitude close to the centre my map, Portugal in this case;
- L_1 is the arc length from Greenwich Meridian to the longitude position of the point in analysis.
- L_2 is the arc length from equator until to latitude position of the point in analysis.

As known, our planet despite being flatted in the poles is a sphere and it is possible to project a distance between two points in terms of both an angle and a linear distance. The arc length (L) was obtained by using that method, using equation 5.4:

$$L = \frac{2\pi \times R \times A}{360} \tag{5.4}$$

Where,

- R is the Earth's radius equal to 6371 kilometres;
- A is the longitude data for x or the latitude data for y, for equations 5.2 and 5.3, respectively.

It is important to remind that do not exist any isometric map that transforms the exact sphere that Earth is into a plane. Converting the latitude and longitude coordinates to an XY system will affect the lengths and some deformation may appear, meaning some errors in the approximation will be present. But, since this work is using a small area from the globe, namely Portugal country area, the simple projection used, equirectangular projection, is sufficient for the purpose.

In the end, it is obtained a graphic similar to the one in figure 5.3. Imposing some restrictions, such as the minimum number of elements per cluster, and the maximum distance of the two furthest points, the program runs and creates clusters based on the distance of each company to the other.

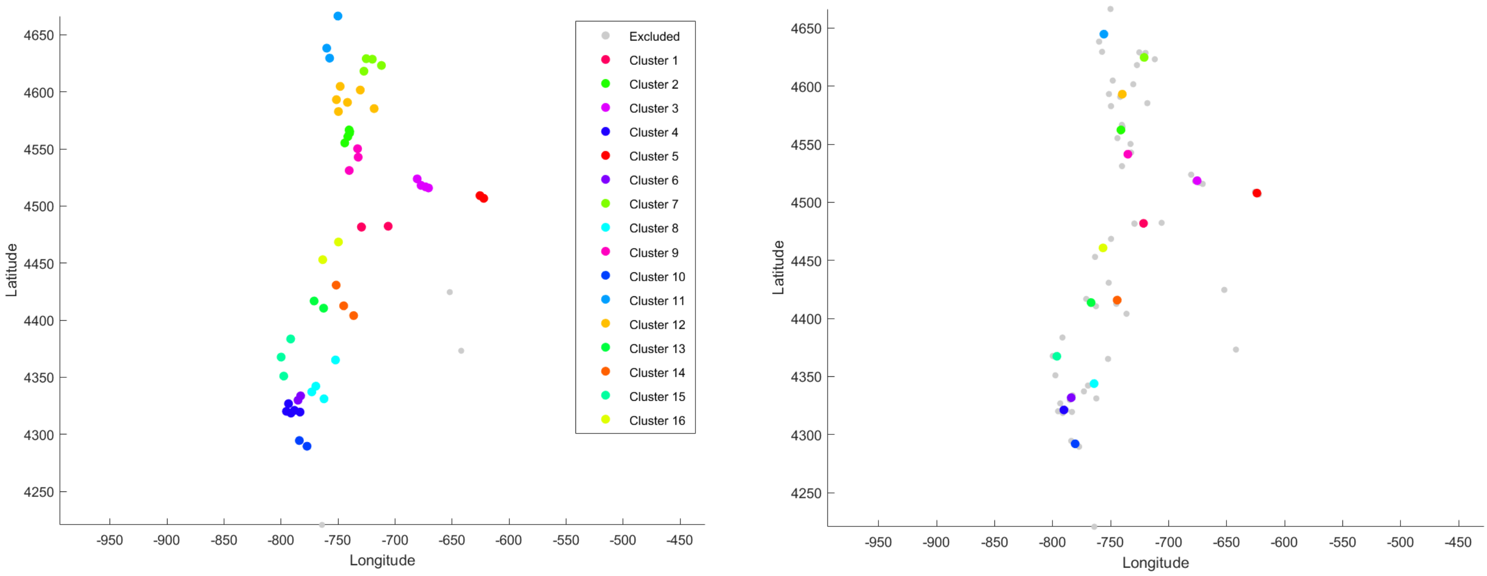

Figure 5.3: Clustering process. Clusters with a minimum of 2 elements and with a maximum distance of 50 kilometres.**(Left)** Respective clusters centroids.**(Right)**

In figure 5.3, on the left, it is demonstrated the clustering formation, by limiting them with a minimum number of elements equal to two and a maximum distance equal to 50 kilometres. This means that to form a cluster it must have at least two companies less than 50 kilometres apart. In fact, this will be my minimum condition that will be evaluated in this study. Maximum distance will vary between 50 to 20 kilometres and the minimum number of elements per cluster between 2 to 5. Besides the clusters, the program also returns the centroid of each cluster, as it can be seen in figure 5.3, on the right.

Besides the maps display, it is also obtained the coordinates of the elements present in each cluster and the coordinates of each cluster centroids. The second is particularly interesting. The centroid is the point that is located in a certain position that stands apart equally from all elements in the cluster. This could be very advantageous information if one of the purposes of this work would be to build a hydrogen refuelling infrastructure that could be strategically located for all companies in each cluster. But, this works assumes that one of the companies is going to obtain the technology and use their infrastructure of them, for the first stage of development.

Compared with the map display of figure 5.1, it was a good conversion of the positions of the freight companies to an XY equal-area system. In the figure 5.4 it is possible to visualize the overlapping of the map of figure 5.1 and the clustering and see that both of them match.

After doing the clusters, it was necessary to finally decide which of the companies will be responsible to install the technology. So, since in this case, distance is not the main issue anymore, the size of the company becomes the major deciding factor. The logic here is that the largest company (the company with the largest fleets), will have bigger infrastructures and spaces, hence, easier it is to implement and accommodate the electrolysis technology. Besides this, the largest companies will have more capital investment to implement it. Table 5.4 summarizes the results obtained in this step.

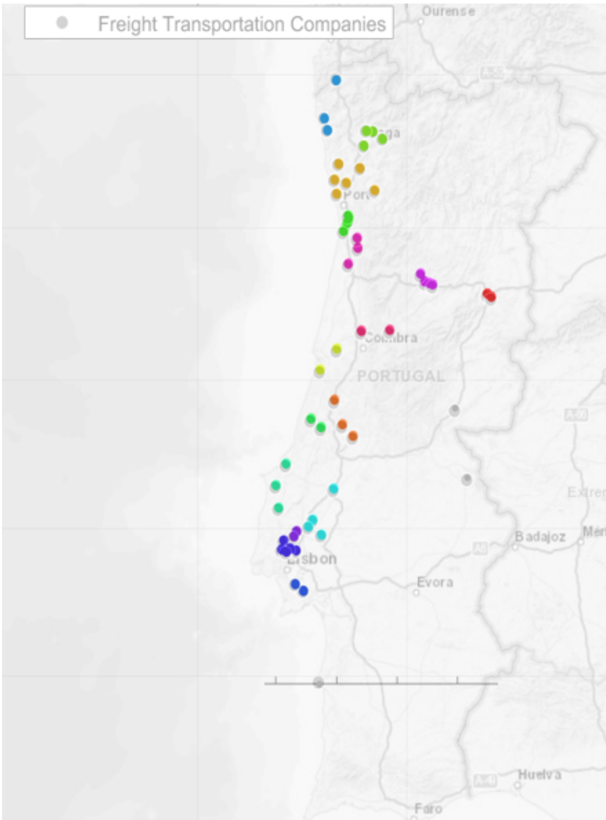

Figure 5.4: Overlap of the map with the display of the freight Portuguese companies and the clusters map.

Table 5.4: Summary of the applied restrictions and the obtained results.

Nº Element per cluster Max distance (km)	**2**	**3**	**4**	**5**
50	16 clusters were formed. 3 elements don't belong to any cluster.	11 clusters were formed. 13 elements don't belong to any cluster.	6 clusters were formed. 28 elements don't belong to any cluster.	3 clusters were formed. 40 elements don't belong to any cluster.
35	16 clusters were formed. 3 elements don't belong to any cluster.	11 clusters were formed. 9 elements don't belong to any cluster.	6 clusters were formed. 28 elements don't belong to any cluster.	3 clusters were formed. 40 elements don't belong to any cluster.
20	15 clusters were formed. 9 elements don't belong to any cluster.	9 clusters were formed. 21 elements don't belong to any cluster.	5 clusters were formed. 33 elements don't belong to any cluster.	3 clusters were formed. 41 elements don't belong to any cluster.

5.3.3 Oxygen demand - Hospitals

For the water electrolysis, it is necessary water as well as electricity, as previously mentioned. In terms of numbers, it requires about 9L of water to produce 1kg of H_2 and around 8kg of O_2, as by-product [16].

The O_2 generated from water electrolysis has a very high level of purity. In literature, it is already mentioned that this oxygen can be sold to health care units or the industrial sector [74]. There is no direct relation between using oxygen for medicine and the improvement of the energy sector but medical oxygen is very costly, due to the need for high purity levels, being compressed, and so on, and its sales help bridge the cost of green hydrogen production, by water electrolysis [74]. Taking this information into consideration, for this model, was considered that the oxygen produced from water electrolysis is sold to hospitals until their demand is fully satisfied.

It was necessary to look for some Portugal databases about hospitals. In the year 2019, and according to Pordata [75], a total of 10766292 kg of O_2 was consumed by a total of 238 hospitals, with a total 35000 beds, which gives a normal oxygen consumption per bed in a year of 450 kg of O2/bed.year. After 2019, the value of oxygen consumption increased about 30% [76] due to the Covid-19 pandemic crisis, and due to this disease affecting the respiratory system and it becomes necessary to provide oxygen to the patients to help them to breathe. Since this was a particular situation that change the normal consumption values, this study will use the data from 2019 to consider normal values of oxygen consumption.

For this work, all hospitals will be considered and so, the total need/demand of them will be equal to 10766292 kg, the last available data from Pordata [75].

Oxygen Revenue:

$$BP^{Profit} = BP_0 \times UOSP \quad (5.5)$$

- The equation 5.5 was adapted from [66];
- BP_0 is the total by-product (oxygen) Hospital demand [kg / y];
- UOSP is the unit of oxygen selling price [€ / kg];

5.3.4 Hydrogen production cost

Green hydrogen is a very important energy vector and can do easy replace the use of fossil fuels. Hydrogen can be obtained through renewable sources, electrolysis of water, SMR, gasification (coal, biomass), pyrolysis, among other technologies, what we called green hydrogen can only be produced from clean sources, with low or zero GHG emissions and low environmental impacts, such as renewable sources and from water electrolysis. For the H_2 economy to be able to develop and continue to grow, it is important to have economically viable H_2 production, so the type of feedstock and the technology that is used, are the main factors that influence the economic viability of H_2 production.

Water electrolysis, as explained previously in the work [Chapter 2], is simply the separation of water molecules (H_2O) into hydrogen and oxygen (O_2). In order to realize this separation, it is necessary to give energy to the process to the molecule to break, and due to the fact of being an endothermic process, an amount of energy, namely electricity, is required.

Here we can see one of the things that affect the hydrogen production cost is the price/cost of the electricity that is consumed during the reaction. The electricity price depends on the energy source, the time of the day that the energy is being consumed, the energy market and its variations, oil and gas prices, and so on. The energy market is not constant, neither are their prices.

For this work it is assumed that all energy that is used for hydrogen production is from renewable sources. It is assumed that a contract has been done with the energy producer and only renewable energy is supplying this process. So, the electricity that feeds the hydrogen production comes directly from the grid and it is guaranteed that is 100% carbon-free. In this contract is also agreed that the price charged for the electricity remains constant.

Water electrolysis can be defined by the source of electricity that uses (fossil fuels, wind, solar, nuclear, etc) and by the type of electrolyte that is being used, being the most known ones the Proton Exchange Membrane (PEM), Alkaline (AE) and Solid Oxide (SOEC). In this model it will be considered that all production sites will be using the Alkaline Electrolysis because is a mature technology and can achieve an efficiency of production of 70%.

Hydrogen Production Total cost:

$$HP^{Cost} = \frac{ELCTR}{1000} + \frac{CAPEX}{10} \times \frac{1}{HPY} \times \frac{33.33}{EFF} \tag{5.6}$$

- The equation 5.6 was adapted from [77].
- HP^{Cost} is the hydrogen production total cost [€/y]
- ELCTR is the electricity price consumed during the electrolysis [€/MWh]

- CAPEX is the total investment in the Alkaline electrolysis technology [€/kW]
- The 10 years is considering the life-time of the technology;
- EFF is the efficiency of the Alkaline electrolyser
- 33,33 is the theoretical minimum power consumption [kWh/kg] if the electrolyser was 100% efficient

The electricity considered in equation 5.6 is produced from renewable sources.It is assumed that there is power generation all year, to produce the electricity for the electrolyzer that will work, at least, 2100h, during all year. Concerning the percentage of oxygen sold, it is possible to do a sensitivity analysis in order to understand how much oxygen needs to be sold to pay the process of hydrogen production, but the purpose is to sell 100% of the oxygen to medical care, more specifically to hospitals.

Concerning the lifetime of the technology, alkaline electrolysis, namely its stack, is able to work a maximum of 90000 hours. Considering the 365 days in a year, with 8760 hours, it means that the alkaline stack has a lifetime of around 10 years [16].

An example of an alkaline electrolyser that can be considered is represented in figure 5.5.

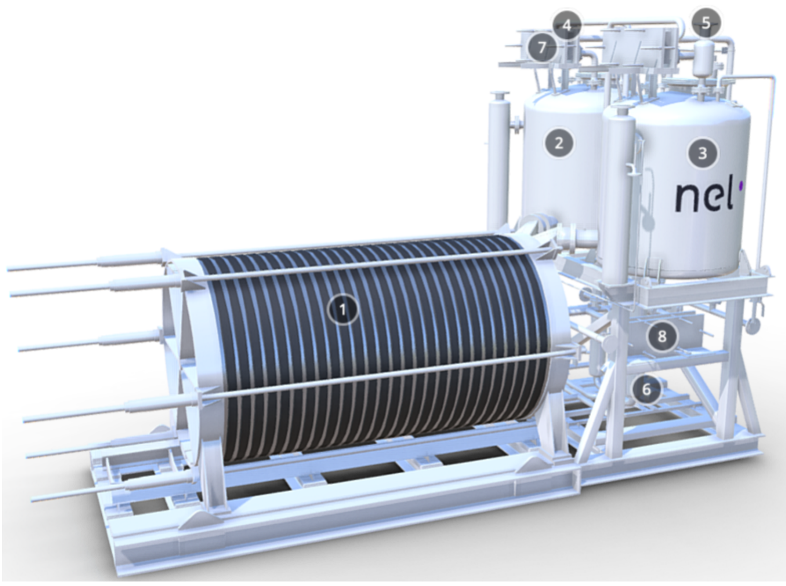

Figure 5.5: Atmospheric Alkaline Electrolyser. Nel Hydrogen. [78]

The components present are numbered from 1 to 8, being 1 the cell stack, 2 and 3 separator tanks one for hydrogen and the other for the oxygen, respectively, 4 and 5 the flanges, one for the hydrogen and the other for oxygen, respectively, 6 is the lye circulation pump, 7 is the gas cooler and finally, 8 is the lye cooler. This electrolyser is one of the most efficient in the world with low power consumption, around 3.8 kWh/Nm^3 (42 kWh/kg of H_2), and able to produce more than 8 tons of hydrogen per day [78].

Capital Expenditure, also called CAPEX, represents the monetary investment that companies must do to acquire the technology, it is the price that each producer must invest to obtain the electrolyser. There are a lot of available data about different CAPEX for water electrolysis, being alkaline electrolysis included, and this occurs due to the fact CAPEX depends on the performance of the technology that is being considered [79]. After the producer has the equipment, the costs that are being associated with it are the costs of operation and maintenance, and the day-to-day expenses (also called OPEX). These last three will not be considered, in order to simplify the model.

