

Hydrogen-Powered Long-Distance Transportation for Portugal

Karan Ramesh Narayan

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Supervisors: Prof. Paulo Manuel Cadete Ferrão Dr. Rui Pedro da Costa Neto

Examination Committee

Chairperson: Prof. Francisco Manuel da Silva Lemos Supervisor: Dr. Rui Pedro da Costa Neto Member of the Committee: Dr. Ana Filipa da Silva Ferreira

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RESUMO

O objetivo deste trabalho é explorar o hidrogénio como um futuro portador de energia para meios de transporte pesados. Para fazer isso, existem alguns fatores diferentes que precisam ser considerados. Em primeiro lugar, a viabilidade de diferentes métodos de transporte que o hidrogénio pode suportar. Isso envolveria determinar os reguisitos técnico-económicos e a viabilidade geral de mudar para o hidrogénio verde em modos como autocarros de passageiros, camiões e comboios. Além disso, para garantir o sucesso da implementação de tal sistema, a infraestrutura de distribuição precisa ser examinada. Uma avaliação técnico-económica da infraestrutura de distribuição ajudaria a tirar conclusões. A realização de uma análise de custos (CAPEX, OPEX, NPV, custo nivelado de H2) ajudará a fornecer uma perspetiva mais abrangente. Durante o curso deste estudo, foi descoberto que o método de distribuição da Eletrólise Descentralizada mostrou-se mais promissor quando combinado com a abordagem de cenário realista. Um valor de LCOH de 4,92 € / kgH₂ foi alcançado com potencial para baixá-lo ainda mais. A falta de confiança em camiões ou oleodutos para distribuir o combustível hidrogénio tornou possível atingir esse valor de LCOH viável. Além disso, consolidou-se a importância da comercialização do subproduto oxigênio, pois sem ele a viabilidade económica do estudo seria quase impossível. A análise de sensibilidade realizada sobre os valores LCOH determinou que o valor era diretamente dependente dos preços da eletricidade e do CAPEX. O estudo permitiu confirmar que o H₂ tem um futuro viável no setor da mobilidade, dadas as condições e caminhos adequados para a sua implementação.

Palavras-chave: Produção de hidrogénio; métodos de distribuição; capacidade de conversão de transporte; análise energética e económica

ABSTRACT

The purpose of this work is to explore hydrogen as a future energy carrier for heavy modes of transportation. In order to do this, there are a few different factors that need to be considered. Firstly, the viability of different transportation methods that hydrogen can support. This would involve determining the techno-economic requirements and overall feasibility of switching to green hydrogen for modes such as Buses, Trucks and Trains. Furthermore, to ensure the success of implementing such a system, the distribution infrastructure needs to be examined. A techno-economic assessment of the distribution infrastructure would help in drawing conclusions. Conducting a cost analysis (CAPEX, OPEX, NPV, Levelized cost of H₂) will help provide a more comprehensive outlook. During the course of this thesis it was discovered that the Dispersed Electrolyser distribution method showed the most promise when combined with the realistic scenario approach. An LCOH value of 4.92 €/kgH₂ was achieved with potential to get it down further. The lack of reliance on trucks or pipelines to distribute the hydrogen fuel made it possible to achieve such a feasible LCOH value. Furthermore, the importance of selling the by-product oxygen was consolidated as the economic viability of the study would be almost impossible without it. The sensitivity analysis conducted on the LCOH values determined that the value was directly dependent on electricity prices and the CAPEX. The study was able to confirm that H₂ has a feasible future in the mobility sector given the right conditions and pathways for its implementation.

Keywords: Hydrogen production; distribution methods; transport conversion capability; energy and economic analysis

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Nomenclature

EU	European Union
IEA	International Energy Agency
LCOE	Levelized Cost of Electricity
LCOH	Levelized Cost of Hydrogen
PEM	Polymer Exchange Membrane
ТСО	Total Cost of Ownership
TPD	Tons per day
CAPEX	Capital Expenditure
OPEX	Operational Expenditure
HRS	Hydrogen Refuelling Station

INTRODUCTION

Literature review

RENEWABLE ENERGY IN THE EU

Energy systems around the world are undergoing substantial changes. Many of these changes are being driven by deliberate government policies, whether these are to put a country on a low-carbon transition path, reduce air pollution, secure energy independence and security, or reduce costs and improve efficiencies.

The EU is a leader in renewable energy technologies. It holds 40% of the world's renewable energy patents and in 2016 almost half of the world's renewable electricity capacity (excluding hydropower) was located within its borders. [8]

The 2030 Climate and Energy Policy Framework that preceded the EU contribution to the Paris Agreement was adopted in October 2014. It set three key targets:

- a mandatory target of at least 40% reduction in greenhouse gas emissions by 2030 compared to 1990, for the EU
- (ii) a mandatory EU-level target of at least a 32 % share of renewable energy in 2030
- (iii) an indicative EU-level target to improve energy efficiency by at least 32.5 % in 2030 compared to projections of future energy consumption [9]

Based on Figure 1, as of 2018, most of the European nations have reached or are close to reaching their 2020 targets for renewable energy share in their final energy consumption mix. These percentages are likely to grow rapidly over the next few decades.

Renewable energy technologies/sources (hydropower, wind power, solar power, marine energy, geothermal energy, heat pumps, biomass and biofuels) are alternatives to fossil fuels that contribute to reducing greenhouse gas emissions, diversifying energy supply and reducing dependence on fossil fuel markets, in particular oil and gas.

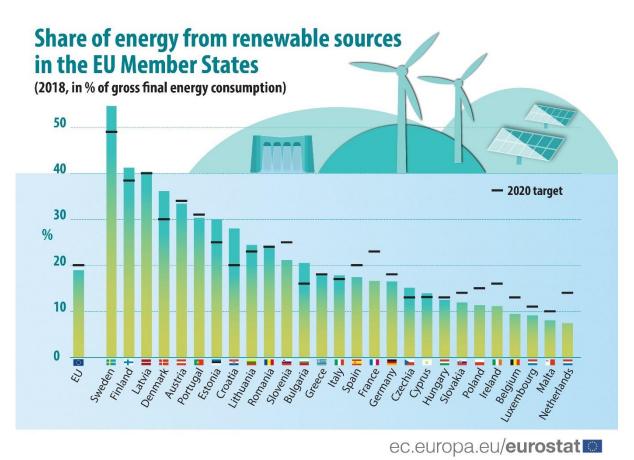


Figure 1:EU Nations 2020 targets for Renewable Energy share in their final energy consumption [7]

The EU 2020 targets are imperative to the 2030 climate and energy targets. In order to maintain its status as a global leader in the climate change revolution and ensure its leadership position in the renewables sector, all EU nations must double down on their efforts to increase the percentage of renewable energy capacity in their energy mix. This has help put them on a sustainable path towards meeting the 2030 targets [7].

GREEN FUELS

With the clear and determined focus on renewable energy to power the future, the biggest question that always gets raised is its intermittent nature. The idea of using clean electricity as a fuel for industry and transport and the technologies that facilitate it have become a major topic of research and discussion in recent times.

Declining costs in available technologies have propelled interest in green fuels forward like never before. The price of lithium-ion batteries for Battery Electric Vehicles (BEV) has fallen by about 80% over the past five years. The global EV fleet is expected to reach 10,5 million by the end of 2020 [21].

Despite some major benefits of battery-based storage for clean electricity, like efficiency, the energy density of the technology poses a serious issue when considering its use in Industry and Heavy Transportation modes. Diesel has an energy density of 45.5 megajoules per kilogram (MJ/kg). On the other hand, hydrogen has an energy density of around 120 megajoules per kilogram. In terms of energy,

the hydrogen energy density translates to 33.6 kWh/kg. Whereas, diesel contains about 12-14 kWh per kg[25]. Lithium-ion batteries have an energy density of around 1 MJ/kg. Hence, for heavy transport modes where weight plays a major factor, a huge amount of batteries would weigh down the vehicle in order to provide the same kind of range that diesel or hydrogen fuel cells would. Therefore, the topic of Hydrogen as a fuel for heavy modes of transport has caused a stir in the energy sector.

PORTUGUESE ENERGY MIX

Having set targets of achieving 80% renewable electricity by 2030 and establishing a carbon neutral economy by 2050, Portugal aims to consolidate its position as a world leader in integrating renewable energy generation from wind and solar PV. In order to achieve these goals, Portugal will need to ensure better interconnection with the rest of Europe and practice clear policy making that will support effective markets [20].

Portugal's national energy and climate plan for 2030 and Roadmap to Carbon Neutrality by 2050 lay out ambitious plans to decarbonise the energy sector. The government needs to ensure that policy will support the development of effective markets to guarantee de-carbonisation goals are met in a cost-effective manner. A strong effort must also be placed on electricity to unlock the potential of Portugal's solar and wind resources to support local economic development and European energy security.

Portugal must also continue with market reforms to ensure stable, transparent and efficient energy markets that can attract the investment needed to achieve its energy sector targets while maintaining affordable energy prices.