5.3.5 Water supply cost

Water is one of the main components for green hydrogen production, through electrolysis. Since it is necessary 100% pure water, it is assumed that each production site will have a desalination infrastructure to purify the water that will be used for hydrogen production. For this model, the water that will be used will come directly from the Portugal Water Grid.

Portugal is a country that is surrounded by seawater and has a lot of rivers traveling through it. So, water is not a limitation or a constrain for Portugal to produce H_2, it is only required the right technology to help this process. If seawater was used, the purification would be more difficult and the costs would rise, would be necessary more energy to sustain this process. This is why it will be used water directly from the grid. As mentioned in chapter 2, there are two main methods to purify the water and for this work, the reverse osmosis technology would be considered. The implementation of this technology, if used, would be considered as part of the fixed cost, part of the capital investment.

As previously explained, to produce one kilogram of hydrogen it is necessary to use 9kg of water. This way, knowing the total amount of hydrogen that will be produced, it is possible to know the total annual amount of water that will be used for the process. Meaning, the total amount of water necessary for each producer is nine times higher than the amount of hydrogen that each of them committed to producing.

Water Total Cost:

$$W_{Supply} = UWS_G \times WD_T \tag{5.7}$$

Where,

- WD_T= 9 $\times H_{produced}$

- UWS_G is the unit price of water supply from the grid per kilogram of hydrogen [€ / kg H_2]
- WD_T is the water total demand for the hydrogen production [kg]
- $H_{produced}$ is the total amount of hydrogen, kg, that each producer will produce.

5.3.6 Hydrogen transportation cost

It is being considered a decentralized production, where some production sites will produce the hydrogen to other companies.

Decentralized production has the advantage of being distributed for several regions, facilitating the consumer to access the product and avoiding traveling long distances to reach it. Another advantage lays in the fact it does not require a huge amount of space or large infrastructures, which would be costly, which occur in a centralized production. But in opposition, a larger scale production has a lower cost of producing hydrogen, because allows producing higher quantities and the electrolyte is working more hours (the higher the number of hours, the lower is the cost), but the transportation of the product would be expensive because one single unit would have to distribute for all the others.

One thing that affects the transportation of H_2 is the form under with it will be transported. There are two possible ways of transporting hydrogen, in liquid form or gaseous form. For long distances, the liquid form is a more suitable option, but it is necessary to compress the hydrogen, which would influence the cost because the cost of compressing liquid hydrogen would need to be considered. For smaller distances, hydrogen can easily be transported in gaseous form. Transporting the hydrogen under gaseous form also eases the process because the fuel cell vehicles use hydrogen gas, so the hydrogen that is produced and then distributed is ready to be used from the moment that reaches the consumer, and it is not necessary to do a extra compression step to transport it, as it happens fot the liquid form.

Transportation Cost:

$$HT^{Cost} = Dist \times GHD_{Cost} \times HD_{Cost} \tag{5.8}$$

Where,

- The equation 5.8 was adapted from [66];
- Dist is the distance of each producer to each consumer [km];
- GHD_{Cost} is the gaseous hydrogen delivery cost to specific industry per km [€ / km / kg]
- HD_{Cost} is the amount of hydrogen to be deliver in each consumer per year [kg H_2 / y]

To simplify the model, it is considered that all hydrogen is transported to the other companies in gaseous form. The cost of transportation is based on the distance between each producer to each consumer.

The distance from one company to others was determined using MATLAB Software using the geographical coordinates of each of the companies in the study. The distance calculated was the linear distance between a point and the other, meaning the linear distance between the position of one company to the position of the other. In the end, it was obtained a matrix of 56 companies per 56 companies, with zeros diagonal (because the distance of the company to itself is zero), where it is presented the distance in kilometres from a company to all others. Table 5.5 shows a part of the matrix of 56 per 56, where the numbers, as explained previously, represent the raking position that each company occupies.

Table 5.5: Representation of the matrix of distance between one company to others.

Companies	**1**	**2**	**4**	**5**	**6**	**8**	**10**
1	0	33.969	191.116	28.462	198.798	26.598	29.479
2	33.969	0	217.905	7.002	230.769	11.973	30.976
4	191.116	217.905	0	210.904	66.899	215.864	188.814
5	28.462	7.002	210.904	0	224.049	12.534	24.484
6	198.798	230.769	66.899	224.049	0	225.357	206.329
8	26.598	11.973	215.864	12.534	225.3570	0	34.595
10	29.479	30.976	188.814	24.483	206.329	34.595	0

6

Results and Discussion

Contents

6.1 Results 56
6.2 Discussion 69

6.1 Results

The purpose of this work was to find the optimal locations to implement the first hydrogen refuelling stations in Portugal and to understand the economic investment necessary for that.

Firstly, it was important to understand which sector would be more advantageous to implement and after some research, it was easy to conclude that the transportation sector, namely long-distance, would benefit from this implementation. Hydrogen is a good alternative to diesel, gasoline and natural gas, and hydrogen fuel cell vehicles besides having higher efficiencies compared to internal combustion engines, it has zero emissions, allowing the sector to decrease its GHG emissions. Concerning electric battery vehicles, the traveling distances are too long and the truck would need to stop several hours to recharge the battery to be able to reach the final destination. That would delay the deliveries, in opposition to hydrogen fuel, which has a refuelling time similar to gasoline or diesel, which is efficient.

After understanding which sector was a more suitable candidate for the study, it was necessary to develop the problem. The data was collected, assumptions were made and the simulations started. From a ranking of 100 companies, only 56 were able to participate in the simulations. At a first sight, a very interesting thing to highlight is that the majority of the companies being evaluated are located close to all coast of the country, where the density of people is higher. Clusters were formed in order to understand how it was possible to organize the companies into groups to transform the supply chain more efficiently, having two or more companies refuelling from the same production site. Just with these constraints the number of companies in the study decreased from 56 to 53, because 3 of them were too far from the others, being more isolated, not able to belong to any group. The results showed that to be able to cluster all remaining 53 companies, 10 companies need it to be organized in groups of 2, 15 organized in clusters of 3, 12 into groups of 4, 10 in groups of 5 and 6 in a group of 6.

The problem was always unbalanced, this means that suppliers were never able to satisfy all their consumers, 100%. In other words, the demand of the consumers was never completely suppressed. This enables to conclude that there is no feasible solution due to the fact there is not enough hydrogen produced to reach all consumers.

6.1.1 Geographical Assessment

The clustering method was selected for the companies in this study and this way several producers are distributed along with the territory, that get in line with the Portugal's goal of having a decentralized green hydrogen production. For the approach where the mean distance was the only criteria to take into account, it showed that this way all producers were located in the same region, as it is possible to verify in figure 5.2, and that would not allow an efficient distribution and it would not be congruent with Portugal perspectives and targets for hydrogen implementation. Figure 6.1 shows all 56 companies arranged into 19 clusters, without any element being excluded.

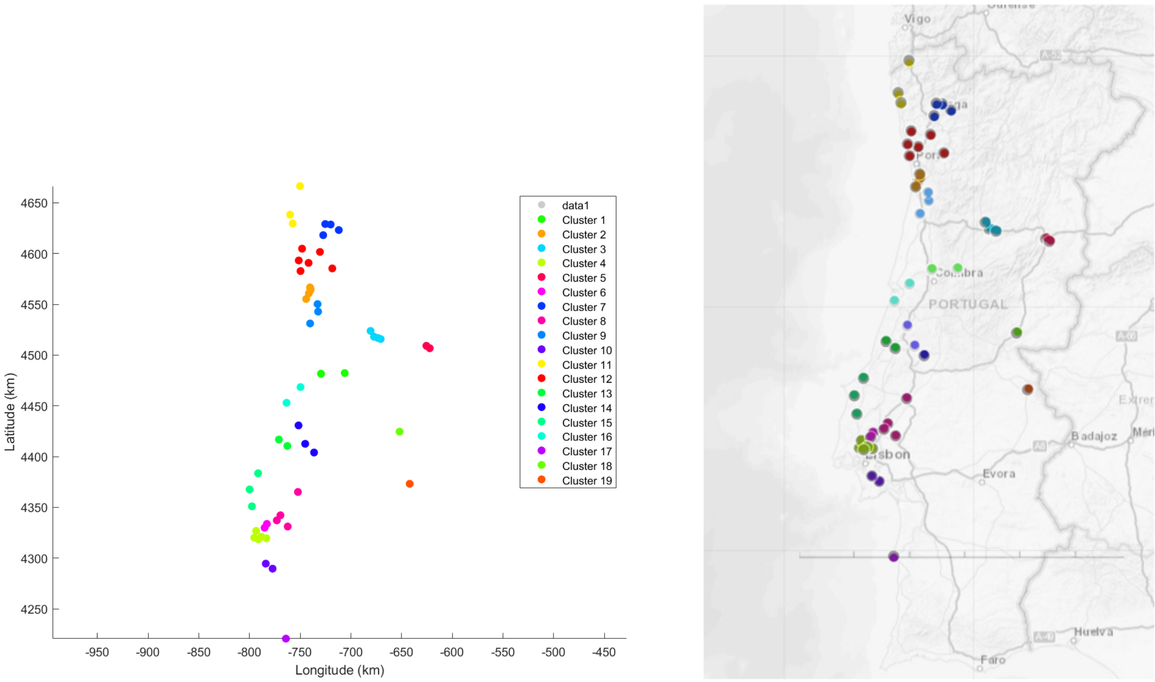

Figure 6.1: Clustering method. 56 companies arranged into 19 clusters. Portugal map overlay **(on the right)**

After the method selection, it was conducted a sensitivity analysis in order to understand how the number of clusters vary and how the elements of each cluster were affected. For the first stage of the creation of hydrogen refuelling stations, it would not make sense to have hydrogen production sites that would supply only one element, it would make more sense to implement production sites, also called refuelling stations in locations where more than one consumer can easily access. For this reason, the number of elements per cluster only varies between a minimum number of 2 and a maximum of 6 elements. Since the results showed that only one cluster was formed with 6 elements, it would be redundant to run the program for this restriction. With that in mind, the number of elements will only vary from 2 to 5.

With distance variation, it was decided to vary the distance from 20 kilometres to 50 kilometres, changing 15 kilometres per case, meaning that the distances in consideration were 20 kilometres, 35 kilometres, and 50 kilometres. The table 5.4 shows the summary of all results obtained and it is possible to verify that for a distance equal to 35 and distance equal to 50, nothing changes, the results are exactly the same. Because of that, and to not being redundant once again, it was only considered the distances equal to 20 and 50 kilometres. The distance equal to 50 kilometres was preferred, in opposition to a distance equal to 35 kilometres, because this way it is possible to put a production site in a cluster with a larger diameter, meaning that will have a greater operation area of supply, which will enable to other companies, in a more mature time, to be easily inserted in these clusters. Taking into consideration the assumptions described, the results obtained are briefly summarized in figure 6.2.

Figure 6.2: Total number of clusters formed in each scenario.

The higher number of clusters formed is, as expected, when the minimum number of elements per cluster is 2, with the two furthest companies at a distance of up to 50 kilometres ([2, 50]), and the lowest number is for minimum elements equal to 5, for both distances. But, even for the case where the restriction of the minimum number of elements per cluster was the same (only the distance was being changed), the companies were being eliminated from the study. It is possible to see in figure 6.3 the number of elements that were excluded in each case.

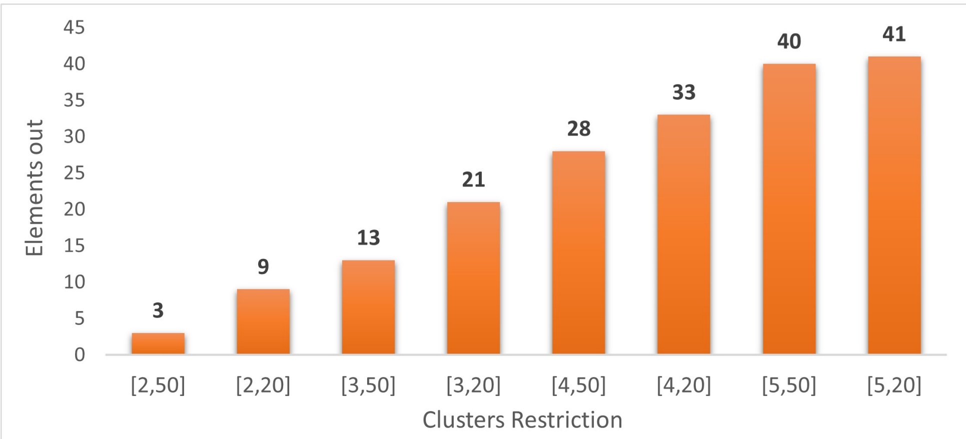

Figure 6.3: Number of companies excluded from the clustering process due to don't fit in the restrictions imposed.

As the restrictions get tighter, the number of elements that are being excluded increases. And, as

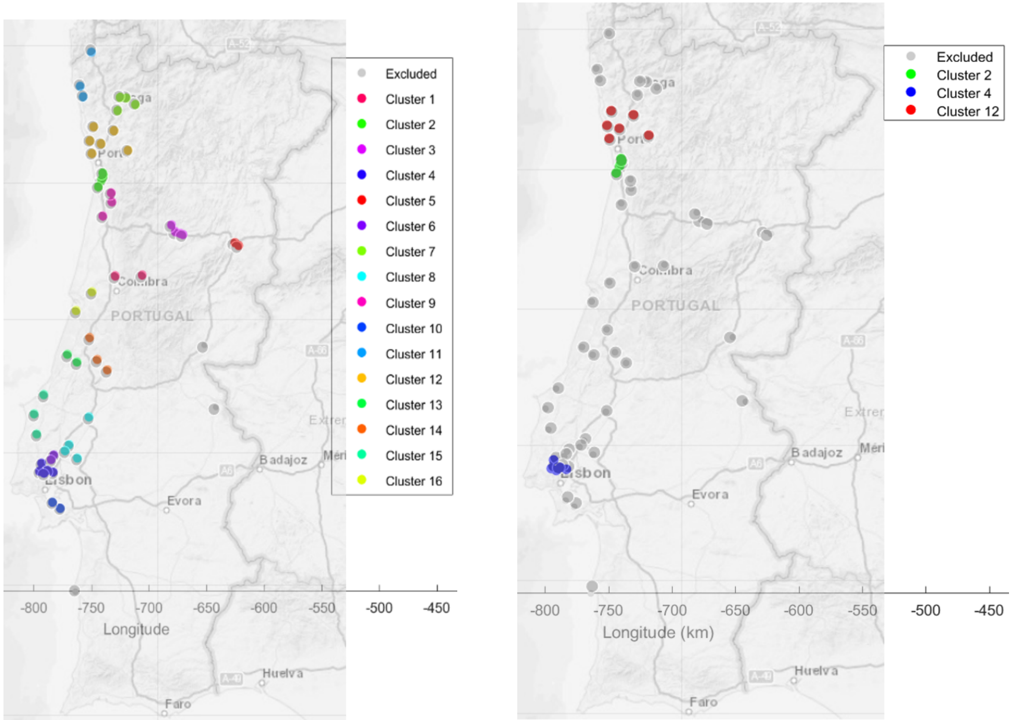

Figure 6.4: Clustering process. Minimum elements equal to 2 and maximum distance equal to 50km.**(Left)** Minimum elements equal to 5 and maximum distance equal to 20km.**(Right)**

expected, the case where the number of elements excluded is higher is for the case where the minimum elements per cluster are equal to 5 and the maximum distance between the two furthest companies is 20 kilometres ([5, 20]), obtaining a percentage of exclusion equal to 73.2%. Figure 6.4 it is possible to visualize two scenarios, side by side, and see how the constraints affect the number of clusters formed, where the grey points displayed to represent the elements that were excluded from the clustering, and the colored points are the points that belong to a cluster. To differentiate, each cluster has a different color. It is important to mention that each case has advantages and disadvantages, it depends on what the main goal is.

The cases exposed in figure 6.4 are the extreme cases evaluated, and from the original 16 clusters (from [2,50]), only three of them "survive to all restrictions". The results, for all different restrictions can be find in figures 6.5, 6.6, 6.7 and 6.9. As it was possible to see in the previous figures, for this work, the clusters were organized by numbers (Cluster 1, Cluster 2, and so on), in order to simplify the organization. The clusters that are formed are always the same, what changes are the elements inside of each of them, depending on if they are in line with the restrictions imposed or not.

Observing figure 6.5, which illustrates the case study for clusters limited to a minimum of 2 elements

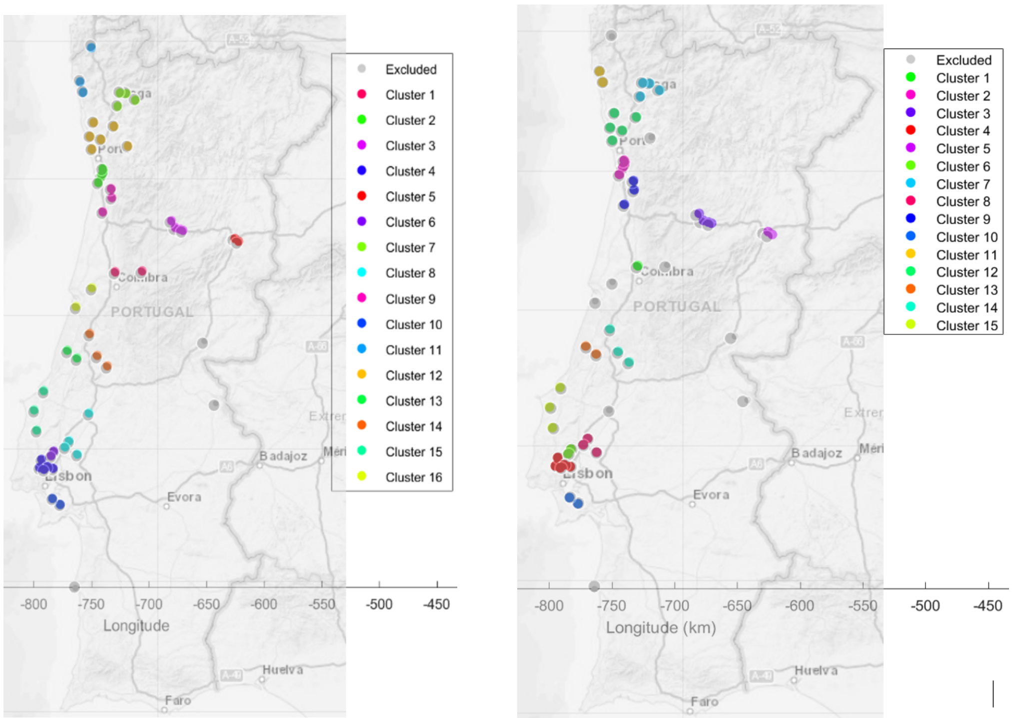

Figure 6.5: Clustering process. Minimum elements equal to 2 and maximum distance equal to 50km.**(Left)** Minimum elements equal to 2 and maximum distance equal to 20km.**(Right)**

for two distances (50 kilometres on the left and 20 on the right), it is possible to see that there was a decrease in the number of clusters formed and the number of total elements able to fit in those, comparing to figure 6.1, from a total of 19 clusters to a total 16, and having already 3 elements left out. Comparing the clustering with minimum elements equal to 2, by only changing the maximum distance from 50 kilometres to 20, one cluster was not able to form, namely cluster 16, and the number of companies left out increased to 9, as posted in figure 6.3.

The analysis performed in the previous paragraph can be applied to the remaining following cases, represented in figures 6.6, 6.7 and 6.9, and it shows that the number of clusters will successively decline. This happens because by increasing the minimum amount of elements per cluster and by restricting the distance, for clusters that are formed with that minimum value, if the furthest points are over the maximum distance, that cluster will disappear.

In the scenario displayed in figure 6.6 it is possible to highlight an advantage in comparison to the scenarios of [2,50] and [2,20], even when the distance change, the same clusters remain present, there is no decrease of clusters. But the negative side is that despite this, every cluster is not fully satisfied either, as it is possible to conclude by comparing the total number of clusters formed displayed in graphic 6.2 and the number of fully satisfied clusters in graphic 6.8.

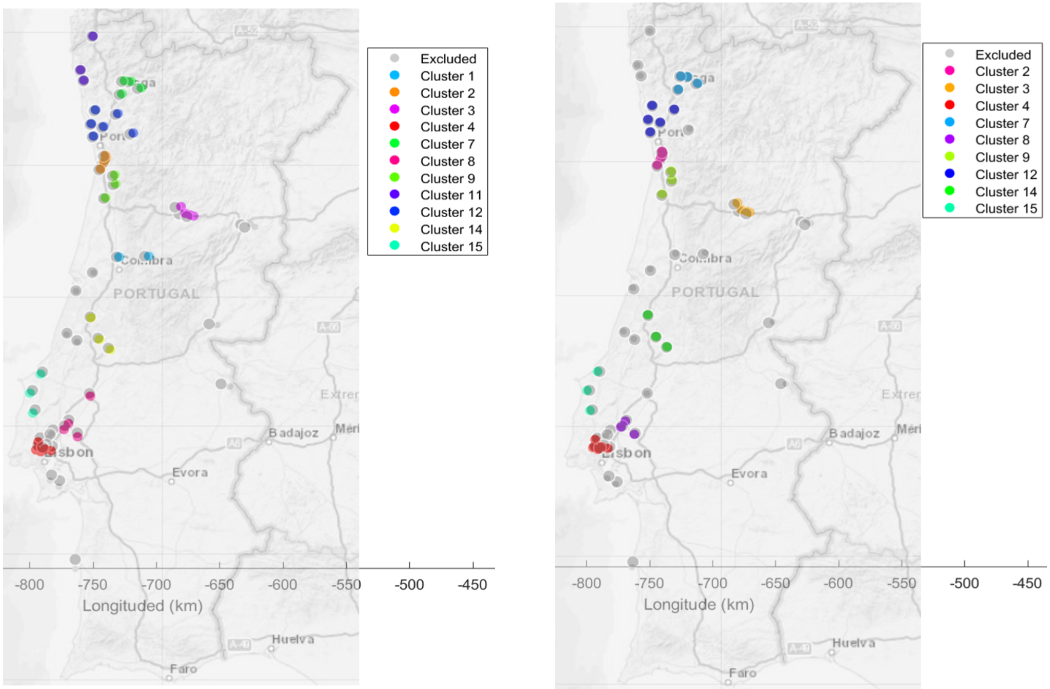

Figure 6.6: Clustering process. Minimum elements equal to 3 and maximum distance equal to 50km.**(Left)** Minimum elements equal to 3 and maximum distance equal to 20km.**(Right)**

By varying the distance from 50 to 20 kilometres, the number of clusters remained the same but the number total number of elements that formed those decreased. Even with this decrease of elements, not all producers were able to supply the needs of the consumers. The scenarios for clustering with 2 and 3 minimum elements are interesting because even when the number of consumers decreases by restricting the distance and even for the first case there is a loss of one cluster, the number of totally satisfied clusters remains the same.

The figure 6.7 represents the case for clustering process limited to a minimum of 4 elements per cluster and it is possible to understand the same occurs as previously as in figure 6.5. The number of clusters reduces, and consequently, the number of elements of the clusters is also eliminated. In opposition to what occurs in scenarios with the minimum of 2 and 3 elements, here the number of fully satisfied clusters decreases, as demonstrated in the graphic exposed in figure 6.8. This was interesting because by decreasing the number of elements it would be expected that the satisfaction of the clusters would be higher but that is not the case because the cluster that was eliminated was the one who was able to fully supply the consumer's need.

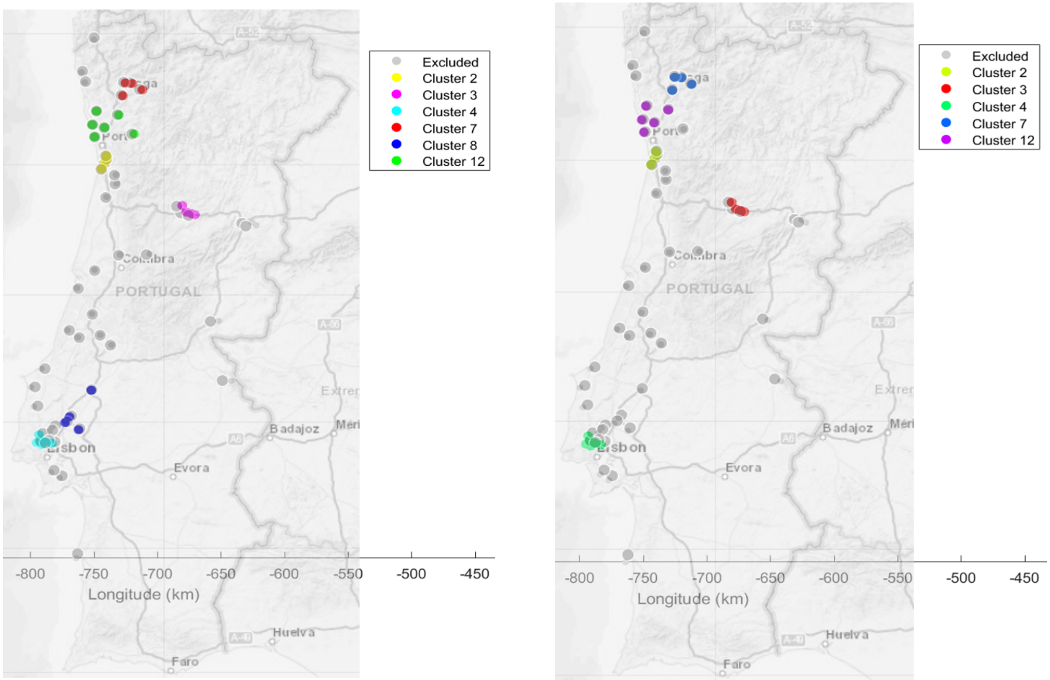

Figure 6.7: Clustering process. Minimum elements equal to 4 and maximum distance equal to 50km.**(Left)** Minimum elements equal to 4 and maximum distance equal to 20km.**(Right)**

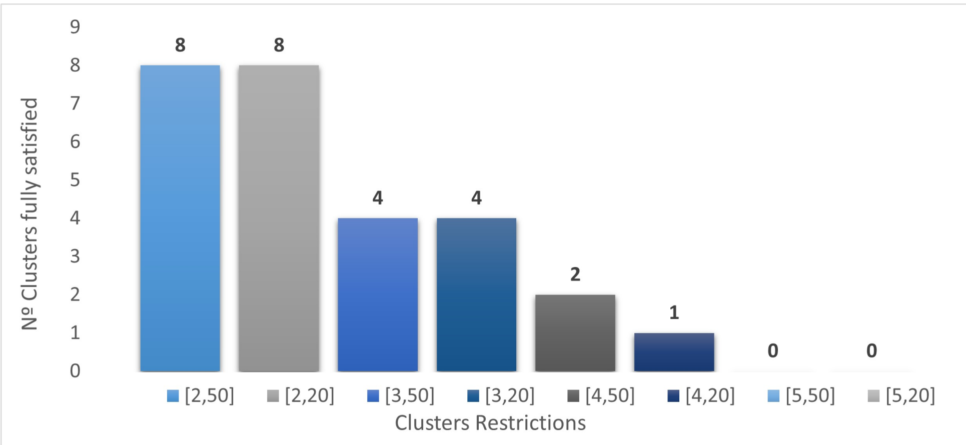

Figure 6.8: Number of clusters that are able to satisfy their hydrogen demand per scenario.

Finally, it is presented the last scenario in figure 6.9, where the clusters are limited to a minimum of 5 elements each. Here, for both distances, the producers were never able to fully satisfy their consumer's demands. This is not a particular situation of this scenario, but it comes highlighted here because are the only clusters that can answer to the constraints imposed.

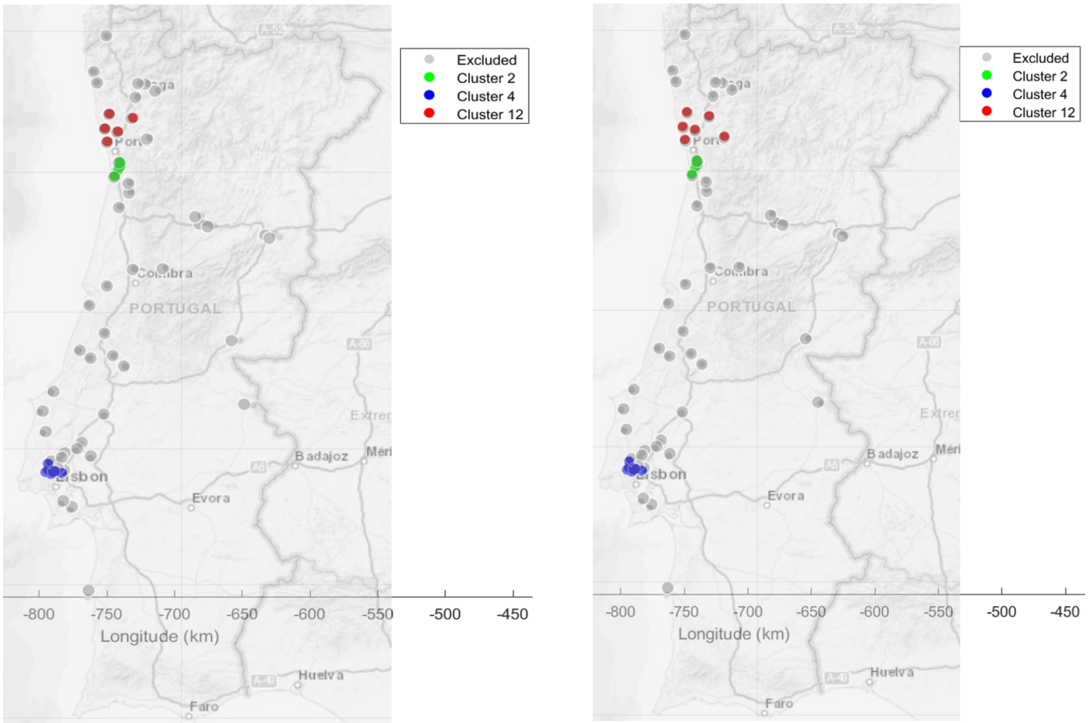

Figure 6.9: Clustering process. Minimum elements equal to 5 and maximum distance equal to 50km.**(Left)** Minimum elements equal to 5 and maximum distance equal to 20km.**(Right)**

Meaning that these clusters were never able to satisfy the consumers even in the previous scenarios. This happens due to the fact of being the more numerous clusters, clusters composed with a greater number of elements, which makes it difficult to meet the needs of all consumers taking into consideration the producer's capacity. But the supply chain will be analyzed in more detail further in the following subsection 7.1.2.

Besides evaluating the number of clusters that are fully satisfied, as presented in graphic 6.8, is more interesting to evaluate the percentage of clusters satisfaction, presented in table 6.1. For the same scenarios, by varying the distance, the number of clusters change declines but the number of fully satisfied clusters didn't. Meaning, for limiting the number of elements with a minimum equal to 2 or 3, the percentage of satisfaction increased from 50% to 53% (from 50 kilometres to 20 kilometres) and from 36% to 44% (from 50 kilometres to 20 kilometres), respectively.