In 2018, Portugal emitted 17 Million tons of CO₂ just from their transport sector. In 2019, electricity generation from wind power was 13.738 GWh and from solar was 1275 GWh [20]. As a country, they recognize the need for not just green electricity but also, for green fuels. This is evident in their recent efforts to plan for a solar-powered green hydrogen plant that will cost an estimated \in 5 billion and have a capacity of 1 GW [13].

This is a major step in the efforts to push towards energy independence as, producing green hydrogen in Portugal is estimated to lead to a reduction of natural gas imports that currently cost € 300-600 million annually. Furthermore, according Matos Fernandes, current Minister of Environment, the green hydrogen will also be used as an energy vector for transport with the simultaneous creation of Hydrogen refuelling stations.

PORTUGUESE TRANSPORT SECTOR

- 37.2% of the total primary energy consumption in 2017
- In 2017, the fuel consumption of road transport reached 5.5 million tons of oil equivalent (toe)
- Electricity consumption of heavy rail transport reached 307.5 million kWh
- Diesel consumption of rail transport was 6.8 million litres
- Portuguese airlines consumed a total of 1.26 million tons of fuel in aircraft operation [30]

The main focus of this thesis is to analyse the possible impact Hydrogen can have on this sector of Portugal's economy. Transportation is a major contributor to climate change, emitting 32% of CO_2 emissions in the EU. To achieve the 2-degree scenario, the region needs to eliminate about 72% of CO_2 from the EU transportation fleet by 2050, equal to roughly 825 Mt [11].

A key technological question is how to store large amounts of energy at low weight and in a restricted space within the vehicle. While for some modes of transportation the battery will be the energy storage of choice, other applications require higher energy density for lightweight energy storage or longer driving ranges and faster recharging times.

The second key issue revolves around recharging/refuelling infrastructure. Energy needs to be efficiently distributed from renewable sources to vehicles. While a small share of EVs can be served with the current power grid, meaningful decarbonization requires either a different way of distributing energy, or massive upgrades to power grids.

Hydrogen is the most promising decarbonization option for trucks, buses, ships, trains, large cars, and commercial vehicles for four reasons.

- Hydrogen provides a way to achieve to full decarbonization, where other technologies only act as bridge technologies.
- Having a high energy density, Hydrogen is more suited to provide power for long ranges and high payloads.
- Despite the lack of infrastructure acting as a barrier, faster refuelling, flexible loading and smaller space requirements prove a compelling argument.
- Finally, hydrogen is the best alternative for trains and ships while, hydrogen-based synthetic fuels have the potential to decarbonize aviation [11].

HYDROGEN ECONOMY

Hydrogen is one of the most promising clean and sustainable energy carriers and emits only water as a by-product without any carbon emissions. Hydrogen having many attractive properties as an energy carriers and high energy density which is more than two times higher than typical solid fuels. Presently, the entire worldwide hydrogen production is around 500 billion cubic meter (m³) per year [32]. The produced hydrogen is mostly used in many industrial applications, such as fertilizers, petroleum refining processes, petrochemical, fuel cells, and chemical industries. Hydrogen has been produced from various renewable and non-renewable energy resources such as fossil fuels, especially steam reforming of methane, oil/naphtha reforming, coal gasification, biomass, biological sources and water electrolysis, Figure 3. Steam reforming is the most common method of hydrogen production today, followed by partial oxidation. Based on the data given in Figure 2, it can be observed that this is because the efficiency and cost of the two methods are very attractive. Steam reforming has an efficiency range of 74-85% with a low cost of 2,00 ϵ /kg of H₂. Partial oxidation also has a high efficiency range of 60-75% and a very low cost of 1,30 ϵ /kg of H₂. In comparison, electrolysis matches up to the high efficiency range of the other two methods. It's efficiency range is 60-80%. However, the cost of the hydrogen is where the other two methods are significantly better as, hydrogen has a high cost of 9,06 ϵ /kg of H₂.

Hydrogen production Method	Advantages	Disadvantages	Efficiency	Cost [\$/kg]
Steam Reforming	Developed technology & Existing infrastructure	Produced CO, CO ₂ Unstable supply	74-85	2,27
Partial Oxidation	Established technology	Along with H ₂ Production, produced heavy oils and petroleum coke	60-75	1.48
Auto thermal Reforming	Well established technology & Existing infrastructure	Produced CO ₂ as a byproduct, use of fossil fuels.	60-75	1.48
Bio photolysis	Consumed CO ₂ , Produced O ₂ as a byproduct, working under mild conditions.	Low yields of H ₂ , sunlight needed, large reactor required, O ₂ sensitivity, high cost of material.	10-11	2.13
Dark Fermentation	Simple method, H ₂ produced without light, no limitation O ₂ , CO ₂ -neutral, involves to waste recycling	Fatty acids elimination, low yields of H ₂ , low efficiency, necessity of huge volume of reactor	60-80	2.57
Photo Fermentation	Involves to waste water recycling, used different organic waste waters, CO ₂ -neutral.	low efficiency, Low H ₂ production rate, sunlight required, necessity of huge volume of reactor, O ₂ -sensitivity	0.1	2.83
Gasification	Abundant, cheap feedstock and neutral CO_2 .	Fluctuating H ₂ yields because of feedstock impurities, seasonal availability and formation of tar.	30-40	1.77-2.05
Pyrolysis	Abundant, cheap feedstock and CO_2 -neutral.	Tar formation, fluctuating H ₂ amount because of feedstock impurities and seasonal availability	35-50	1.59-1.70
Thermolysis	Clean and sustainable, O ₂ -byproduct, copious feedstock	High capital costs, Elements toxicity, corrosion problems.	20-45	7.98-8.40
Photolysis	O_2 as byproduct, abundant feedstock, No emissions.	Low efficiency, non-effective photocatalytic material, Requires sunlight.	0.06	8-10
Electrolysis	Established technology Zero emission Existing infrastructure O ₂ as byproduct	Storage and Transportation problem.	60-80	10.30

Various Hydrogen production methods along with their advantages, disadvantages efficiency and cost [Refs. [2,4,5]].

Figure 2: Various Hydrogen Production Methods [33]

HYDROGEN PRODUCTION METHODS

Steam Reforming

The most common way to produce hydrogen in Steam-methane reforming. It also accounts for almost all the commercially produced hydrogen in the United States. Steam reforming is used by commercial hydrogen producers and petroleum refineries to separate hydrogen atoms from carbon ones in methane. High temperatures in the range of 704°C to 982°C are used in conjunction with 3-25 bar pressure to generate hydrogen, carbon monoxide and small amounts of carbon dioxide, Figure 4 [42].

A water-gas shift reaction consists of a steam and carbon monoxide reaction using a catalyst to generate carbon dioxide and hydrogen. The next step called pressure-swing adsorption enables carbon dioxide and other impurities to be extracted from the gas leaving almost pure hydrogen. Ethanol, propane and gasoline can also be used in steam reforming to produce hydrogen [6].

The following equations represent the balance of reactions:

- Steam-methane reforming reaction CH₄ + H₂O (+ heat) → CO + 3H₂
- Water-gas shift reaction $CO + H_2O \rightarrow CO_2 + H_2 (+ \text{ small amount of heat})$

Partial Oxidation

Partial oxidation is process during which methane and other hydrocarbons react in a oxygen-poor environment that enables incomplete oxidation. This converts hydrocarbons to carbon dioxide and water. With the lack of sufficient oxygen, the products of the reaction contain mainly hydrogen and carbon monoxide and tiny amount of carbon dioxide.

This process is exothermic in nature. It takes place much faster than steam reforming and requires less space for the reaction. However, this process generates less hydrogen per unit of the input fuel than with steam reforming.

The following equations represent the balance of reactions:

• Partial oxidation of methane reaction

 $CH_4 + {}^{1\!\!}_{2}O_2 \rightarrow CO + 2H_2 \text{ (+ heat)}$

• Water-gas shift reaction

 $CO + H_2O \rightarrow CO_2 + H_2$ (+ small amount of heat)

Electrolysis [5]

Electrolysis shows promise when considered for hydrogen production using renewable electricity. The process involves splitting water using electricity to produce hydrogen and oxygen. This process takes place in an electrolyser. These come in many different sizes and can be used for a variety of different purposes. From appliance sized to large-scale industrial purpose scale, electrolysers can be used in conjunction with renewable energy sources.

They consist of an anode and a cathode separated by an electrode. The type of electrolyte used in the process decides how a particular electrolyser works. Figure 3 represents a PEM electrolyser diagram. The water is pumped to the anode where it is split into oxygen (O_2) , protons (H^+) and electrons (e⁻). The protons travel to the cathode via the membrane. The electrons exit from the anode to the power circuit. At the cathode, the protons and the electrons combine again to form hydrogen gas molecules.