For the clustering process with a minimum equal to 2, despite losing one cluster (cluster 16), that was fully satisfied, due to the loss of some elements, turns out possible for the producers to allocate the product (namely hydrogen) to the elements that stayed. For the scenario of minimum elements equal to 3, the clusters that were capable of fully suppressing their demands remain the same, being excluded clusters that could not fully answer to their needs. But unfortunately, the same didn't occur to other clusters. The results showed that even by changing the constraints, the results didn't quite change as would be expected. The elements of each cluster remained practically constant and even with some elements being eliminated, there was still not enough hydrogen to suppress the consumer's demand, so in all simulations, it was always the same elements that were being supplied. The only thing that changed was in fact the number of clusters formed.

Table 6.1: Percentage of clusters fully satisfied.

Clusters restrictions	% of clusters totally satisfied
[2,50]	50%
[2,20]	53%
[3,50]	36%
[3,20]	44%
[4,50]	33%
[4,20]	20%
[5,50]	0%
[5,20]	0%

6.1.2 Supply chain - Economic analysis

The second main goal of this work was to try to evaluate the distribution of hydrogen from the producers to the consumers. After the clusters were formed, a study of distribution based on the capacity of the producer and the demand of each consumer was performed. With this, it was possible to obtain the total cost of hydrogen grid implementation per scenario and the implementation cost associated with each cluster. To do it so, a Transportation Assignment method was used in this work.

Transportation Assignment is a linear programming optimization method where the problem can be solved by formulating a linear model. This method can be easily disassembled by using an algorithm called Simplex. Simply, transportation problems deal with the distribution of a product from a source (producer) to a receptor (consumer) and it aims to a final distribution process where the total cost of it is minimal. This method looks to help to create a supply chain and minimize its costs. [80]. The demand corresponds to the necessity of hydrogen to replace 5% of companies fleet and the capacity of the producers to produce hydrogen is assumed to be equal to 10% of their fleet.

The problem is solved based on the lowest distribution cost, which means that for each consumer there is a cost associated for the producer to supply to them. In this work, and as explained in section 5, the distribution costs takes into consideration the cost of hydrogen production, the cost of distribution considering the distance from the producer to the consumer, and the costs of water consumption, and each of these costs is per each of kilogram of hydrogen distributed, considering the needs and capacities of each cluster. The problem was solved by using Excel tool Solver. An example of the process can be found in table 6.2.

Table 6.2: Transportation assignment example. Excel Solver tool. Cluster 1 from scenario of minimum of 2 elements per cluster with 50km maximum distance.

Producer/ Consumer	13	39	68	Capacity	
13	4,34	7,32	4,37	4887412	Total demand
Demand	2443706	1529934	1529934		5503575

Producer/ Consumer	13	39	68	Supply	Capacity
13	2443707	913772	1529934	4887412	4887412
Demand	2443706	913772	1529934		
Demand	2443706	1529934	1529934		
	Totally satisfied	56% satisfied	Totally satisfied		
Total cost	**23972207**				

Difference Demand-Capacity	Total oxygen produced (kg)
-616162	39099299

After the clusters were formed, it was necessary to analyze each element that belonged to each cluster and select from that group which company would be the best to be a producer, as explained in chapter 5. In the particular case represented in table 6.2, cluster 1 is formed by the companies 13, 39 and 68. These numbers represent the position of each of the companies in the ranking used for the selection. From these 3 companies, company 13 was selected to be the producer due to the fact of being the one with the largest fleet having about 350 vehicles (the other two have 179 and 100, respectively). So, company 13 will be producing hydrogen for itself and the other 2. The demand and the capacity were determined as mentioned in chapter 5 in subsection 5.2.2 and the previous method was applied to the remaining clusters.

On the first half of the table 6.2, there is the cost of distribution from the producer (13) to each consumer (13 itself, 39 and 68). It is easy to see and understand that the cost of distribution from producer to itself is the lowest one because the distance is equal to zero but it takes into consideration the remaining factors. What Solver will do, is analyze the demand of each consumer and the cost of supplying each of them, and considering the total capacity of the producer, will allocate hydrogen to the receptor. At the end of the run, it is obtained the total cost of distribution and the respective quantities allocated to each consumer. The consumer can be totally satisfied, partially satisfied, or not satisfied at all. The column of supply can be different from the column capacity if, for example, the capacity of the producer can be higher than the total demand of the cluster, so it will be hydrogen left over. In this particular case, is possible to see that it will be a deficiency in hydrogen supply because the difference between capacity and demand is negative, which gives an unbalanced case. If there was more capacity that consumers need the problem would be also unbalanced. A case is only balanced when the supply meets the exact demand. This process was repeated for every cluster of every scenario.

As mentioned in subsection 7.1.1, the total number of clusters was never fully satisfied in any of the cases present. But it is important to understand if the clusters which they need were not met, if all elements were not supplied or if they were partially supplied. A cluster not being fully satisfied means that all elements that belong to it didn't have their needs 100% satisfied, but it can be present elements that were fully, partially, or not supplied at all. All cases can happen in the clusters. Tables 6.3, 6.4, 6.5 and 6.6 show the results. This is important because even though the supply is not complete (in the sense that are consumers that are not supplied, complete or partially), that the distribution that occurs to the other elements doesn't count for the total cost of distribution.

Table 6.3: Characteristics of scenarios [2,50] (left) and [2,20] (right).

Min. 2 elements and max. distance 50km	
Satisfied	38
Partially satisfied	7
Not satisfied	8
Companies used	53
Total companies	56

Min. 2 elements and max. distance 20km	
Satisfied	36
Partially satisfied	7
Not satisfied	4
Companies used	47
Total companies	56

Table 6.4: Characteristics of scenarios [3,50] (left) and [3,20] (right).

Min. 3 elements and max. distance 50km	
Satisfied	29
Partially satisfied	6
Not satisfied	8
Companies used	43
Total companies	56

Min. 3 elements and max. distance 20km	
Satisfied	24
Partially satisfied	5
Not satisfied	3
Companies used	32
Total companies	56

What happens is that clusters that have a higher number of elements will have a similar cost of implementation as clusters with lower elements because the capacity of the producer is not enough for all of them. The selection of which companies were supplied or not, can be based on two criteria, one the cost of distribution and the other the demand of the consumer itself.

The first criteria is easy to understand, the program will choose to supply the consumer for which the producer will have the lower cost to distribute, to minimize the cost. For the second criteria, if there is not enough hydrogen for all consumers, for example, a case where there is a cluster of 5 elements, and the producer only have hydrogen to satisfy 3 consumers, but can satisfy (fully or partially) 3 consumers that have a distribution cost higher and higher demands (which means that will be largest companies), or satisfy the 3 closest companies with lower demands, and the program chooses the first option. Running the program, both of these criteria were being used, so it was necessary to force it to only simulate under one of them. When the lowest path was chosen, the results could remain, when the other criteria were being evaluated, I force the program to select intermediate values, meaning, to choose companies that had an average distribution cost with average demand.

Table 6.5: Characteristics of scenarios [4,50] (left) and [4,20] (right).

Min. 4 elements and max. distance 50km	
Satisfied	18
Partially satisfied	4
Not satisfied	6
Companies used	28
Total companies	56

Min. 4 elements and max. distance 20km	
Satisfied	14
Partially satisfied	4
Not satisfied	4
Companies used	20
Total companies	56

Table 6.6: Characteristics of scenarios [5,50] (left) and [5,20] (right).

Min. 5 elements and max. distance 50km	
Satisfied	8
Partially satisfied	3
Not satisfied	5
Companies used	16
Total companies	56

Min. 5 elements and max. distance 20km	
Satisfied	8
Partially satisfied	3
Not satisfied	4
Companies used	15
Total companies	56

The total oxygen produced as a by-product is obtained by multiplying the total amount of hydrogen supplied (not the total capacity) per 8, taking into consideration the stoichiometry of the water electrolysis reaction. The graphic presented in figure 6.10 shows the total amount of oxygen produced for each scenario of hydrogen supply network implementation. It is easy to understand that the higher is the number of clusters formed, the greatest will be the hydrogen production and consequently, the greater will be the amount of oxygen, as a by-product produced. Since the oxygen selling is what makes decreases the cost of implementation of the network, it is important to sell the biggest quantity of oxygen possible. But the problem is related to oxygen demand. The oxygen selling is conditioned to the oxygen demand, and in this work, is limited to medical oxygen need.

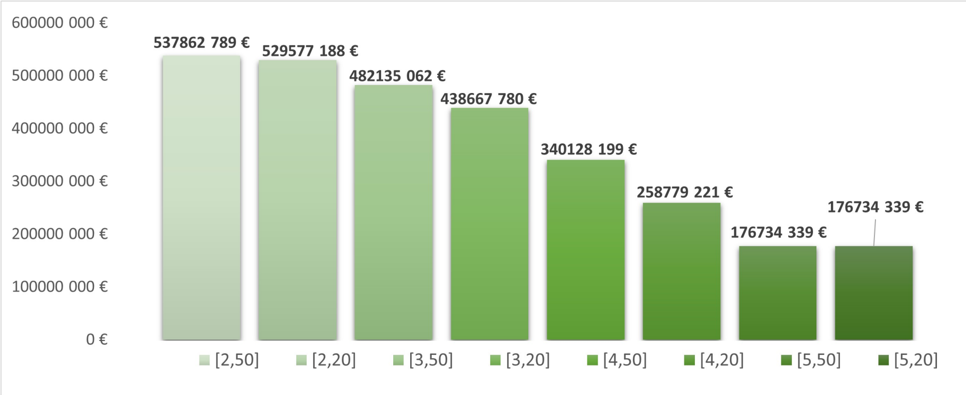

Figure 6.11: Total cost of implementation of hydrogen supply chain for the different scenarios.

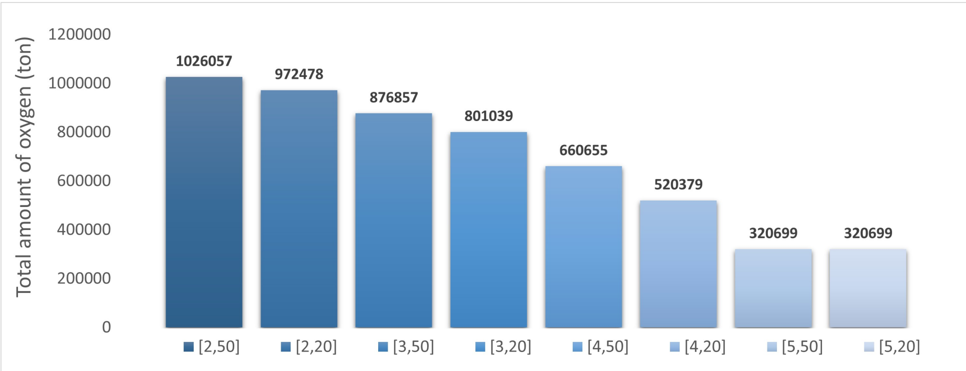

Figure 6.10: Total amount of oxygen produced as by-product in kilograms per each scenario.

Besides the demand, oxygen has another very important factor associated. The selling price. In Portugal, the expensive amounts of oxygen are associated with medical care consumption and apart from that, is the sector at which oxygen has the higher cost, as mentioned in chapter **??**.

Running all case studies, it is obtained the total cost of implementation of a hydrogen supply network per each. The cost of implementation is represented in figure 6.11.

It is easy to understand the decrease in the total cost of implementation as the constraints change. If the number of clusters and elements declines, the costs of hydrogen supply will be lower. It is necessary to understand if from all scenarios which would be more advantageous to implement on the first stage of implementation, taking into consideration cost and the number of clusters formed, and the total number of companies supplied.

6.2 Discussion

From this study, it was possible to see that the higher the number of elements per cluster, the more difficult it was for the producer to supply them all. For example, in the particular case of the only group of 6 elements (only formed when the maximum distance was equal to 50 kilometres, for 20 kilometres one element was excluded), the producer is not capable to produce enough hydrogen for all elements, being only satisfied (totally or partially) 3 of those 6 elements. In opposition to the majority of the clusters of 2 elements that had a percentage of supply and satisfaction higher. When the restriction increase from a minimum of 2 elements to 3, the number of fully satisfied clusters decreased to half. These results show that having clusters too crowded is not a good option, at least not in the first stage.

Due to the results obtained, it was necessary to select the ones where it would be the most advantageous sites to implement the technology and would be the most efficient clusters, allowing to development of an efficient network supply. The criteria used for the selection of the cluster were simple. Only clusters that had their elements being supplied (completely or partially) were chosen. If any element of the clusters was not supplied at all, that group was not considered. This has the purpose of trying to pick the best sites for a first implementation, where all the elements are being supplied with hydrogen. With this, it is obtained the final selection of eleven clusters being them 1, 3, 4, 5, 6, 8, 9, 10, 13, 15, and 16. They can be found marked in the map represented in figure 6.12.

From the map, in figure 6.12, it is possible to highlight the clusters per region or district. In Lisbon there are 3 clusters, in Santarém there is 1 cluster, in Leiria, there are 2 clusters, in Coimbra, there are 2 clusters, in Aveiro, there is 1 cluster, in Viseu, there is also 1 cluster and finally in Guarda there is 1 cluster. One good thing important to mention is that for a first implementation, although the distribution is not perfect, there are several clusters along with the territory and even in its interior, which is very important. It will help to dynamize the economy the interior and enable this region to be more attractive, helping decrease human desertification, which is a concern in Portugal.

Taking into consideration those sites, table 6.7 shows the clusters characteristics, namely it cost of hydrogen implementation and the amount of oxygen, as by-product, that is produced.

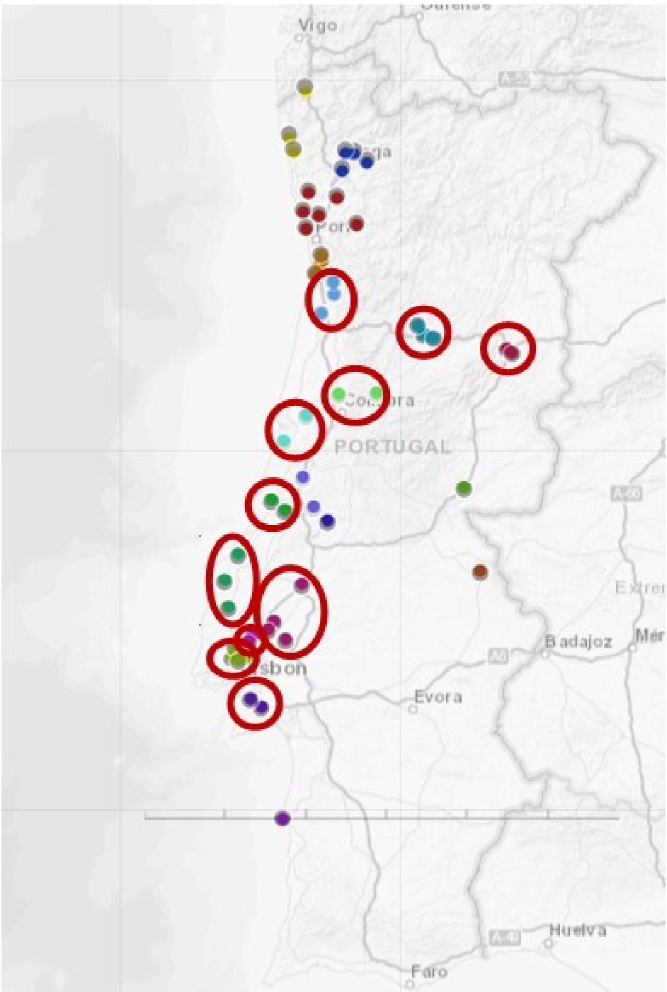

Figure 6.12: Best sites for refuelling stations.