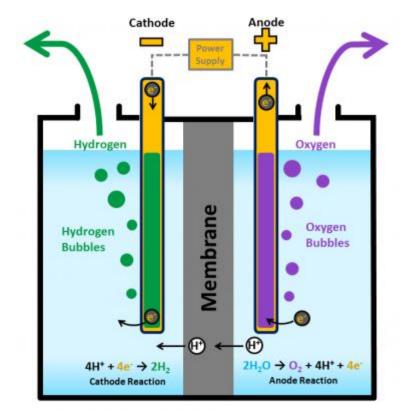


Figure 5: PEM Electrolyser Diagram [5]

Depending on the source of the electricity, electrolysis can produce hydrogen that has zero greenhouse gas emissions. When analysing the benefits and economic viability of hydrogen via electrolysis, the source of the electricity must be taken into account along with a few other factors such as cost, efficiency and emissions.

Potential for synergy with renewable energy power generation:

Hydrogen production via electrolysis offers a solution for renewable energy technologies that face problems of intermittency. For example, despite the cost of wind power declining, the variable behaviour of wind is a major issue that prejudice the efficiency. If hydrogen is generated in combination with renewable energy, in times of excess production of electricity, the excess power can be used to generate and store hydrogen that can be used at a later time when the renewable source of electricity cannot meet the demand.

ELECTROLYSERS (AEC vs. PEM vs. SOEC)

Both alkaline electrolysers (AEC) and proton exchange electrolysers (PEM) can deliver on site and on demand pressurized hydrogen without the use of compressors. However, each one of these methods have certain properties that make them suitable for different applications.

Table 1: Electrolyser Properties [27]

	Units	AEC	PEM	SOEC
Electrolyte	-	Aq.	Polymer	Yttria stabilised
		Potassium	membrane	Zirconia (YSZ)
		hydroxide	(e.g. Nafion)	
		(20–40 wt%		
		KOH)		
Cathode	-	Ni, Ni-Mo	Pt, Pt-Pd	Ni/YSZ
		alloys		
Anode	-	Ni, Ni-Co	RuO2, IrO2	LSM/YSZ
		alloys		
Current Density	A cm ⁻²	0.2-0.4	0.6-2.0	0.3–2.0
Cell Voltage	V	1.8-2.4	1.8-2.2	0.7–1.5
Voltage Efficiency	%HHV	62-82	67-82	<110
Cell Area	m²	<4	<0.3	<0.01
Operating Temperature	٦°	60-80	50-80	650–1000
Operating Pressure	Bar	<30	<20	<25
Production Rate	m ³ _{H2} h ⁻¹	<760	<40	<40
Stack Energy	kWh _{el} m ⁻³ H2	4.2-5.9	4.2-5.5	>3.2
System Energy	kWh _{el} m ⁻³ H2	4.5-6.6	4.2-6.6	>3.7
Gas Purity	%	>99.5	99.99	99.9
Lower Dynamic Range	%	10-40	0-10	>30
System Response	-	Seconds	Milliseconds	Seconds
Cold-start Time	min.	<60	<20	<60
Stack Lifetime	h	60,000-	20,000-60,000	<10,000
		90,000		
Maturity of Technology	-	Mature	Commercial	Demonstration

AEC is the most mature technology from the list. It is commonly used for industrial-scale applications. These systems are readily available, are robust and have a lower capital cost compared to the technologies. However, lower current density and the required operating pressure create issues that affect system size and production costs. The time to start-up and fluctuations in power input are weaknesses that limit the system efficiency and gas purity. Hence, most development around this technology focuses on improving current density and operating pressure to enable dynamic operations such as working with renewable sources. Future cost reductions are expected to be linked to achieving economies of scale which would mean increasing the production by 100 times of units/year, fully automated assembly lines and increasing in the size of electrolysers by 4 times.

General Electric first introduced the PEM system, which is based on the solid polymer electrolyte concept, in the 1960s. This was done in an attempt to overcome the drawbacks of AECs. This

technology is less mature than AECs and is mostly used for small-scale operations. The higher power density, cell efficiency, flexible operation and highly compressed and pure hydrogen are its main benefits. This comes at a cost though, with disadvantages such as expensive catalyst and fluorinated membrane materials and a high complexity due to a high-pressure environment requirement. It also has a shorter lifespan than AEC. As a result, current development efforts are aimed at reducing the complexity of the system in order to scale the system and reduce capital costs through cheaper materials and more sophisticated stack manufacturing processes.

SOEC is the least mature technology available. There is no commercially availability as yet. However, it has been developed for demonstrations on a laboratory scale. This technology uses solid-ion conducting ceramics as the electrolyte which allows for operations to take a much higher temperatures. The advantages are low material cost, a possibility to function in a reverse manner as a fuel cell with and high electrical efficiency. One of the main disadvantages is the rapid material degradation as a direct consequence of high operational temperatures. Ongoing research is focused on stabilising the component materials and also developing new materials. Furthermore, research is being conducted to try and bring down the operating temperature to enable commercial operations.

Most experts believe that there will be a shift in adoption of technology as PEM will become the preferred technology over AEC around 2020. This is mainly due to its compatibility with renewable generation [27].

ELECTROLYSIS COUPLING WITH WIND/SOLAR

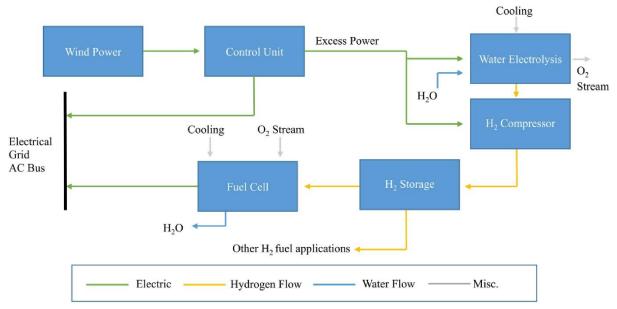
The need to produce green hydrogen for reducing the intermittence of renewable power sources is imminent. Hence, it is important to understand the technical and economic conditions of coupling electrolysers to green power sources such as Wind and Solar.

Solar Coupling

The Solar PV and electrolyser coupling system is an encouraging approach for large-scale hydrogen production. There are two different methods for going about this process. The direct coupling and the indirect coupling. In the indirect coupling system, there is a PV cell, an electrolyser, a DC converter, a fuel tank and a battery. However, this approach requires larger investment and has higher maintenance costs. Hence, there is a greater focus on the direct coupling method. Direct coupling method is when the solar PV system is connected directly to the electrolyser. There are no additional components required in between the two systems [28].

Based on research papers published recently, most experimental papers prefer PEM electrolysers for their low operational temperature, high pressure density, solid membrane, long life and its likeliness to be the most commercial type of electrolyser. This technique can achieve the efficiency of 13% concerning conversion of solar radiation into hydrogen. The experimental results also indicate a direct relation between solar irradiance and hydrogen production [28].

At the end 2018, Portugal has 670 MW of solar installed which represented 2.2% of total power generation in 2019. However, during the period of 2019-2023, the expected growth in installed solar power for Portugal is expected to be around 3865 MW. In the Portuguese market, 75% of electricity consumption came from renewable energy in 2018 [41].



Wind coupling

Wind power is considered to be the most important energy source for the future in many 2050 scenarios. Wind-coupled electrolysis generate lower Carbon dioxide emissions than other renewable energy-electrolyser coupling methods, Figure 7. The system almost achieves the 1 kg of CO₂ per kg of H₂ produced target.

The LCOE for wind power is well below the average cost of conventional fuels, since it goes as low as 26,4 €/kWh. Hydrogen as a storage medium also shows great promise as its seasonal storage cost varies from 44 to 916 €/MWh. This is much lower than other renewable energy storage technologies.

Even though the wind-electrolysis coupling comes in at a cost that is slightly higher than the cheapest conventional fuel source, the social cost of implementing clean energy, including storage, makes it worthwhile. It is possible to maximise profit from wind power by enabling storage and export of electricity using hydrogen at as an outlet at specific hours during operations.

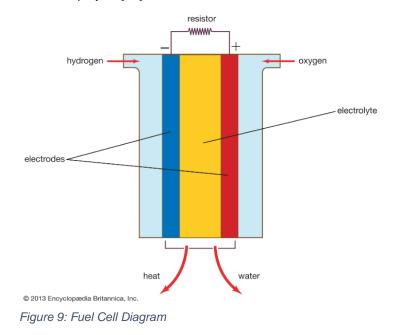
Portugal's wind power is expected to grow to around 7 GW by 2030, which is enough to cover almost 40% of the country's electricity consumption. In 2019, wind power represented 27.5% of total electricity generation [14].

Figure 6: Wind Power Operational chart [4]

FUEL CELLS

Fuel cells have almost the same components as a battery. Each cell of fuel cell consists of a matching pair of electrodes, Figure 8. The anode supplies the electrons and the cathode absorbs them. Both the electrodes must be in contact with the electrolyte and must also be separated by it. The electrolyte can be either a solid or a liquid. It facilitates the conduction of ions between the electrodes. Hydrogen, a common fuel, is supplied to the anode where it gets oxidized and produces hydrogen ions and electrons. Oxygen is supplied at the cathode, where the hydrogen ions from the anode are reduced by electrons and this reaction produces water.

Various types of fuel cells have been developed. They are generally classified on the basis of the electrolyte used, because the electrolyte determines the operating temperature of a system and in part the kind of fuel that can be employed [34].



Alkaline fuel cells

These have an liquid solution of sodium hydroxide or potassium hydroxide as the electrolyte. The fuel is usually hydrogen gas, with oxygen used as an oxidizer. Zinc or aluminium can also be used as an anode if the metal is supplied continuously in strip or powder form. The operating temperature range for fuel cells is usually under 100 °C (212 °F) and they are constructed of metal and certain plastics. Electrodes are fashioned from carbon and a metal such as nickel [34].

Phosphoric acid fuel cells

They use an orthophosphoric acid electrolyte that accommodates operational temperatures of up to about 200 °C (400 °F). They can even use a hydrogen fuel contaminated with carbon dioxide and an oxidizer of air or oxygen. The electrodes are made up of catalysed carbon. The framing structure for this assembly of cells is made of graphite, which significantly raises the cost [34].

Molten carbonate fuel cells

The fuel is made up of a mixture of hydrogen and carbon monoxide that is produced using water and a fossil fuel. The electrolyte is molten potassium lithium carbonate, which operates at a temperature of about 650 °C (1,200 °F). Warming up to operational temperatures takes several hours, making this type of fuel cell incompatible for vehicles. The electrodes are usually metallic in nature, and the containment structure is made of metals and specially engineered plastics. Molten carbonate fuel cells are expected to be useful in both local uses and larger-scale power stations [34].

Solid oxide fuel cells

The cell materials are made up of special ceramics with a small amount of nickel. The electrolyte is an ion-conducting oxide such as zirconia treated with yttria. The fuel for the anode is pure hydrogen or hydrogen combined with carbon monoxide. The cell products are water vapour and carbon dioxide. Due to the high operating temperatures, the electrode reactions proceed very quickly. Achieving overall efficiency of about 60% is a within the realm of possibility. [34]

Proton exchange membrane (PEM) fuel cells

Pressurized hydrogen gas is passed through a catalyst, typically made of platinum, on the anode. Here, electrons are extracted from the hydrogen atoms and carried by an external electric circuit to the cathode. The hydrogen ions then pass through the proton exchange membrane to the catalyst on the cathode side. Here the reaction, with oxygen and electrons from the circuit, takes place to form water vapour and heat [19].

Applications for each type of fuel cell

Table 2 suggests the best applications for each type of Fuel cell. For example, Alkaline fuel cells are best suited for large scale stationary use. Hence, this could be a suitable option for industrial scale gas to power conversion. For the purpose of mobility, Table 2 suggest that PEM fuel cells are the best option due to a variable electrical output.

Table 2: Fuel Cell Applications based on type [19]

Туре	Applications
AFCs	Tend to have large footprint and are better for stationary uses. Used on
	NASA shuttles throughout the space programme
PAFCs	Used in stationary power generators (100 kW to 400 kW). Low electrical
	efficiency but overall efficiency can be over 80% if waste heat is utilized
MCFCs	Used in stationary power generators (100 kW to 400 kW). Low electrical
	efficiency but overall efficiency can be over 80% if waste heat is utilized
SOFCs	Auxiliary power units in vehicles, Stationary power generation (100 W to 2
	MW), Uses with heat engine energy recovery devices or combined heat
	and power, which further increases the overall fuel efficiency.
PEMFCs	Electrical output can be varied making it ideal for road transport (cars,
	buses, trucks, residential cogeneration, etc.)

OXYGEN BY-PRODUCT ECONOMIC BENEFIT

During the water electrolysis process, half the moles of oxygen are produced along with the desired hydrogen as a by-product. Hence, in large scale operations of water electrolysis, large amounts of by-product oxygen will be produced alongside the hydrogen. This presents an opportunity to use this oxygen commercially. Oxygen is an important industrial gas that is used for many different processes such as wastewater treatment and combustion. As environmental concerns and awareness increases, demand for oxygen is rising for processes like electric furnaces and glass melting [38].

Europe's liquid oxygen capacity is close to 31.000 tons per day (tpd). Total demand (including all industrial uses) is around 24.500 tpd. Medical oxygen is needed at a rate of 3.150 tpd [29]. Considering 741 million the Europe pollution, and 10 million the Portuguese pullulation, that represents around 1,3 % of the Europe population. It would be plausible that the Oxygen demand in Portugal would be: medical 41 tpd, the industrial uses would be 328 tpd, that will make the Portuguese total daily need of oxygen 370 tpd.

For example, when electrolysis efficiency is 70%, 5000 kWh of electricity would produce 1000 Nm³ of hydrogen and 500 Nm³ of oxygen. If oxygen by-product is used to meet some of the demand in Europe, it could help bring down the capital costs of electrolysis and make it an attractive option.

In this case, the balance between by-product oxygen and oxygen demand is very important. In hydrogen production by water electrolysis, if the oxygen demand is not too large relative to the possible supply of by-product oxygen, large quantities of by-product oxygen must be wasted. Oxygen itself is an important industrial gas used in many industries such as blast furnaces, electric furnaces and glass melting. The by-product oxygen can thus be sold to these industries, reducing the nominal cost for producing hydrogen by electrolysis. On the other hand, if a large oxygen consumer produces oxygen by electrolysis, it can put the hydrogen on the market.

It will be key factor to bring down to the overall costs of implementing a hydrogen-based transportation network in Portugal. This thesis will be incorporating the oxygen benefit in the cost analysis for the hydrogen plant investment in order to understand how significant of an impact it could make.

TRANSPORT SECTOR

Trains

Hydrogen's energy density advantage makes it the preferred renewable option for trains. In Europe, many commuter and freight trains run on diesel. The electrification of these train lines is the most logical solution. However, the upgrades to the existing tracks are quite expensive. In order to accommodate electrification equipment, tunnels need to be widened and bridges need to be altered. Furthermore, the necessary performance requirement rules out batteries as an option for electrification. This is where hydrogen trains do well. It has no carbon emissions and hardly any noise emissions. Since, the refuelling can take place in large quantities in a handful of locations, the infrastructure can be developed with ease and economically [11].

Since, Portugal has taken up multiple projects to electrify most of their train lines, it makes the most sense to focus on the few train lines that will not be electrified in the near future. Here the diesel trains can simply be replaced with fuel cell trains without having to change the infrastructure for the railways. [17].

For long-haul road transport, PEMFCs are the ideal choice of powertrain system due to their compactness in comparison to the other variants of fuel cell systems.

Buses

As far as road transport is concerned, public transport buses are the most commonly tested for hydrogen applications. Several hundred buses have been tested since the 1990s and continue to run on hydrogen all around the world.

Hydrogen was initially used in buses with internal combustion engines. However, now most bus developers are solely focused on fuel cell bus applications. The use of fuel cell buses is currently being used to promote clean air policies in urban areas.

These buses, through years of testing and development, have acquired a high level of maturity. They are still not in continuous production yet. The small production batches is the reason behind the high cost of fuel cell buses where their diesel counterparts are much cheaper [10].

Depending on annual production numbers, production costs for FCEBs should continue to fall, however, in future projects. The production costs for 12-metre buses are projected to fall to around 650,000 EUR by 2020 and to approx. 350,000 EUR by 2030, bringing them within reach of diesel hybrid buses [35].

Fuel cell buses today have two fuel cells stacks that they draw power from. Each has a capacity of around 100 kW. Furthermore, a small traction battery is also fitted to them that helps recover energy from braking. The fuel tank capacity is anywhere from 30 to 50 kg of compressed hydrogen which is stored at 350 bar pressure.

The range for a fuel cell bus today is typically in the range of 300 to 450 km and hence offers the same capabilities of a diesel bus. The newer fuel cell buses have an average consumption of about 8 to 9 kg of hydrogen per 100 km. This gives fuel cell buses an edge over its diesel counterpart as it is 40% more energy efficient [10].

Trucks

Almost all lorries are fitted with diesel engines; this is especially true of the heavy goods vehicles used for long-distance road haulage. Alternative drives and fuels – mostly gas vehicles (CNG and LPG) – are only used for light commercial vehicles, and even then, only in small numbers as yet. Electric drives have so far been unable to achieve significant numbers in lorries because of the weight and volume of the batteries needed to provide the necessary range reduces the payload to an unacceptable level. However, a gradual increase in hybridisation/electrification is anticipated in the future for light commercial vehicles.

For heavy and long-distance trucking, FCEVs are the superior solution. For these trucks, the low energy density of batteries is a significant disadvantage. A battery for a 40-ton truck would add around three tons of payload to the vehicle, already accounting for the advantage of the electric motors compared to the combustion engines. A hydrogen powertrain would end up weighing similarly or slightly more than a combustion engine. Fuel cells also demand significantly fewer raw materials compared to batteries and combustion engines. They are cobalt free, and research targets are to use less platinum than in a comparable diesel vehicle.