Table 6.7: Clusters informations.

Cluster	Implementations Cost (€)	Oxygen produced (ton)
1	21 214 343 €	39099
3	59 712 469 €	118957
4	140 966 445 €	256000
5	14 480 632 €	28928
6	14 336 269 €	28253
8	79 965 952 €	140276
9	47 087 080 €	82639
10	19 467 658 €	39111
13	10 465 326 €	18879
15	28 486 279 €	48947
16	25 464 121 €	45519
Total	461 646 574 €	846609

Considering that results showed in the previous table 6.7, and summing the total cost of each cluster it is obtained a cost of implementation of this network equal to 461 646 574 € that is less than the total cost for the same number of clusters for the case scenario of minimum elements equal to 3, with a maximum distance equal to 50km represented in the graphic present in figure 6.11.

Another analysis that is crucial for this work is the study of how oxygen selling affects the costs of hydrogen implementation. In table 6.7 there is presented also the amount of oxygen that is produced as a by-product. If all oxygen was able to be sold, a total of 846609 tons, the producers could put a selling price equal to 0.55€ to have the hydrogen grid implementation with a cost equal to zero. So, it would be possible to pay the implementation of the hydrogen supply, and selling the oxygen at this price is very competitive in the market. It would be oxygen with a high level of purity being sold at a very low price. That this is not the case. Unfortunately, the amount of oxygen produced is massive compared with what the real demand is. In 2019 the total oxygen consumption in the hospital sector was equal to 10766 tons, and according to Infarmed reports, there was a total expense equal to 10 409 294€ [81], which give a cost of around 0.97€/kg of oxygen. Comparing the perspective of the amount of oxygen that will be produced, 846609 tons, with the amount that is consumed by this sector, it corresponds only to a 1.3% of the total production of the by-product. It is a very small consumption. So the profits associated with oxygen selling will be around 10 409 294€. But it is important to have a market competitive price to guarantee that the sector will prefer the oxygen that is produced in Portugal. By decreasing the unit price of oxygen by 0.17€/kg, that will give revenue of 8 613 034€. However, this only saves 1,9% of the entire implementation cost, which would not make the companies invest in the business.

It is important to show how will companies benefit from this change. If hydrogen implementation will be only a cost, it would be a very unattractive investment or deal and the companies would not accept it just because it was a green alternative, it must be also economically feasible for them.

6.2.1 Net Present Value

Most heavy-duty trucks work with an internal combustion engine running with diesel fuel. Some companies already started to adopt some trucks that run with natural gas, because it has lower carbon emissions but it is just a representative number. So, assuming that all trucks that are being replaced in this work, in each of the companies, run with diesel fuel, it is possible to compare the diesel consumption in a year and its costs with the hydrogen. A work developed in association with a transportation company, where the consumption of the vehicles was evaluated, it is referred that the desired consumption for a truck is 30L/100km [82]. To simplify the calculation, this was the value considered for all vehicles. Knowing the number of trucks that would be replaced and the total number of kilometres they do in a year, it was obtained the total diesel consumption (in a year), for that same amount of vehicles. Assuming the average value of road diesel price given in Pordata, equal to 1.30€/L [83], the total cost of that fuel consumption was obtained. For this study was important to understand how replacing diesel trucks with hydrogen fuel cells ones would be advantageous, the investment in new trucks needed to be also considered. The same study where it was obtained the desired consumption, also presents the costs of acquiring a heavy-duty truck with hydrogen fuel cell technology in the current days. The acquisition price is around 160 000€ [82]. For the clusters chosen, it obtained the following results shown in table 6.8

Table 6.8: Costs of hydrogen implementation, diesel consumption, and fuel cell vehicles acquisition per each cluster, in a year.

Cluster	Implementations Cost (€)	Diesel Cost (€)	Fuel Cell Vehicles Cost
1	21 214 343 €	23 548 217 €	4 236 800 €
3	59 712 469 €	68 121 497 €	19 040 000 €
4	140 966 445 €	156 048 429 €	46 240 000 €
5	14 480 632 €	17 628 000 €	3 200 000 €
6	14 336 269 €	17 216 797 €	5 280 000 €
8	79 965 952 €	85 480 468 €	26 560 000 €
9	47 087 080 €	50 358 429 €	9 600 000 €
10	19 467 658 €	23 832 981 €	6 720 000 €
13	10 465 326 €	11 569 772 €	1 264 000 €
15	28 486 279 €	29 827 328 €	12 800 000 €
16	25 464 121 €	27 738 429 €	6 240 000 €
Total	461 646 574 €	511 370 348 €	141 180 800 €

A good tool that helps to understand if this investment is good or not is the Net Present Value (NPV). It is an economical-financial tool of capital budgeting that to analyzes the viability of a project or investment, considering its profitability of it. NPV is calculated through the difference between the present value of cash inflows and outflows, for a while. Can be calculated using the expression 6.1, where *n* correspond to the period in years considered for the project and *r* is the discount rate, which was assumed to be 5%.

$$NPV = \sum_{n=1}^{N} \frac{Inflows - Outflows}{(1+r)^n} - I_0 \tag{6.1}$$

For a project to be viable or profitable, NPV must assume a value higher or at least equal to zero. If NPV assumes a negative value it means that the investment will always be an expense, and no return will come from it. For this work, the inflows correspond to diesel fuel savings (that are annual), the outflows to the costs of hydrogen supply network (also annual) and the initial investment (I_0) correspond to the acquisition of the hydrogen fuel cell vehicles, presented in table 6.8. The inflows and outflows are considered constant per year. It is assumed this way because it is assumed that the consumption (the number of kilometres per year) is practically the same. The NVP was calculated for different periods, from 1 to 10 years and the results are represented in the graphic of figure 6.13.

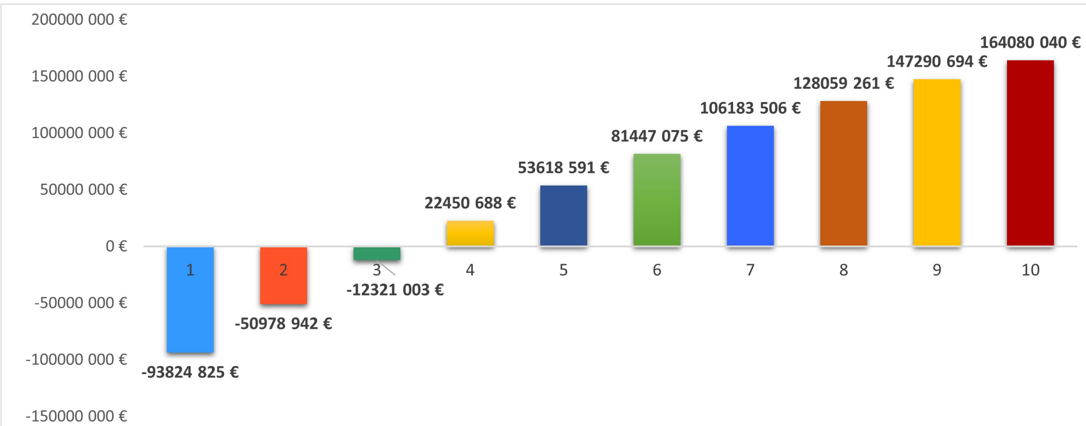

Figure 6.13: NPV of the project along 10 years, no oxygen selling.

Considering the investment that is necessary to do to acquire all the vehicles and the annual costs of producing and distributing hydrogen, it takes between 3 to 4 years to have some return on that investment. After the 4th year, the companies start to see the financial advantage of changing to hydrogen fuel. So, besides being a green alternative to diesel consumption that is a fossil fuel that requires to be imported to the country, hydrogen fuel is more efficient and environmentally friendly. It allows to run the same amount of kilometres in a year with lower costs and enables to have a ”home production”, reducing the necessity of material imports, improving Portugal economy, and allowing it to be more self-sufficient.

The addition of oxygen selling, with the conservative unit cost of 0,80€, will help to down the price. This oxygen selling is considered as an inflow, that is constant per year. Figure 6.14 shows the NPV for the different periods of time, from 1 to 10 years. The change that becomes easier to see is the NPV for 3 years, with the selling of the by-product (oxygen) the NPV increases from -12 321 003 € to 9 999 784 €, and becoming a viable project.

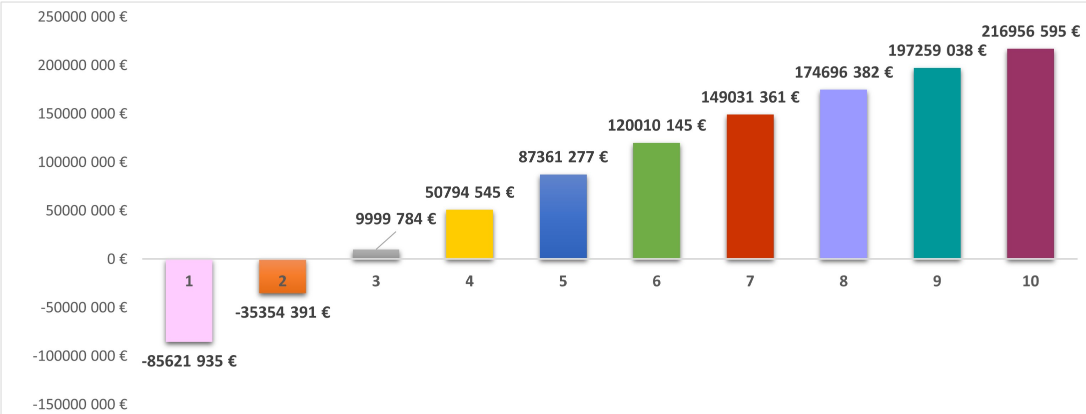

Figure 6.14: NPV of the project along 10 years, with oxygen selling at 0.80€/kg.

According to the Portuguese National Plan for Hydrogen, there is the intention of building 50 hydrogen refuelling stations by 2050. This works focus its attention on 11 production sites (where they can also be considered refuelling stations because they serve other companies) and will provide economic analysis for 10 years.

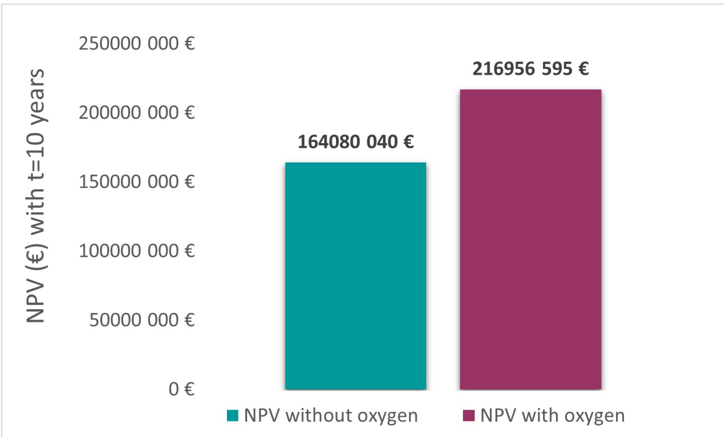

Figure 6.15: NPV of the project for 10 years, considering and not considering the oxygen selling.

As is possible to verify by the figure 6.15, the NPV is positive for both scenarios, considering the selling (in dark purple) or not (in green), which indicates that both scenarios are viable cases for a profitable investments.

6.2.2 Internal Rate of Return and Payback

The internal rate of return (IRR) helps to evaluate the profitability of the project and of the investments and helps to decide if the investors should accept the project or not. IRR corresponds to the discount rate that makes the NPV equal to zero. The higher it is the IRR the more attractive and desirable is to invest in the project.

For a project to be accepted, the IRR obtained needs to be higher than the rate of return (5%) used to calculate the NPV. IRR is calculated as the following:

$$NPV = 0 \tag{6.2}$$

Which means,

$$\sum_{n=1}^{N} \frac{Inflows - Outflows}{(1 + IRR)^n} - I_0 = 0 \tag{6.3}$$

That gives,

$$\sum_{n=1}^{N} \frac{Inflows - Outflows}{(1 + IRR)^n} = I_0 \tag{6.4}$$

By using the equation 6.4 it is obtained the results exposed in figure 6.16.

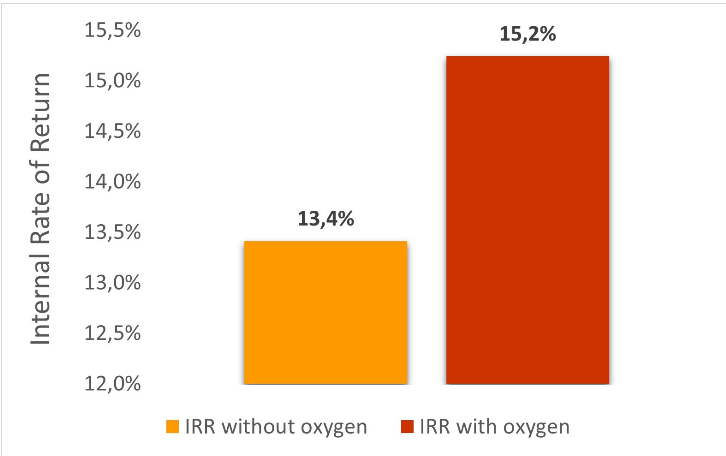

Figure 6.16: Internal Rate of Return (IRR), considering and not considering the oxygen selling.

For both cases IRR is higher than the rate of return used to calculate the NPV (5% <13,4% and 5% <15,2%), which means that for both cases, selling or not the oxygen, the implementation of the hydrogen network is a good project to invest, being more attractive with the oxygen selling, helping to pay the project faster. That can be more easily observed through the payback time.

The payback corresponds to the period that it takes to pay (or recover) completely the initial investment. The simplest way to determine the payback period is by dividing the cash flow (input minus the outputs) by the total initial investment. Taking this into consideration, the results are presented in figure 6.17.

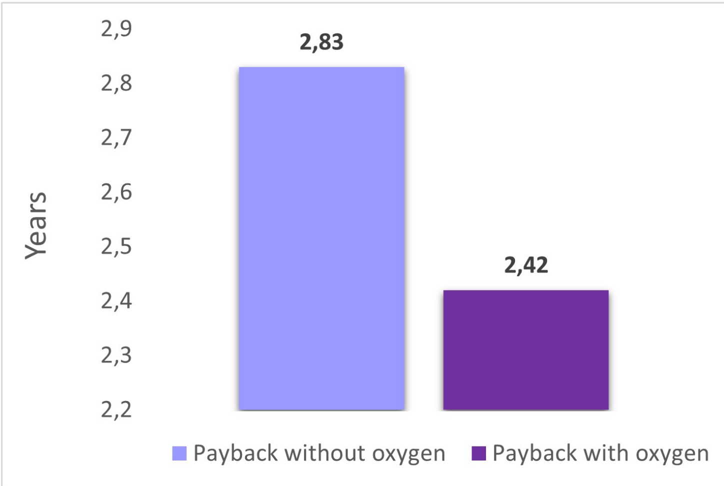

Figure 6.17: Payback time, considering and not considering the oxygen selling.

As expected, by selling the oxygen produced as a by-product, the amount of time that is necessary to recover the investment is lower because the selling helps to depreciate the costs. The simple payback calculation has a limitation of not accounting for the time value of money.

In finalization, all this study performed is a rough approximation that intends to demonstrate the feasibility of the implementation of a hydrogen network supply chain in Portugal. The major highlight is that only considering the oxygen selling as a way to be able to depreciate the costs of initial investment and annual and constant costs of the grid is not possible but, when looking for the bigger picture, and understanding how efficient hydrogen fuel can be in relation to diesel having a lower cost and able to run the same number of annual kilometres, companies will understand the viability of adopting this technology and fuel. But, it is important to mention that the oxygen selling has also a huge contribution in helping decrease the costs of hydrogen production and distribution and helping to recover the initial investment, as represented in the previous figures 6.15, 6.16 and 6.17.