PLACEMENT OF HYDROGEN PRODUCTION SITES

The three largest ports of Portugal are the Port of Sines, Port of Lisbon and the Port of Leixões by scale of operations. Portugal has three more important ports that are smaller in operations but are considered very important for the economy. These are the ports of Aveiro, Douro and Setubal.

Port of Setubal has even been recognised as a "Green Port" by the European Sea Ports Organisation (ESPO) for their excellent environmental quality.

The vehicle traffic in and out of these ports is very large and can hence be an ideal place to situate the large scale alkaline electrolysers to generate hydrogen. This hydrogen can then be used by trucks and trains that work closely with the ports. Hydrogen fuelling stations can be set up near parking bays for trucks and near loading stations for the cargo trains. This would allow a network of hydrogen generation and fuelling stations along the coastline of Portugal. A network near the coastline is highly beneficial as

75% of Portugal's energy consumption and electricity demand come from the coastal regions of the country. It also makes sense as majority of Portugal's population resides in the major cities that are situated along the coast.



Figure 10: Port Map of Portugal [2]

This could be an ideal solution for further expansion of the hydrogen use case as placing hydrogen generation sites near the port allows for the natural progression of hydrogen use for the maritime industry as well.

METHODOLOGY

In order to achieve a comprehensive study of Hydrogen's Transport sector potential, the analysis of data conducted will be divided into two main sections. They are as follows:

<u>Transport Conversion Scenarios</u>: Using three different scenarios, with varying assumptions, in order to predict what the future of hydrogen based heavy transport could look like. Using these scenarios will help calculate the amount of hydrogen fuel required to support the transport sector. The next step would analyse the use of three different methods to distribute the produced hydrogen fuel to assess the best and most economical way to supply the transport sector's need.

<u>Determining the TCO for each transport mode</u>: In order to assess the viability of running long distance transportation on hydrogen fuel, the total cost of ownership (TCO) needs to be considered and evaluated against the those of traditional diesel vehicles and electric vehicles.

For the purpose of this thesis, the scenarios will start in the year 2022 and end in the year 2050. This is done to account for the COVID-19 pandemic and allow the Portuguese government the year 2021 to set their plans in place to execute hydrogen mobility projects.

Once the results for these two sections are calculated and obtained, the aim is to use them to gain an economic perspective and draw conclusions for the future of hydrogen-based transport in Portugal.

ASSUMPTIONS

For any scenario-based study, it is imperative to start by establishing a comprehensive set of parameters and assumptions. These helps define the boundary conditions for the study.

Parameter	Value Assumed	Reasoning
Available Electricity	11-12 GWh	Studying the electricity data for Portugal's energy
Supply	(average)	grid, it was determined that the amount of surplus
		renewable electricity that goes unutilized in non-
		peak hours can be redirected towards hydrogen
		fuel generation. The value assumed is what is
		available daily on average [31]
Electricity Cost	9,27 € Cents /	Based on the standard industrial electricity price in
	kWhel (average)	Portugal [37]
Electricity Requirement	54 kWh/kg H ₂	Based on the current AEC efficiency data [23]
for H ₂ Production		
Number of Buses	15.000	Based on government data [1]
Number of Trucks	120.000	Based on government data [1]
Number of Diesel	59	Based on government data [3]
Trains		

Table 3: Scenario Assumptions

Based on the number of vehicles of each transportation type, an assumption was made to split the hydrogen fuel production which would service the future fuel-cell versions of those vehicles. This production split is as follows:

- Trucks: 85% of hydrogen fuel production
- Buses: 10% of hydrogen fuel production
- Trains: 5% of hydrogen fuel production

TRANSPORT CONVERSION SCENARIOS

The best approach to model future events is to anticipate multiple outcomes and analyse each one. For the purpose of this thesis, three scenarios were chosen to cover the broad range of possible events that could occur. They are as follows:

Pessimistic Scenario:

The first scenario portrays a slow adoption of the hydrogen-based technology. This would mean an introduction of fewer fuel cell vehicles and subsequently, lesser hydrogen fuel generation. In order to do this, the following conditions were set:

- Buses: 10% of all buses in Portugal would be replaced by hydrogen fuel cell buses by 2050
- Trucks: 20% of all cargo trucks in Portugal would be replaced by hydrogen fuel cell trucks by 2050
- Trains: 20% of all diesel trains in Portugal would be replaced by hydrogen fuel cell trains by 2050

Realistic Scenario:

The second scenario explores a moderate adoption of the hydrogen-based technology. This would mean a compelling number of vehicles would be replaced by fuel cell vehicles. And to support this growth, there would be a need for a significant amount of hydrogen fuel generation. To study this scenario, the following conditions were set:

- Buses: 40% of all buses in Portugal would be replaced by hydrogen fuel cell buses by 2050
- Trucks: 40% of all cargo trucks in Portugal would be replaced by hydrogen fuel cell trucks by 2050
- Trains: 50% of all diesel trains in Portugal would be replaced by hydrogen fuel cell trains by 2050

Very Optimistic Scenario:

The third and final scenario tests a complete takeover of the heavy transport sector with hydrogen technology. This would suggest that Portugal would become a hydrogen pioneer in Europe and around the world and generate massive amounts of hydrogen fuel to support this move. The following conditions were assumed:

- Buses: 100% of all buses in Portugal would be replaced by hydrogen fuel cell buses by 2050
- Trucks: 100% of all cargo trucks in Portugal would be replaced by hydrogen fuel cell trucks by 2050

 Trains: 100% of all diesel trains in Portugal would be replaced by hydrogen fuel cell trains by 2050

Once the general assumptions are set, the modelling of the scenarios can begin. The first step is to decide a starting point for the amount of electricity available for hydrogen generation via electrolysis.

DETERMINING AVAILABLE ELECTRICITY FROM THE GRID

Using Portuguese Electricity Market data, determine an average amount of electricity surplus available. Using this figure as a reference, an estimation of **10%** of total surplus electricity is assumed to be available for hydrogen production. Next, using a simple equation 1,

Equation 1: Hydrogen production equation

 $Hydrogen \ Produced \ (kg \ H_2) = \frac{Electricity \ Available \ (kWh)}{Electricity \ Required \ per \ kg \ of \ H_2(\frac{kwh}{kg \ H_2})}$

and the standard electricity requirement value used for AECs, the initial daily hydrogen production is determined. The data used is found in Table 4.

Table 4: Electricity Grid Data

Daily Electricity Load	121.055 [31]	MWh
Daily Electricity Generation	133.375 [31]	MWh
Available Electricity Supply	12.320	MWh
AEC Electricity Requirement	54 [23]	kWh/per kg H ₂
Daily Hydrogen Generation	22.815	kg H₂/day
Capacity		

This initial daily hydrogen production will provide a baseline to kick-off the different scenarios for calculating the percentage of transport that hydrogen fuel can potentially support.

MAPPING OUT THE TRANSPORT CONVERSION SCENARIOS

The three scenarios for this section are analysed using assumptions made earlier in the methodology along with some crucial data pertaining to the three different modes of transportation. This crucial data consists of:

- Total number of existing fossil fuel based trucks, buses and trains
- Fuel tank capacity for trucks, buses and trains
- Scenario specific percentage data of serviceable number of each mode of transport

The data used can be found in Table 5.

Table 5: Transport Data Table

	Units	Trucks	Buses	Trains
Total number of		120.000 [1]	15.000 [1]	59 [3]
vehicles				
Fuel Tank	kg H ₂	70 [22]	40 [10]	99 [36]
Capacity				

Next, taking 22.815 kg of daily hydrogen generation capacity and splitting it between the three modes of transport, based on the assumed percentage split of 85:10:5, gives the amount of hydrogen available for each mode of transport for the first year of the scenarios.

In order to determine the number of each type of vehicle for each year, the total number of vehicles of each type is multiplied by the assumed percentage of vehicles that should be converted to hydrogenbased by 2050. Once the 2022 and 2050 values are obtained, a linear interpolation for the years in between help determine the annual increase in vehicle conversions.

Once the scenarios are mapped out over the selected time period, the corresponding amount of yearly fuel required is calculated for each transport mode. By multiplying the fuel tank size data and the number of vehicles that can be serviced per day, the total daily required fuel is calculated for each mode and each scenario. This is then converted to an annual value of hydrogen fuel required. The equation for this is as shown below,

Equation 2: Fuel Requirement Equation

Fuel required (ton
$$H_2$$
) = $\frac{Fuel tank capacity * Number of vehicles * 365 days}{1000 kg/ton}$

When this is done for each year for each mode of transportation, the fuel required for all 3 modes of transport are summed to get a total amount of annual fuel required for each scenario. These total annual fuel values will form the basis for the economic analysis for each scenario.

ECONOMIC ANALYSIS

To conduct an economic analysis, the following data is required as can be seen in Table 6.

Table 6: Economic Analysis Data

Hydrogen Output for 1 MW system	20 [47]	kg/h
Hours of Operation	8.000 [47]	h/yr
Hydrogen Output for 1 MW system	160.000	kg/yr
Capital Cost of AEC	800 [46]	€/kWel
Cost of Industrial Electricity	9,27 [37]	Euro cents/kWh
Electricity required	54 [23]	kWh/per kg H ₂
Cost of Hydrogen (without cost of electricity)	6,75 [23]	€/kg
Cost of electricity	5 [23]	€/kg
AEC Fixed O&M Cost	5% [43]	of CAPEX
AEC Variable O&M Cost (Raw Materials)	2,80 [43]	€/kg
Stack Replacement Cost	25% [43]	of Capex
Sale price of Hydrogen	2 [47]	€/kg

Once this data is obtained, the next step is to list out the economic cost factors that need to be considered for a comprehensive analysis. These factors are as follows:

- Electrolyser Capacity Required: The total AEC capacity required to provide the annual hydrogen fuel requirement. This is calculated by dividing the total fuel requirement by the hydrogen output of a 1MW AEC system.
- Electrolyser Capital Cost Decline: The cost of AEC systems is predicted to fall steadily from 800 €/kW down to 450 €/kW by 2050 [46]. This needs to be taken into account when calculating CAPEX costs for the scenarios.
- Total Electrolyser CAPEX: The product of the AEC required capacity and the Electrolyser predicted capital cost for that particular year.
- Stack Replacement Cost: Each AEC stack needs to be replaced after 80.000 hours of operation [47]. This would mean that there is an additional cost factor to consider for previously installed electrolysers after they've been operational for a few years. However, the stack replacement

cost is taken as 25% of CAPEX cost at the time of replacement. So that makes it cheaper to replace per megawatt as the capex cost continues to drop.

• Fixed and Variable O&M cost: These costs are a part of the operation of this technology and need to be considered.

The Net system cost also incorporates the benefit of selling the produced hydrogen at a competitive price. While this price might not be the ideal price producers might look for, it needs to be set at a level where hydrogen can compete with other alternatives such as petrol and diesel. This price is set at 2 \in /kg of hydrogen. This price is then multiplied by the amount of hydrogen produced annually to give a total cost benefit that helps reduce the Net system cost.

Finally, the last factor that needs to be considered is the oxygen benefit as mentioned in the introduction section. Based on the following chemical reaction,

$$9kg H_2 O \xrightarrow{}_{Electrolysis} 1kg H_2 + 8kg O_2$$
 [47]

it is evident that for every kilogram of hydrogen, produced from electrolysis, 8 kilograms of oxygen is also obtained. This oxygen is very pure and can be sold to multiple industries for a profit that offsets the Net system cost further. Hence, in an experiment to see the effect of the oxygen benefit, the Net system cost will be reviewed with and without the oxygen benefit. This will hopefully display the benefit of taking it into consideration. Current oxygen prices are shown in Table 7. [47] The oxygen split assumed is in favour of industrial use as the demand is much higher. Another assumption is made to have a more realistic value for the oxygen benefit. It is assumed that offloading the oxygen for a profit to a gas distributor will come at a price. Hence, only 70% of the total oxygen benefit is used for calculations where, 30% is reserved for partnership payments for gas distributors.

	Units	Oxygen Price	Oxygen Purity	Oxygen Split
Industrial	€/kg	0,10	99,50%	90%
Medical	€/kg	9,00	99,99%	10%

Table 7: Oxygen Data [47]

Once all this data has been calculated, it is displayed in a graphical manner to be reviewed in the results section of this thesis.

After dealing with the transport conversion scenarios, the next task is to plan the steps for distributing the hydrogen that is produced. This is done with the help of three distribution methods. Each method explores a different technology for which the cost and effectiveness will be calculated in order to make an informed decision regarding which technology is best suited for distributing the hydrogen for transport mobility.

HYDROGEN DISTRIBUTION METHODS

There are various ways to store and distribute hydrogen. Hydrogen can be compressed and dispersed through pipelines, compressed and distributed in gas tanks on trucks and can also be liquified by cooling to -235°C to be transported by truck [26]. While liquefying hydrogen is a useful technique, the temperatures at which it needs to be stored is highly energy intensive to maintain and would not be ideal for transport applications. Hence, the following three options are considered to be the best possible methods for hydrogen distribution suited for Portugal.

Portugal's electrical grid consists of 71.015 km (44.127 miles) of high/medium voltage transmission lines and 112.074 km (69.640 miles) of low voltage lines [15]. Hence, it makes sense to design the hydrogen network by making use of the readily available extensive grid connections.

Using electricity straight from the grid to power the alkaline electrolysers that are installed near logistical parks and ports to reduce transportation costs for hydrogen. Transportation of produced hydrogen will be carried out one of three ways:

- Trucks: Transport hydrogen from parks and ports to refuelling stations along major highways and within cities. Assuming a 70:30 split for hydrogen utilization where, 70% can be reserved for use at fuelling stations on site at logistical parks and ports. The remaining 30% can be transported using trucks to refuelling stations. This allows for a significant amount of hydrogen to be used directly on site for industrial purposes and for the majority of heavy-vehicles that are usually located near such centres. The cost of using distribution trucks will be analysed in order to assess its viability. The data required to do so can be found in Table 8.

CAPEX	162,8	€ thousand
Annual OPEX	12%	% of CAPEX
Depreciation Period	12	years
Truck Fuel Capacity	420	kg H ₂
Fuel pressure	200	bar

Table 8: Estimated Portugal Truck Data [46]

Using this data, the annual cost of owning and operating one truck can be calculated. The number of trucks needed to distribute the 30% of total hydrogen is also determined using the truck fuel capacity. Once the number of trucks required is established, the total cost can be calculated for using this distribution method. The cost of the electrolysers is in addition to this investment. Hence, the total generation and distribution infrastructure cost will also be compared later on.

- Pipeline: The pipeline will follow the same distribution split as the trucks. However, as the pipeline requires fixed infrastructure, it is important to connect the logistical parks and ports to the refuelling stations in major cities along the coast. This would follow the gas pipeline plan as seen in the figure 7 below. (E64, E65 and E43) [39].



Figure 11: Pipeline Map of Portugal [39]

The cost of implementing pipeline infrastructure for distribution requires data outlined in Table 9. To make for an easier implementation, the hydrogen pipeline is assumed to be following the same route as the gas pipelines. This will allow for easier construction as pipelines are already in place. This also allows for the assumption that the hydrogen pipeline is the same length as the gas pipelines. While the pipeline will distribute the hydrogen fuel efficiently in the industrial areas, the major highways will still need to be serviced with hydrogen fuel with the use of trucks. This is because the pipeline will not cover the internal areas of Portugal away from the coast. A 85:15 split is assumed for the distribution, where 85% will be handled by the pipeline and the 15% will be handled by the trucks needed to distribute fuel to the regions of Portugal that are further inland.

Table 9: Estimated Portugal Pipeline Data

Lifetime [46]	40	years
Inlet pressure [46]	80	bar
Capex [46]	0,44	€ million/km
Design Throughput [46]	38	kton H ₂ /yr
E64 [39]	209	km
E65 [39]	179	km
E43 [39]	150	km
Total	550	km

Using the data in the table, the total cost of implementing the pipeline can be calculated for the identical length of existing gas pipeline infrastructure. The pipeline is a permanent structure that cannot be altered based on demand and supply. Hence, the pipeline costs will not be calculated based on the three main scenarios. The calculation will be a one-time investment for the cost of the overall pipeline. The cost of the electrolysers is in addition to this investment. Hence, the total generation and distribution infrastructure cost will also be compared later on.

- Dispersed Electrolysers: The final method explores the idea of minimizing the need for hydrogen transport by dispersing the production across the country. Using the grid to power large scale electrolysers near the ports and industrial areas in combination with small scale electrolysers at fuel stations both along highways and in cities. The use of large scale alkaline electrolysers for cargo and logistical hubs will be beneficial due to the lower cost of the technology. The small scale electrolysers ensure each of the targeted fuel stations have enough hydrogen fuel to supply the demand and also minimize the need for hydrogen fuel to be transported to those locations.

As mentioned in the introduction, PEM electrolysers are well suited for small-scale applications. Hence, they would be the ideal choice to implement for the smaller electrolysers that are being considered for this distribution method. Small PEM electrolysers and large AEC electrolysers will combine to form the foundation of this distribution method.

Table 10 shows the data used to calculate the PEM values for this distribution method. And the AEC values will be the same as the ones represented in Table 6. Since the PEM electrolysers are for small scale use, the assumption is made that each system has a 100 kW capacity. As it is a smaller capacity, the capital cost is on the higher end of spectrum.

Table 10: PEM Electrolyser Data

Hydrogen Generation for 1 MW system	20 [47]	kg/h
Hours of Operation	8000 [47]	h/yr
Hydrogen Generation for 1 MW system	160.000	kg/yr
Capital Cost	1300 [46]	€/kWel
Cost of Industrial Electricity	9,27 [37]	Euro cents/kWh
Electricity required	39,4 [45]	kWh/per kg H₂
Price of Hydrogen	2 [47]	€/kg
PEM Fixed O&M Cost	5% [43]	of CAPEX
PEM Variable O&M Cost (Raw Materials)	2,80 [43]	€/kg
Stack Replacement Cost	30% [43]	of Capex

Using this data, the cost of the dispersed electrolyser method is determined for each of the three main scenarios. Since the electrolyser act as distributors, there is no need for transportation. In this distribution method, there won't be a need to add the additional electrolyser costs like in the other two methods.