Besides the oxygen selling, another factor that will affect the hydrogen economy, is carbon taxes, namely their savings. Carbon taxes are fees that are charged to companies for their carbon and greenhouse gas emissions. The higher the carbon emission, the higher the amount the company has to pay for its emission. As it happens with diesel savings, the fact of companies are not paying these taxes, is a cost that the companies are not paying, so it can be seen as revenue, and if they assume to transform part of their fleet to hydrogen fuel cell vehicles, they will be emitting less carbon, paying less. Right now, Portugal has settled a value of around 80€ per ton, [7], of carbon emitted to the atmosphere. However, it is predicted that this situation will tend to increase as a way of encouraging companies to pollute less and take on greener alternatives. By being more sustainable and emitting less, companies will be saving money, and that can count as a "revenue". Other factors that can be included and explored also in the future and in more detailed works are the compression and storage costs, the operations and maintenance costs of the hydrogen fuel cell vehicles, and the savings of the operations and maintenance operations of the diesel vehicles. The purpose of this work is the create a simple model that can be easily adapted to more complex cases, being only necessary to adapt new factors into it and analyze the new results.

7

Conclusions

In this study, a Linear Programming model, Transportation Assignment, the formulation is proposed for a transportation sector in a Portuguese context, to decrease the GHG emissions and fossil fuel dependency by using a green hydrogen economy. The model takes into consideration the cost related to hydrogen production, where considers the electricity price and consumption, the investment in electrolysis technology (CAPEX), the number of hours that the electrolyte is working, the cost of hydrogen distribution to the companies, and water supply cost as a raw material. For the revenues, first, it is only considered the selling of oxygen to hospitals until their demand is fully satisfied, but the addition of the savings of fuel consumption (diesel) improved the model.

With this very simple model was possible to see that the hydrogen integration in Portugal is be very costly. And besides that, even considering a small number of companies, there is excess of oxygen production as by.product. This will intensify for large scale production. It's expensive to implement this technology (large initial capital investment), so to make it attractive with the analysis of the savings in diesel consumption. It helped to understand how hydrogen is more efficient and can benefit in a shorter period.

Regarding the oxygen, the producers can easily supply the oxygen demand of all hospitals in Portugal. The problem is the huge amounts of that are produced. Hydrogen is required and Portugal can produce it but the question is what to do with the excess of oxygen. It is necessary to reach new markets and to supply to other consumers such as water treatment stations (the usage of oxygen helps the purification of water to be more efficient instead of using air, that has a lower oxygen content - 21%), pulp industry, glass industry, metallurgic industry. Besides reaching new sectors, it is indispensable to reach international markets to be able to leak the excess product that Portugal has, for example selling to its neighbour, Spain. It is a very close country, so the costs of oxygen transportation would not be too high.

The savings in diesel costs, equal to 511 370 348€, and considering the acquisition of hydrogen fuel cell trucks, assuming a value equal to 141 180 800€ with 160 000 €/truck, can easily transform this project attractive. Looking at NPV results, even not considering the oxygen selling, it was possible to conclude that this was a viable project that would generate profit and with a payback time lower than 3 years. The results obtained for the IRR were also positive (13.4% without selling oxygen and 15.2% by selling it), being higher than the return rate used (5%) for NPV calculations, which helped confirm once again the viability of the network (NPV >0). The oxygen selling alone is not enough to make the companies adapt the technology and change to hydrogen as fuel, only considering the hospitals demands. But, the addition of diesel savings is the game changer.

It's important to highlight also the unitary price of hydrogen production that was obtained in this model, assuming the value equal to 3.81€/kg, which is a very competitive price considering the world's average price mentioned at the beginning of the work. This price can decrease more if the electrolyzer works more than 2100h (having in mind that will decrease its lifetime). The electricity price will decrease in the next years, renewable sources will have a higher share in the energy mix, and being more mature will allow decreasing its unitary price. The same will occur also with electrolyzer prices, by the years this type of technology will be more efficient and accessible, allowing to decrease even more the production price of hydrogen.

In conclusion, it's possible to see that the implementation of a hydrogen supply chain network is economically attractive in Portugal. Unfortunately, due to the lack of data, and the missing collaboration of Portuguese companies, it was not possible to develop a greater grid and correspond to Portugal. But, besides being a simple model and a rough approximation, building a network with 11 production sites for the next 10 years showed to be achievable and attractive. The expansion of the network will occur in proportion to what was established in the study, and to increase the grid, efficiently, it will be necessary that the other producers (that were excluded) have higher production capacities. Another thing that would be interesting to consider is to develop refuelling stations in favourable regions that coincide with the transit routes of the heavy trucks or in the zones near to the country's border, allowing other international companies to refuel their trucks because, like Portugal, other countries in Europe intend to explore more sustainable alternatives and reach the decarbonisation goal of 2050. To finalize, Portugal intends to finance and support projects that will contribute to achieving the target of decarbonisation by 2050 (allocating 30% of the overall spending budget), which includes the energy transition and can help even more the development and implementation of the hydrogen supply chain network. So, Portugal has all the resources necessary available: water, energy/electricity, funding, the right reasons, and the right sector to implement, with the huge advantage of this being an attractive project and investment.

Bibliography

[1] C. F. Guerra, L. Reyes-Bozo, E. Vyhmeister, J. L. Salazar, M. J. Caparrós, and C. Clemente-Jul, "Sustainability of hydrogen refuelling stations for trains using electrolysers," *International Journal of Hydrogen Energy*, no. xxxx, 2020.

[2] G. Akhmat, K. Zaman, T. Shukui, and F. Sajjad, "Does energy consumption contribute to climate change? Evidence from major regions of the world," *Renewable and Sustainable Energy Reviews*, vol. 36, pp. 123–134, 2014.

[3] IEA (2021), "Net zero by 2050 plan for energy sector is coming, iea, paris, [accessed: 16.03.2021]." [Online]. Available: https://www.iea.org/commentaries/net-zero-by-2050-plan-for-energy-sector-is-comings

[4] G. Kakoulaki, I. Kougias, N. Taylor, F. Dolci, J. Moya, and A. Jäger-Waldau, "Green hydrogen in Europe – A regional assessment: Substituting existing production with electrolysis powered by renewables," *Energy Conversion and Management*, vol. 228, no. July 2020, 2021.

[5] Fuel Cell and Hydrogen (FCH), *Hydrogen Roadmap-Europe, A Sustainable pathway for the European energy transition*, January, 2019, [accessed: 19.05.2021]. [Online]. Available: https://www.fch.europa.eu/sites/default/files/HydrogenRoadmapEurope_Report.pdf

[6] D. Y. Lee, A. Elgowainy, A. Kotz, R. Vijayagopal, and J. Marcinkoski, "Life-cycle implications of hydrogen fuel cell electric vehicle technology for medium- and heavy-duty trucks," *Journal of Power Sources*, vol. 393, no. January, pp. 217–229, 2018.

[7] Trading Economics. European carbon permits. [accessed: 30.12.2021]. [Online]. Available: "https://tradingeconomics.com/commodity/carbonr"

[8] MIBGAS. Mercado ibérico del gas. [accessed: 29.12.2021]. [Online]. Available: "https://www.mibgas.es/en"

[9] S. Shiva Kumar and V. Himabindu, "Hydrogen production by PEM water electrolysis – A review," *Materials Science for Energy Technologies*, vol. 2, no. 3, pp. 442–454, 2019.

[10] Z. Navas-Anguita, D. García-Gusano, J. Dufour, and D. Iribarren, “Revisiting the role of steam methane reforming with CO 2 capture and storage for long-term hydrogen production,” 2021.

[11] A. Velazquez Abad and P. E. Dodds, “Green hydrogen characterisation initiatives: Definitions, standards, guarantees of origin, and challenges,” *Energy Policy*, vol. 138, no. August 2019, p. 111300, 2020.

[12] I. Dincer, “Green methods for hydrogen production,” *International Journal of Hydrogen Energy*, vol. 37, no. 2, pp. 1954–1971, 2012.

[13] EIA (2021), “Hydrogen explained, production of hydrogen, [accessed: 05.04.2021].”

[14] M. A. Qyyum, R. Dickson, S. F. Ali Shah, H. Niaz, A. Khan, J. J. Liu, and M. Lee, “Availability, versatility, and viability of feedstocks for hydrogen production: Product space perspective,” *Renewable and Sustainable Energy Reviews*, no. September 2020, p. 110843, 2021. [Online]. Available: https://doi.org/10.1016/j.rser.2021.110843

[15] P. Nikolaidis and A. Poullikkas, “A comparative overview of hydrogen production processes,” *Renewable and Sustainable Energy Reviews*, vol. 67, no. January 2018, pp. 597–611, 2017.

[16] IEA, “The Future of Hydrogen - Seizing today’s opportunities, IEA for the G20, Japan,” *The Future of Hydrogen, no. June, 2019 [accessed: 18.05.2021]*. [Online]. Available: https://www.iea.org/reports/the-future-of-hydrogen

[17] O. Schmidt, A. Gambhir, I. Staffell, A. Hawkes, J. Nelson, and S. Few, “Future cost and performance of water electrolysis: An expert elicitation study,” *International Journal of Hydrogen Energy*, vol. 42, no. 52, pp. 30 470–30 492, 2017.

[18] R. Chauvy, L. Dubois, P. Lybaert, D. Thomas, and G. De Weireld, “Production of synthetic natural gas from industrial carbon dioxide,” *Applied Energy*, vol. 260, no. November 2019, 2020.

[19] Elementar. DessalinizaÇÃo: A solução para falta de Água no mundo?, [accessed: 14.04.2021]. [Online]. Available: https://www.youtube.com/watch?v=305JREWkkQ4

[20] H. Cherif and J. Belhadj, “Chapter 15 - environmental life cycle analysis of water desalination processes,” in *Sustainable Desalination Handbook*, V. G. Gude, Ed. Butterworth-Heinemann, 2018, pp. 527–559.

[21] L. Malaeb and G. M. Ayoub, “Reverse osmosis technology for water treatment: State of the art review,” *Desalination*, vol. 267, no. 1, pp. 1–8, 2011.

[22] P. M. N. G. J. L. J. M. C. B. Edited by Agata Godula-Jopek, Foreword Detlef Stolten and B. Guinot, *Hydrogen Production by Electrolysis*.

[23] U.S Department of Energy. Alternative fuels center: How do fuel cell electric vehicles work using hydrogen?, [accessed: 10.08.2021]. [Online]. Available: https://afdc.energy.gov/vehicles/how-do-fuel-cell-electric-cars-work=

[24] D. Akal, S. Öztuna, and M. K. Büyükakın, "A review of hydrogen usage in internal combustion engines (gasoline-Lpg-diesel) from combustion performance aspect," *International Journal of Hydrogen Energy*, vol. 45, no. 60, pp. 35 257–35 268, 2020.

[25] P. E. Dodds, I. Staffell, A. D. Hawkes, F. Li, P. Grünewald, W. McDowall, and P. Ekins, "Hydrogen and fuel cell technologies for heating: A review," *International Journal of Hydrogen Energy*, vol. 40, no. 5, pp. 2065–2083, 2015.

[26] KEYOU. Hydrogen [accessed: 25.10.2021]. [Online]. Available: "https://www.keyou.de/hydrogen/?lang=en0"

[27] P. D. A. v. W. Jorgo Chatzimarkakis, Constantine Levoyannis and F. Wouters, "April 2021 Hydrogen Europe, [accessed: 09.08.2021]," no. April, 2021.

[28] I. A. Hassan, H. S. Ramadan, M. A. Saleh, and D. Hissel, "Hydrogen storage technologies for stationary and mobile applications: Review, analysis and perspectives," *Renewable and Sustainable Energy Reviews*, vol. 149, no. July, p. 111311, 2021.

[29] P. Speers, "Hydrogen Mobility Europe (H2ME): Vehicle and hydrogen refuelling station deployment results, ," *World Electric Vehicle Journal*, vol. 9, no. 1, 2018.

[30] European Commission. A European strategy for low-emission mobility, [accessed 10.05.2021]. [Online]. Available: https://ec.europa.eu/clima/policies/transport_en

[31] IEA. Transport sector CO_2 emissions by mode in the Sustainable Development Scenario, 2000-2030, [accessed: 11.08.2021]. [Online]. Available: "https://www.iea.org/data-and-statistics/charts/transport-sector-co2-emissions-by-mode-in-the-sustainable-development-scenario-2000-2030"

[32] ——. Tracking transport 2020, [accessed: 13.08.2021]. [Online]. Available: "https://www.iea.org/reports/tracking-transport-2020"

[33] Z. Navas-Anguita, D. García-Gusano, J. Dufour, and D. Iribarren, "Prospective techno-economic and environmental assessment of a national hydrogen production mix for road transport," *Applied Energy*, vol. 259, no. October 2019, p. 114121, 2020.

[34] E. Mulholland, J. Teter, P. Cazzola, Z. McDonald, and B. P. Ó Gallachóir, "The long haul towards decarbonising road freight – A global assessment to 2050," *Applied Energy*, vol. 216, no. January, pp. 678–693, 2018.

[35] European Commission. Reducing CO_2 emissions from heavy-duty vehicles, [accessed: 20.08.2021]. [Online]. Available: "https://ec.europa.eu/clima/policies/transport/vehicles/heavy_en"

[36] A. Ferrara, S. Jakubek, and C. Hametner, "Energy management of heavy-duty fuel cell vehicles in real-world driving scenarios: Robust design of strategies to maximize the hydrogen economy and system lifetime," *Energy Conversion and Management*, vol. 232, p. 113795, 2021.

[37] I. Staffell, D. Scamman, A. Velazquez Abad, P. Balcombe, P. E. Dodds, P. Ekins, N. Shah, and K. R. Ward, "The role of hydrogen and fuel cells in the global energy system," pp. 463–491, 2019.

[38] J. Kast, R. Vijayagopal, J. J. Gangloff, and J. Marcinkoski, "Clean commercial transportation: Medium and heavy duty fuel cell electric trucks," *International Journal of Hydrogen Energy*, vol. 42, no. 7, pp. 4508–4517, 2017.

[39] P. Schäfer, "Hyundai baut Wasserstoffinfrastruktur für Brennstoffzellen-Lkw. (German)," *Springer Professional*, 2019, [acessed: 25.10.2021]. [Online]. Available: "https://www.springerprofessional.de/brennstoffzelle/schwere-lkw/hyundai-baut-wasserstoffversorgung-fuer-brennstoffzellen-lkw-auf/17221340"

[40] J. Kast, G. Morrison, J. J. Gangloff, R. Vijayagopal, and J. Marcinkoski, "Designing hydrogen fuel cell electric trucks in a diverse medium and heavy duty market," *Research in Transportation Economics*, vol. 70, no. November 2016, pp. 139–147, 2018.

[41] J. Marcinkoski, R. Vijayagopal, J. Kast, and A. Duran, "EVS29 Symposium Driving an Industry : Medium and Heavy Duty Fuel Cell Electric Truck Component Sizing," vol. 8, pp. 78–89, 2016.

[42] P. Partidário, R. Aguiar, P. Martins, C. M. Rangel, and I. Cabrita, "The hydrogen roadmap in the Portuguese energy system – Developing the P2G case," *International Journal of Hydrogen Energy*, vol. 45, no. 47, pp. 25 646–25 657, 2020.

[43] Energizer. Portugal needs to invest in green hydrogen, [accessed: 13.05.2021]. [Online]. Available: https://www.energiser.pt/en/forward/2020-12-04-Portugal-needs-to-invest-in-green-hydrogen

[44] Portuguese Government, "Roadmap for Carbon Neutrality 2050 (RNC2050) Long-Term Strategy for Carbon Neutrality of the Portuguese Economy by 2050," *Report R 262/2019*, vol. 2050, p. 102, 2019.