With transport conversion, generation and distribution covered the only that remains is to analyse the refuelling stations. The costs associated with them are in addition to the remaining investment and can significantly impact the overall economic outcome.

REFUELLING STATIONS

The data used to determine refuelling stations is divided into two sets. The first set applies to large scale refuelling stations that can be used at ports and logistic parks. The first set data is shown in Table 11. The HRS cost shown in this table covers the cost for the compressor, storage and dispenser. [11]

Table 11: HRS Data

HRS Cost (€ mil)	2,59
HRS Offloading Capacity (per day)	1 ton

The second of data is used for the fuel stations that along major highways and within cities that would require smaller quantities of hydrogen fuel. For the first two methods of distribution, this data is used to calculate the additional cost of infrastructure at the fuel stations. As, the hydrogen fuel must be produced

at the large-scale electrolysers and then transported to these fuel stations where the compression, storage and dispenser infrastructure must be in place. For the third method, the production is simply divided between large and small electrolysers and there is no need for additional infrastructure. Table 12 shows the second set of data for smaller refuelling stations.

Compressor Cost	5.437	€/kW
Storage Cost	578	€/kg
Dispenser Cost	15.000	unit

Table 12: Smaller hydrogen refuelling stations (HRS) Component Costs

For the three main scenarios, another assumption is made with respect to refuelling stations. There are approximately 220 fuel stations in Portugal. For the realistic scenario, 20% of fuel stations are assumed to be fitted with an HRS. In the same manner, 10% of fuel stations are assumed for the pessimistic scenario and 40% of stations are assumed for the optimistic scenario. This assumption helps distinguish the three scenarios from each other and give a wider view on the possible outcomes for the future.

In order to cover a comprehensive overview of the hydrogen transport network, it is imperative to look at the cost of ownership of hydrogen-fuel based trucks, buses and trains. Since the infrastructure being built is to service the future owners of such vehicles, it is important to understand how expensive is a hydrogen-based vehicle going to be own and operate in comparison to the other existing alternatives on the market. Hence, a TCO analysis is conducted to answer that question.

TOTAL COST OF OWNERSHIP ANALYSIS

Using the following data in Table 13, an estimate TCO value for Fuel cell buses is determined:

Table 13: Fuel cell (FC) Buses Data [12]

CAPEX	375.000	€
OPEX	0,3	€/km
Range	400	km
Cost of H ₂	5 to 7	€/kg
Tank Capacity	35	kg
Lifespan	12	years
Daily Distance	250	km
Discount Rate	8	%

Using the following data in Table 14, an estimate TCO value for Fuel cell trucks is determined:

Table 14: Fuel cell (FC) Truck Data [44]

CAPEX	320.000	€
OPEX	0,5	€/km
Range	480	km
Cost of H ₂	5 to 7	€/kg
Tank Capacity	70	kg
Lifespan	8	years
Daily Distance	400	km
Discount Rate	8	%

Using the following data in Table, an estimate TCO value for Fuel cell trains is determined: (REFF)

Table 15: Fuel cell (FC) Train Data [44]

CAPEX	5.100.000	€
OPEX	0,72	€/km
Range	700	km
Cost of H ₂	5 to 7	€/kg
Tank Capacity	224	kg
Lifespan	15	years
Daily Distance	400	km
Discount Rate	8	%

Once these values are established, a sensitivity analysis is conducted to understand the significance of Capex values and daily distance driven.

LEVELIZED COST OF HYDROGEN

The last step in the analysis section of this thesis is to test the LCOH sensitivity against two different factors: 1) Annual Operational Hours and 2) Electricity Price. This process is done using a sample 1MW AEC system in order to establish the behaviour of an electrolysis system's output and what it could mean for the future of green hydrogen.

Firstly, the process starts with setting the AEC system characteristics. They are shown in the Table 16 below.

Capex of AEC system	800	€/kW
Fixed Opex	5% of Capex	%
Variable Opex	2,8	€/kg of H ₂
Electricity Cost	0,0927	€/kWh
Efficiency	54	kWh/kg of H ₂
Annual Operational hours	8.000	h

Table 16: Levelized cost of hydrogen (LCOH) Data

The key part of this section is the equation for LCOH [24] which is,

Equation 3: LCOH Equation

$$LCOH = \frac{\sum_{n=1}^{N} (I_n + M_n + F_n) * (1+i)^{-n}}{\sum_{n=1}^{N} (E_n) * (1+i)^{-n}}$$

Here I_n stands for Initial investment, M_n stands for maintenance cost, F_n stands for fuel cost, E_n stands for energy generation, *i* is the discount rate, *n* is the specific year and *N* stands for lifetime.

Hence, using this equation and varying the values of Annual Operational hours and Electricity price, the behaviour of the LCOH value can be studied. This will allow for the adjustment of future project parameters in order to achieve a better LCOH.

RESULTS AND DISCUSSION

Following the methodology and doing the necessary calculations provides valuable insight into the possibilities of Hydrogen technology. The results mapped onto graphs will help showcase these possibilities and enable observations to be made.

TRANSPORT CONVERSION SCENARIOS

Pessimistic Scenario Results

Based on the assumptions made, the number of vehicles of each type that could be serviced by the current grid capacity was determined, Figure 13. They are as follows:

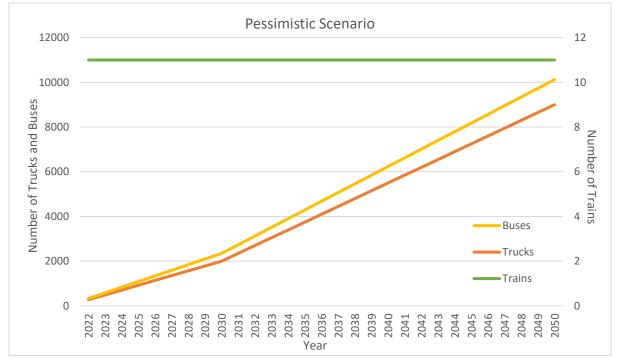


Figure 12: Pessimistic Scenario Transport Conversion

The number of trains to be replaced does not grow with each year as most of Portugal railway network has been electrified. Hence, the number of diesel trains that need to be replaced are 11.

Based on the figures above, it is clear that even with a pessimistic approach, the number of hydrogenpowered vehicles that can be serviced is a reasonable amount.

So over the course of this scenario, the percentage of fossil-fuel powered vehicles that could be replaced would be 7.5% for buses & trucks and 20% for diesel trains.

After conducting a financial analysis on the data, the following figure 9 represents the results.

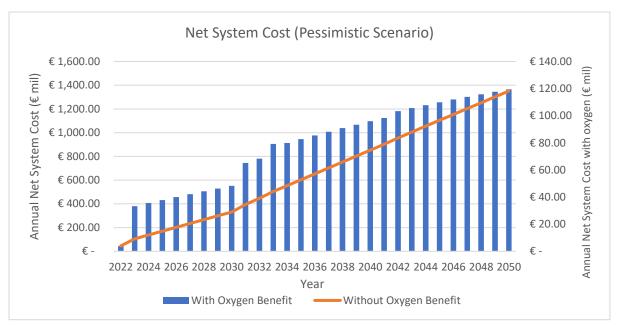


Figure 14: Net System Cost - Pessimistic Scenario

The Figure 15, above assumes the worst conditions to adopt a new technology and the results clearly show the same picture. Regardless of the oxygen benefit, the costs of the system continue to rise with each year. The blue bar chart indicates a system cost much lower than that of the one without the oxygen benefit. Despite, the capital costs of the electrolyser decreasing steadily with each year, the investment costs continue to rise. Part of the reason is due to the fact that the capacity is increasing each year. This is clearly not a suitable scenario to pursue with these conditions and hence, the other scenarios should be looked at as better alternatives.