[45] A. e. A. C. "República Portuguesa and Direção Geral de Energia e Geologia", *Roteiro e plano de ação para o hidrogénio em portugal*, 2019.

[46] J. P. M. Fernandes. The portuguese hydrogen strategy to decarbonise its economy: The project to produce green hydrogen by electrolysis, [accessed: 13.05.2021]. [Online]. Available: https://www.europeanfiles.eu/energy/the-portuguese-hydrogen-strategy-to-decarbonise-its-economy-the-project-to-produce-green-hydrogen-by-electro

[47] Dirário da República (DRE), "PRESIDÊNCIA DO CONSELHO DE MINISTROS. Resolução do Conselho de Ministros 27/2021. Plano Nacional do Hidrogenio," *Diário da República - I Série-B*, no. 27, pp. 5–13, 2019.

[48] Evonik Industries. SEPURAN Green – Evonik's hollow fiber membranes for efficient biogas upgrading [Accessed: 30.12.2021]. [Online]. Available: "https://www.youtube.com/watch?v=C2jW0NkCKmw"

[49] Associação Portuguesa de Empresas Petrolíferas (APETRO). Combustíveis líquidos. compromisso com o futuro, [accessed: 10.10.2021]. [Online]. Available: https://www.apetro.pt/setores-de-atividade/combustiveis/combustiveis-liquidos/1670

[50] Pordata. Venda de combustíveis para consumo, [accessed: 25.09.2021]. [Online]. Available: https://www.pordata.pt/Portugal/Venda+de+combust%C3%ADveis+para+consumo-1131

[51] EUROSTAT, "Energy, transport and environment statistics," 2019, [accessed: 27.09.2021]. [Online]. Available: "https://ec.europa.eu/eurostat/documents/3217494/10165279/KS-DK-19-001-ENN.pdf/76651a29-b817-eed4-f9f2-92bf692e1ed9"

[52] Agência Portuguesa do Ambiente (APA). Relatótio do estado do ambiente, [accessed: 10.09.2021]. [Online]. Available: "https://rea.apambiente.pt/content/transporte-de-mercadorias"

[53] Direção Geral de Energia e Geologia (DGEG). Porquê biocombustíveis?, [accessed: 13.09.2021]. [Online]. Available: "https://www.dgeg.gov.pt/pt/areas-setoriais/energia/eficiencia-energetica/biocombustiveis/porque-biocombustiveis/"

[54] ——. Guia do promotor - legislação e regulação para a economia do hidrogénio" (apa e dgeg), [accessed: 12.09.2021]. [Online]. Available: https://www.dgeg.gov.pt/pt/areas-setoriais/energia/energias-renovaveis-e-sustentabilidade/hidrogenio/guia-do-promotor-apa-dgeg/

[55] DGEG (2020), *Energy Scenarios in support of the Portuguese Strategy for Hydrogen. DEIR Studies on the Portuguese Energy System 002. Directorate-General for Energy and Geology, Divison of Research and Renewables, Lisbon, Portugal. 1st edition June 2020, reviewed February 2021. 50 pp.*, no. October.

[56] B. E. Jiménez Cisneros, T. Oki, N. W. Arnell, G. Benito, J. G. Cogley, P. Döll, T. Jiang, S. S. Mwakalila, Z. Kundzewicz, and A. Nishijima, “Freshwater resources,” *Climate Change 2014 Impacts, Adaptation and Vulnerability: Part A: Global and Sectoral Aspects*, pp. 229–270, 2015.

[57] Agência Portuguesa do Ambiente (APA). Water. surface and groundwater availability, [accessed: 10-09.2021]. [Online]. Available: ”https://pt-espwaterproducts.glopalstore.com/understanding-ro/?utm_campaign=oth_r&utm_source=https://www.espwaterproducts.com&utm_medium=wi_proxy&utm_content=en_US&utm_term=c”

[58] MIBEL. Iberian electricity market – mibel. [accessed: 08.12.2021]. [Online]. Available: ”https://www.mibel.com/en/home_en/”

[59] D. G. de Energia e Geologia (DGEG). Energia em números, edição 2021. [accessed: 09.12.2021]. [Online]. Available: ”https://www.dgeg.gov.pt/pt/destaques/energia-em-numeros-edicao-2021//”

[60] H. UK. Medical oxygen. [accessed: 09.12.2021]. [Online]. Available: ”https://www.bochealthcare.co.uk/en/products-and-services/products-and-services-by-category/medical-gases/medical-oxygen/medical-oxygen.html”

[61] V. Hartley. Pure enriched: The advantages of using oxygen in wastewater treatment processes. [accessed: 09.12.2021]. [Online]. Available: ”https://www.airbestpractices.com/industries/wastewater/pure-enriched-advantages-using-oxygen-wastewater-treatment-processes”

[62] U. I. Gases. Oxygen (o_2) properties, uses and applications oxygen gas and liquid oxygen. [accessed: 09.12.2021]. [Online]. Available: ”http://www.uigi.com/oxygen.html”

[63] P. O. Solutions. Pulp and paper. [accessed: 09.12.2021]. [Online]. Available: ”https://www.pcigases.com/oxygen-solutions/pulp-and-paper”

[64] D. Bellotti, M. Rivarolo, L. Magistri, and A. Massardo, “Feasibility study of methanol production plant from hydrogen and captured carbon dioxide,” *Journal of CO2 Utilization*, vol. 21, pp. 132–138, 2017.

[65] M. Gómez-Chaparro, J. García-Sanz-Calcedo, and L. A. Márquez, “Analytical determination of medical gases consumption and their impact on hospital sustainability,” *Sustainability (Switzerland)*, vol. 10, no. 8, 2018.

[66] M. K. Kazi, F. Eljack, M. M. El-Halwagi, and M. Haouari, “Green hydrogen for industrial sector decarbonization: Costs and impacts on hydrogen economy in qatar,” *Computers and Chemical Engineering*, vol. 145, no. 2021, 2021.

[67] I. DB. Ranking de empresas do setor transportes rodoviários de mercadorias, [accessed: 12.05.2021]. [Online]. Available: ”https://ranking-empresas.dinheirovivo.pt/sector-H49410”

[68] Instituto de Mobilidade e dos Transportes (IMT). Empresas de transporte de mercadorias - nacional / internacional e exclusivamente nacional - por ordem alfabética das empresas, [accessed: 27.10.2021]. [Online]. Available: "https://www.imt-ip.pt/sites/IMTT/Portugues/TransportesRodoviarios/EmpresasLicenciadas/Documents/Dezembro%202017/Mercadorias_31-12-2017_Ordem%20Empresas.pdf"

[69] Interreg North-West Europe H2-Share. Toyota's beta: hydrogen fuel cell electric truck for project portal 2.0s, [accessed: 12.05.2021]. [Online]. Available: "https://fuelcelltrucks.eu/project/toyotas-beta-hydrogen-fuel-cell-electric-truck-for-project-porta-2-0/"

[70] Daimler. Hyundai motor's delivery of xcient fuel cell trucks in europe heralds its commercial truck expansion to global markets, [accessed: 12.05.2021]. [Online]. Available: "https://www.daimler-truck.com/innovation-sustainability/efficient-emission-free/mercedes-benz-genh2-fuel-cell-truck.html"

[71] Hyundai. Hyundai motor's delivery of xcient fuel cell trucks in europe heralds its commercial truck expansion to global markets, [accessed: 12.05.2021]. [Online]. Available: "https://www.hyundai.com/worldwide/en/company/newsroom/hyundai-motor%E2%80%99s-delivery-of-xcient-fuel-cell-trucks-in-europe-heralds-its-commercial-truck-expansion-to-global-markets-00000

[72] Interreg North-West Europe H2-Share. Nikola tre: hydrogen-electric truck for european markets, [accessed: 12.05.2021]. [Online]. Available: "https://fuelcelltrucks.eu/project/nikola-tre/"

[73] Y. M. (2021). Distance-based clustering of a set of xy coordinates, matlab central file exchange. retrieved october 27, 2021, [accessed: 10.09.2021]. [Online]. Available: "https://www.mathworks.com/matlabcentral/fileexchange/56150-distance-based-clustering-of-a-set-of-xy-coordinates"

[74] T. Kato, M. Kubota, N. Kobayashi, and Y. Suzuoki, "Effective utilization of by-product oxygen from electrolysis hydrogen production," vol. 30, pp. 2580–2595, 2005.

[75] Pordata. Hospitais: número e camas, [accessed: 19.03.2021]. [Online]. Available: "https:www.pordata.pt"

[76] Afonso Maria Cordeiro da Silva, "Green Hydrogen and Oxygen Economy developments in Portugal, [2021]."

[77] J. Proost, "Critical assessment of the production scale required for fossil parity of green electrolytic hydrogen," *International Journal of Hydrogen Energy*, vol. 45, no. 35, pp. 17 067–17 075, 2020.

[78] Nel Hydrogen. A series. atmospheric alkaline electrolyser, [accessed: 29.08.2021]. [Online]. Available: "https://nelhydrogen.com/product/atmospheric-alkaline-electrolyser-a-series/?gclid=CjwKCAjw4KyJBhAbEiwAaAQbE-0idYMwPVGqzvQ2aiqJyOZ6FiasZxaa7Z4nCD8DwfTT7QVe436OOhoCd_4QAvD_BwE"

[79] Q. S. Wei, X. Zhang, and B. S. Oh, “The effect of driving cycles and H2 production pathways on the lifecycle analysis of hydrogen fuel cell vehicle: A case study in South Korea,” *International Journal of Hydrogen Energy*, no. 10, pp. 7622–7633.

[80] Open Course Ware Europe, “The transportation problem and the assignment problem, [accessed: 02.07.2021],” pp. 151–204. [Online]. Available: https://ocw.ehu.eus/pluginfile.php/40935/mod_resource/content/1/5_Transportation.pdf

[81] Infarmed. Meio hospitalar, monitorizaÇÃo do consumo de medicamentos. [accessed: 27.11.2021]. [Online]. Available: ”https://www.infarmed.pt/documents/15786/3082402/dezembro/a5437f26-ce4b-5732-6972-ab3d589c984c?version=1.0”

[82] Maria Teresa Ramalho, “Impacte energético e económico de medidas de eficiência energética numa frota de veículos pesados de mercadorias,” 2021.

[83] Pordata. Preços médios de venda ao público dos combustíveis líquidos e gasosos – continente. [accessed: 27.11.2021]. [Online]. Available: ”https://www.pordata.pt/Portugal/Pre%c3%a7os+m%c3%a9dios+de+venda+ao+p%c3%bablico+dos+combust%c3%adveis+l%c3%adquidos+e+gasosos+%e2%80%93+Continente-1265-10032”

[84] Statista. Electricity prices for households in portugal from 2010 to 2020, semi-annually, [accessed 03.06.2021]. [Online]. Available: ”https://www.statista.com/statistics/418111/electricity-prices-for-households-in-portugal/”

[85] Grupo Águas de Portugal (EPAL). Preços de venda de água, [accessed: 15.06.2021]. [Online]. Available: ”https://www.epal.pt/EPAL/menu/clientes/tarif%C3%A1rio/%C3%A1gua”

[86] Green Car Congress. Van Hool to build 40 hydrogen buses for Cologne and Wuppertal (Germany); largest fuel cell bus order in Europe to date, [accessed: 11.06.2021]. [Online]. Available: ”https://www.greencarcongress.com/2018/03/20180301-vanhool.html”

8 Appendix

In the following chapter it is presented the essential data used for this work.

8.1 Table 1

Table 8.1: Transportation companies data

Ranking	Company	County	District	National/ International	Fleet Size
1	DOCTRANS - Transportes Rodoviários de Mercadorias Lda	Azambuja	Lisboa	Both	2000
2	Luís Simões - Logística Integrada, S.A	Loures	Lisboa	Both	2100
3	Lamision - Sociedade de Transportes, Lda	Azambuja	Lisboa	Both	—
4	TJA - Transportes J. Amaral, S.A	Estarreja	Aveiro	Both	800
5	LASO - Transportes	Mafra	Lisboa	Both	2000
6	Patinter - Portuguesa de Automóveis Transportadores, S.A	Mangualde	Viseu	Both	2000
7	Dachser Portugal, Sociedade Unipessoal, Lda	Vila do Conde	Porto	National	—
8	STEF Portugal - Logística e Transporte, Unipessoal, Lda	Vila Franca de Xira	Lisboa	Both	2300
9	TRANSBASE - Transporte e Logística, S.A	Alcacena	Santarém	International	—
10	Transportes Paulo Duarte, Lda	Torres Vedras	Lisboa	Both	1179
11	Transportes Florêncio &Silva, S.A	Mafra	Lisboa	Both	—
12	Transportes Broliveira, Lda	Ourém	Santarém	Both	400
13	Transportes Pascoal	Mealhada	Aveiro	Both	350
14	Dilofar - Distribuição, Transportes e Logística, Lda	Vila Franca de Xira	Lisboa	National	—
15	LUSOCARGO - Transitários	Maia	Porto	Both	—
16	XPO Transport Solutions Portugal, Lda	Vila Nova de Gaia	Porto	Both	—
17	Transmaia	Trofa	Porto	Both	435
18	ZAS - Transportes e Logística, S.A	Mafra	Lisboa	Both	—
19	Transwhite - Transportes, Unipessoal, Lda	Caldas da Rainha	Leiria	Both	170
20	Arnaud - Logis, Soluções Logística Integradas, S.A	Loures	Lisboa	Both	—
21	Torres & CA, Lda	União de Freguesias de Nogueira	Braga	Both	1600
22	Santos da Cunha 6 - Logística e Transportes, Lda	União de Freguesias de Celeiros, Aveleda e Vimieiro	Braga	National	
23	Logista - Transportes, Trnasitários e Pharma, Unipessoal, Lda	Alcochete	Lisboa	National	
24	Transportes Central Pombalense, Lda	Pombal	Leiria	Both	215
25	Empresa de Transportes Àlvaro Figueiredo, S.A	Oliveira de Azeméis	Aveiro	Both	300
26	J.L.S - Transportes Internacionais, S.A	Viseu	Viseu	Both	276
27	VERYFEX, S.A	Póvoa de Lanhoso	Braga	Both	1000
28	Transportes Bernardo Marques, S.A	Guarda	Guarda	Both	280
29	Transportes Paulo Costa & Ferreira, Lda	Arruda dos Vinhos	Lisboa	Both	160
30	Totalmédia - Entregas ao domicílio, S.A	Loures	Lisboa	Both	—
31	Lusifrota - Transportes, S.A	Figueira da Foz	Leiria	Both	700
32	OLANO Portugal - Logística e Distribuição, Lda	Guarda	Guarda	Both	120
33	Santos e Vale Sul - Distribuição, Lda	Arruda dos Vinhos	Lisboa	Both	500
34	Transportes António Frade	Arruda dos Vinhos	Lisboa	Both	210
35	Transportes Machado & Brites, Lda	Leiria	Leiria	Both	—
36	Transportes Magalhães & Bruno, Lda	Loures	Lisboa	Both	100

Ranking	Company	County	District	National/ International	Fleet Size
37	Rodo Cargo - Transportes Rodoviários de Mercadorias, S.A	Vila Franca de Xira	Lisboa	Both	240
38	TALDIS, S.A	Vila Franca de Xira	Lisboa	Both	—
39	Transportes Marginal do Mondego, S.A	Coimbra	Coimbra	Both	179
40	TN - Transportes M. Simões Nogueira, S.A	Vila Nova de Famalicão	Braga	Both	—
41	Francisco Da Silva Borges & CA, Lda	União de Freguesias de Nogueira	Braga		—
42	Neves&Neves	Viana do Castelo	Viana Do Castelo	Both	120
43	Santos & Vale - Norte - Transportes, Lda	Arruda dos Vinhos	Lisboa	Both	same as 33
44	C.M.TIR - Transportes Nacionais e Internacionais	Vila do Conde	Porto	Both	150
45	Transportes Antunes Figueiras, S.A	Pombal	Leiria	Both	—
46	João Pires - Transportes e Logística, Lda	Vila Nova de Cerveira	Viana Do Castelo	Both	180
47	GASOGÁS - Transportes e Logística, Lda	Marinha Grande	Leiria	Both	100
48	C.A.T. - Companhia de Afretamento e de Transportes, S.A	Setúbal	Setúbal	Both	660
49	Transportes Viana & Fernandes, Lda	Pombal	Leiria	Both	—
50	TIEL - Transportes e Logística, S.A	Alvaiázere	Leiria	Both	—
51	Transportes Os TrÊs Mosqueteiros	Sines	Setúbal	Both	205
52	T.W - Truck and Wheel Portugal, Lda	Benavente	Santarém	Both	900
53	Sesé Portugal, Lda	Vila Nova de Gaia	Porto	Both	150
54	Augusto & Afonso da Cunha, Lda	Lousada	Porto	Both	
55	Transportes Rosália, Lda	Loures	Lisboa	Both	68
56	Transneiva Sociedade de Transportes, Lda	Viana do Castelo	Viana Do Castelo	Both	112
57	Lusopaladar - Transporte e Comércio Alimentar, Lda	Lousada	Porto	Both	—
58	Bricotir - Transportes, S.A	Mangualde	Viseu	Both	50
59	Tracocer, Lda	Lisboa	Lisboa		—
60	Serviroad, S.A	Benavente	Santarém	Both	—
61	Transportes Cardoso & Irmão, S.A	Viseu	Viseu	Both	80
62	Transportes Eduardo Cardoso, Lda	Proença-A-Nova	Castelo Branco	Both	145
63	Transportes Vieira Vacas, Lda	Santarém	Santarém	Both	180
64	S.T.I.B. - Sociedadede Transportes Internacionais Bairrada, S.A	Mealhada	Aveiro	Both	—
65	Portugalenses - Transportes, Lda	Vila Nova de Gaia	Porto	Both	
66	Numerbox, Lda	Loures	Lisboa	Both	—
67	Forcargo - Transportes, S.A	Vila Nova de Gaia	Porto	Both	150
68	Transportes Rama, Lda	Mealhada	Aveiro		100
69	Transportes Marquês de Pombal, Lda	Mealhada	Aveiro	Both	—
70	TRANSTDF, Lda	Oliveira do Bairro	Aveiro	Both	—
71	David Neto - Transports, S.A	Ovar	Aveiro	Both	200
72	Transportes Gama	Seixal	Lisboa	Both	186
73	Auto Cabreira, S.A	Braga	Braga	Both	—
74	ATLA - Logística, S.A	Loulé	Faro	Both	—
75	Atlantic Cargo - Sociedade de Transportes, S.A	Benavente	Santarém	Both	—
76	DOHM - Operador Logístico, Lda	Vila Nova de Gaia	Porto	Both	75
77	Bruno-TIR - Transportes, Lda	Amares	Braga	Both	80
78	Transportes Figueiredo & Figueiredo, Lda	Oliveira de Azeméis	Aveiro	Both	106
79	General Logistics Systems Portugal, Lda	Mafra	Lisboa		250

Ranking	Company	County	District	National/ International	Fleet Size
80	Transportes Rodoviários de Mercadorias do Valado, Lda	Nazaré	Leiria	Both	—
81	Transportes S. Luís, Lda	Paredes	Porto	Both	90
82	Transportes Sardão, S.A	Matosinhos	Porto	Both	200
83	Transportadora Internacional Felicio & Filhos, Lda	Torres Novas	Santarém	Both	
84	Barrinho - Transportes, S.A	Leiria	Leiria	Both	—
85	Transportes de Mercadorias Rendufenses, Lda	Amares	Braga	Both	110
86	RNM - Transportes Químicos, Lda	Vila Nova de Famalicão	Porto	Both	247
87	Dias & Filhos - Transportes Internacionais, Lda	Montemor-O-Velho	Coimbra	Both	80
88	COMBUSTOIL - Combustíveis, Lda	Cascais	Lisboa	Both	—
89	Transportes Lemos, Lda	Mangualde	Viseu	Both	—
90	Pinho, Moreira & Lago, Lda	Póvoa de Varzim	Porto	Both	—
91	STOP Trans II Internacional, S.A	Trofa	Porto	Both	280
92	Autotrans Express, Lda	Palmela	Setúbal	Both	—
93	Agro Merchants Lisboa Transport Unipessoal, Lda	Alenquer	Leiria		—
94	Brites&Brites - Transportes de Aluguer, Unipessoal Lda	Torres Novas	Santarém	Both	—
95	Transportes Matos & Filhos, S.A	Barcelos	Braga	Both	90
96	Santos & Vale Lda	Arruda dos Vinhos	Lisboa	Both	—
97	Pelinchos, Lda	Figueira da Foz	Leiria		—
98	Patrovitrans - Transportes, Lda	Batalha	Leiria	Both	80
99	TRANSNIL - Transportes de Mercadorias Nacionais e Internacionais, S.A	Portalegre	Portalegre	Both	130
100	Transpataiense - Transportes Rodoviários de Mercadorias S.A	Alcobaça	Leiria	Both	—

8.2 Table 2

Table 8.2: Companies fleet size, annual kilometres travelled and respective coordinates (latitude and longitude)

Ranking	Fleet Size	kilometres	Latitude	Longitude
1	2000	—	39.050328712536114	-8.911348294111523
2	2100	200 000 000	38.8517904	-9.2099010
3	—	—		
4	800	80 000 000	40.74931887305224	-8.57257234429967
5	2000	50 000 000	38.9126022651527	-9.188897652324412
6	2000	—	40.62038041552847	-7.797603460508856
7	—	—	—	—
8	2300	—	38.84626884245331	-9.071826196343498
9	—	—		
10	1179	45 000 000	39.12955191955096	-9.237307061351135
11	—	—		
12	400	48 500 000	39.68316328830875	-8.62870379258137
13	350	—	40.302962777267204	-8.447180146715604
14	—	—	—	—
15	—	—		
16	—	—		
17	435	—	41.285854262782436	-8.590114337010554
18	—	—		
19	170	934 000	39.42217734226705	-9.16679563867921
20	—	—		
21	1600	31 000 000	41.53148415411215	-8.423127170642127
22				
23				
24	215	—	39.84634551663209	-8.705015077818643
25	300	30 000 000	40.85424653237575	-8.481551188478381
26	276	—	40.63196864046579	-7.842845322764148
27	1000	—	41.57683615351394	-8.245024725775759
28	280	28 700 000	40.55127671815826	-7.244373763378052
29	160	—	38.97386292178871	-9.066120259730793
30	—	—		

Ranking	Fleet Size	kilometres	Latitude	Longitude
31	700	—	40.04670021087796	-8.841544689367295
32	120	16 500 000	40.53014674712086	-7.206462431790242
33	500	25 021 456	38.939464213762776	-9.092346046929192
34	210	28 000 000	38.8598560038449	-9.128024268267794
35	—	—		
36	100	—		
37	240	23 056 508	39.005078325456005	-8.9527068
38	—	—		
39	179	2 000 000 000	40.31027956354686	-8.176972679610756
40	—	—		
41	—	—		
42	120	20 500 000	41.71315108635376	-8.800907331629583
43	same as 33			
44	150		41.30739803494602	-8.702440560482023
45	—	—		
46	180		41.9660142167205	-8.687048960455897
47	100	14 749 223	39.7211352349123	-8.929043303632977
48	660		38.577188608790244	-9.00069506180569
49	—	—		
50	—	—		
51	205	—	37.957411929384236	-8.84880786060888
52	900		38.95065381645155	-8.828500760572288
53	150		41.054355807994355	-8.567199247001087
54				
55	68		38.83779381895207	-9.16436927116362
56	112	60 000 000	41.634389541480004	-8.771342487450799
57	—	—		
58	50		40.61171126014117	-7.766946018181927
59	—	—		
60	—	—		
61	80	11200000	40.683117010932456	-7.882002360506426
62	145		39.79111476977092	-7.551134463250975
63	180		39.25660799286243	-8.711581360560881

Ranking	Fleet Size	kilometres	Latitude	Longitude
64	—	—		
65		8 897 545	41.01613465035974	-8.58664950652999
66	—	—		
67	150		41.043362116019004	-8.56955788932875
68	100		40.305074337691146	-8.448742956811719
69	—	—		
70	—	—		
71	200	20 000 000	40.96610925526573	-8.617778076010389
72	186	9 110 208	38.621906	-9.078817
73	—	—		
74	—	—		
75	—	—		
76	75		41.06885885330081	-8.573637760491371
77	80		41.625992694651956	-8.337881760469404
78	106		40.921039	-8.487446
79	250			
80	—	—		
81	90		41.23690394726658	-8.319501531648378
82	200		41.21375237130051	-8.682047073018278
83		130 000 000	39.60619062873322	-8.527440873169791
84	—	—		
85	110		41.63016489728126	-8.399558757672759
86	247		41.38311347779857	-8.460105860479038
87	80		40.186070	-8.681765
88	—	—		
89	—	—		
90	—	—		
91	280		39.2791705527469	-9.263713731723634
92	—	—		
93	—	—		
94	—	—		
95	90		41.411796978163004	-8.6642433
96	—	—		

Ranking	Fleet Size	kilometres	Latitude	Longitude
97	——	——		
98	80		39.66451862365444	-8.832623902872722
99	130		39.32899116206079	-7.4349187028853905
100	——	——		

8.3 Table 3

Table 8.3: Data for the network. The number of vehicles to be transformed, hydrogen demand, oxygen produced (considering the hydrogen demand), amount of water required, diesel savings, and hydrogen fuel cell trucks acquisition cost.

Ranking	Fleet Size	kilometres	5% fleet	5% fleet	Hydrogen Need (kg)	Oxygen (kg)	Water (kg)	Diesel Consumption (30L/100km)	Diesel price (1,3€ em 2020)	Cost vehicles aquisition (160000€/vehicle)
1	2000	125000000	100	100	10000000	80000000	90000000	37500000	48750000	16000000
2	2100	200 000 000	105	105	16000000	128000000	144000000	60000000	78000000	16800000
4	800	80 000 000	40	40	6400000	51200000	57600000	24000000	31200000	6400000
5	2000	50 000 000	100	100	4000000	32000000	36000000	15000000	19500000	16000000
6	2000	125000000	100	100	10000000	80000000	90000000	37500000	48750000	16000000
8	2300	125000000	115	115	10000000	80000000	90000000	37500000	48750000	18400000
10	1179	45 000 000	58,95	58	3600000	28800000	32400000	13500000	17550000	9280000
12	400	48 500 000	20	20	3880000	31040000	34920000	14550000	18915000	3200000
13	350	30546327	17,5	17	2443706,16	19549649,28	21993355,44	9163898,1	11913067,53	2720000
17	435	30546327	21,75	21	2443706,16	19549649,28	21993355,44	9163898,1	11913067,53	3360000
19	170	934 000	8,5	8	74720	597760	672480	280200	364260	1280000
21	1600	31 000 000	80	80	2480000	19840000	22320000	9300000	12090000	12800000
24	215	30546327	10,75	10	2443706,16	19549649,28	21993355,44	9163898,1	11913067,53	1600000
25	300	30 000 000	15	15	2400000	19200000	21600000	9000000	11700000	2400000
26	276	30546327	13,8	13	2443706,16	19549649,28	21993355,44	9163898,1	11913067,53	2080000
27	1000	52000000	50	50	4160000	33280000	37440000	15600000	20280000	8000000
28	280	28 700 000	14	14	2296000	18368000	20664000	8610000	11193000	2240000
29	160	19 124 178	8	8	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	1280000
31	700	52000000	35	35	4160000	33280000	37440000	15600000	20280000	5600000
32	120	16 500 000	6	6	1320000	10560000	11880000	4950000	6435000	960000
33	500	25021456	25	25	2001716,48	16013731,84	18015448,32	7506436,8	9758367,84	4000000
34	210	28 000 000	10,5	10	2240000	17920000	20160000	8400000	10920000	1600000
37	240	23 056 508	12	12	1844520,64	14756165,12	16600685,76	6916952,4	8992038,12	1920000
39	179	19 124 178	8,95	8	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	1280000
42	120	20 500 000	6	6	1640000	13120000	14760000	6150000	7995000	960000
44	150	19 124 178	7,5	7	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	1120000
46	180	19 124 178	9	9	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	1440000
47	100	14 749 223	5	5	1179937,84	9439502,72	10619440,56	4424766,9	5752196,97	800000
48	660	52000000	33	33	4160000	33280000	37440000	15600000	20280000	5280000
51	205	30546327	10,25	10	2443706,16	19549649,28	21993355,44	9163898,1	11913067,53	1600000
52	900	52000000	45	45	4160000	33280000	37440000	15600000	20280000	7200000
53	150	19 124 178	7,5	7	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	1120000
55	68	19 124 178	3,4	3	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	480000
56	112	60 000 000	5,6	5	4800000	38400000	43200000	18000000	23400000	800000
58	50	19 124 178	2,5	2	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	320000
61	80	11200000	4	4	896000	7168000	8064000	3360000	4368000	640000
62	145	19 124 178	7,25	7	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	1120000
63	180	19 124 178	9	9	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	1440000
65	50	8 897 545	2,5	2	711803,6	5694428,8	6406232,4	2669263,5	3470042,55	320000

67	150	19 124 178	7,5	7	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	1120000
68	100	19 124 178	5	5	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	800000
71	200	20 000 000	10	10	1600000	12800000	14400000	6000000	7800000	1600000
72	186	9 110 208	9,3	9	728816,64	5830533,12	6559349,76	2733062,4	3552981,12	1440000
76	75	19 124 178	3,75	3	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	480000
77	80	19 124 178	4	4	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	640000
78	106	19 124 178	5,3	5	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	800000
81	90	19 124 178	4,5	4	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	640000
82	200	19 124 178	10	10	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	1600000
83	2000	130 000 000	100	100	10400000	83200000	93600000	39000000	50700000	16000000
85	110	19 124 178	5,5	5	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	800000
86	247	30546327	12,35	12	2443706,16	19549649,28	21993355,44	9163898,1	11913067,53	1920000
87	80	19 124 178	4	4	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	640000
91	280	30546327	14	14	2443706,16	19549649,28	21993355,44	9163898,1	11913067,53	2240000
95	90	19 124 178	4,5	4	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	640000
98	80	19 124 178	4	4	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	640000
99	130	19 124 178	6,5	6	1529934,24	12239473,92	13769408,16	5737253,4	7458429,42	960000

8.4 Table 4

Table 8.4: Input data HSCN. The data was converted to euros.

Parameter	Symbol	Value	Reference
CAPEX	CAPEX	1400 $/kW	[16]
Electricity price in Portugal	ELCTR	24$/MWh	[84]
Number of working hours of the electrolyte in a year	HPY	2100	[77]
Efficiency of the alkaline electrolyte	EFF	70%	[16]
Unitary cost of water supply in Portugal	UWS	1.8334€/m^3	[85]
Gaseous hydrogen delivery cost	GHD$_{Cost}$	0.13$/kg/km	[66]
Unit of oxygen selling price	UOSP	0.80€/kg	[66]
Heavy fuel tank capacity		40kg	[86]
Energy Content of Hydrogen (LHV)		33.33 kWh kg^{-1}	[22]