The total cost of the project over the 29 year period is shown in Table 17

Table 17: Total Cost - Pessimistic Scenario

Total Cost	€ 2,26 billion
Total Cost without oxygen benefit	€ 19,34 billion

Optimistic Scenario Results

Based on the assumptions made, the number of vehicles of each type that could be serviced by the current grid capacity was determined. They are as follows:

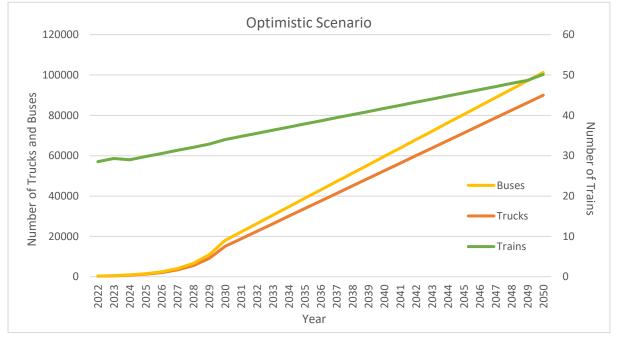


Figure 17: Optimistic Scenario Transport Conversion

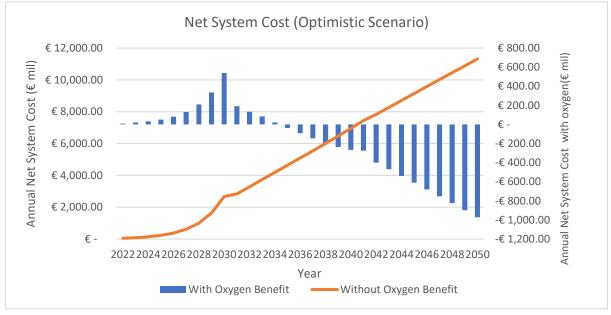


Figure 16: Net System Cost - Optimistic Scenario

Based on the figures 10 and 11 above, a highly optimistic approach yields a very large number of serviceable hydrogen-based heavy vehicles.

So over the course of this scenario, the percentage of fossil-fuel powered vehicles that could be replaced would be 75% for buses and trucks and 85% for diesel trains.

After conducting a financial analysis on the data, the above figure 11 represents the results. The optimistic scenario chooses the most ideal conditions for the system and the results clearly reflect the same. The orange line, which represents the system without the oxygen benefit shows a massive increase as the timeline heads towards 2050. The blue bar chart shows the massive advantage of the favourable conditions chosen for this scenario. As after the year 2035, the net system costs are actually negative. This graph proves that an aggressive push in the direction of green hydrogen is not only feasible but actually profitable.

The total cost of the project over the 29 year period is shown in Table 18.

Table	18.	Total	Cost -	Optimistic	Scenario
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Total Cost	-€ 5,56 billion (Profit)
Total Cost without oxygen benefit	€ 149,17 billion

Realistic Scenario Results

Based on the assumptions made, the number of vehicles of each type that could be serviced by the current grid capacity was determined. They are as follows:

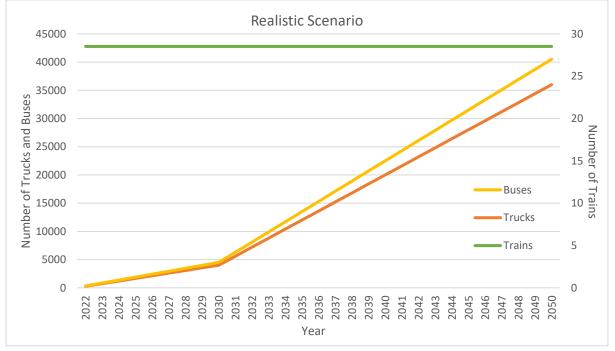


Figure 18: Realistic Scenario Transport Conversion

For the Realistic scenario, Figure 19, the number of serviceable hydrogen-based heavy vehicles is somewhat achievable.

So over the course of this scenario, the percentage of fossil-fuel powered vehicles that could be replaced would be 30% for buses and trucks and 38% for diesel trains.

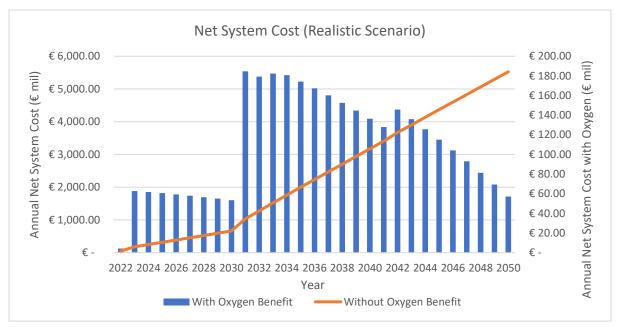


Figure 20: Net System Cost - Realistic Scenario

This Figure 21 represents the total annual cost of the electrolyser system both, with and without considering the oxygen benefit. The chart clearly indicates that the oxygen benefit makes a very significant difference to the overall cost of the system. As the years increase, the cost of system without the oxygen benefit increases rapidly making it highly unfeasible. The blue bar chart, which considers the oxygen benefit, gets cheaper over time and suggests that the system is feasible. The conditions set for this scenario are actually achievable and could make the technology viable for implementation in the timeline that is explored in this thesis.

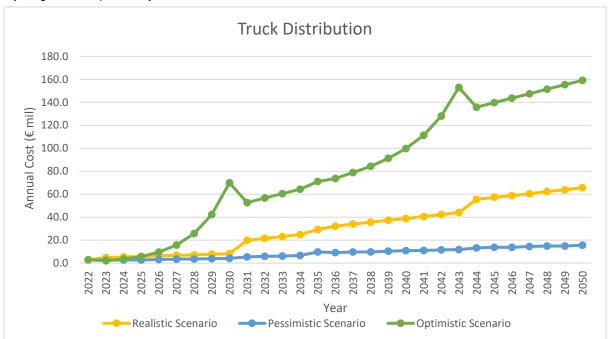
The total cost of the project over the 29 year period is shown in Table 19.

Table 19: Total Cost - Realistic Scenario

Total Cost	€ 3,19 billion
Total Cost without oxygen benefit	€ 69,35 billion

HYDROGEN DISTRIBUTION METHODS

For this section, the results had to consider not only the economic cost of the distribution but also the cost of the Hydrogen refuelling stations. Furthermore, the Truck and Pipeline distribution costs that are shown below are in addition to the electrolyser investment cost required for the production of the hydrogen in the first place. However, the Dispersed Electrolyser method covers the cost of hydrogen production and the distribution costs as well.



Hydrogen Transported by Trucks

Figure 22: Truck Distribution

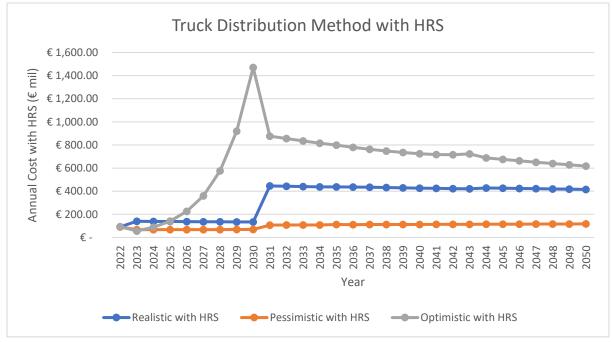


Figure 15: Truck Distribution

The two figures 14 and 15 represent the cost of implementing a truck-based distribution system for all three scenarios. The cost shown in the chart corresponds to 30% of the hydrogen produced in each scenario as the remaining 70% is assumed to be spared for on-site usage in the industrial locations. Another observation that is visible is the major impact of the HRS systems on the annual cost of distribution. These systems have to be considered in order to provide a comprehensive picture of the costs. Table 20 below shows the total cost of distribution over the 29 year period considered for this study.

	Total Cost	€ 0,90 billion
Realistic Scenario	Total Cost with HRS	€ 9,76 billion
	Final Cost with Production	€ 12,95 billion
	Total Cost	€ 0,25 billion
Pessimistic Scenario	Total Cost with HRS	€ 2,88 billion
	Final Cost with Production	€ 5,14 billion
	Total Cost	€ 2,33 billion
Optimistic Scenario	Total Cost with HRS	€ 18,57 billion
	Final Cost with Production	€ 13,01 billion

Table 20: Total Truck Distribution Cost

Table 20 shows not only the total cost of distribution with the HRS costs included, but also shows the final cost of the overall system with the hydrogen production costs included. Upon observation, the optimistic scenario numbers are very close to those of the realistic scenario. This indicates that in the long run, the optimistic scenario will eventually be feasible.

Hydrogen Transported by Pipeline

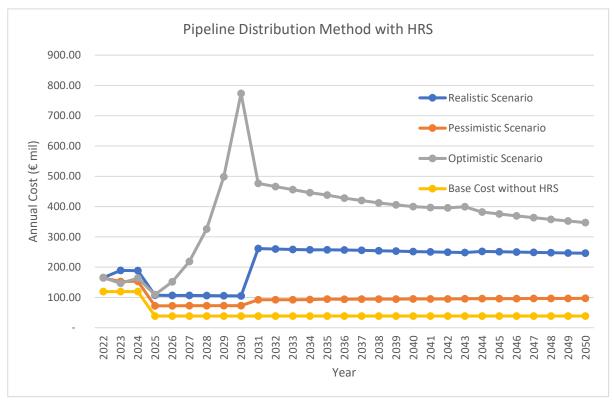


Figure 16: Pipeline Distribution

The figure 16 represents the cost of implementing a pipeline solution for distribution. The yellow line represents the base cost of the pipeline that includes, the capital investment and the operating expenditure. The first three years of the baseline cost include the capital cost of \in 242 million which is split over the three years. The remaining years just show the OPEX cost which stays the same each year. The rest of the three lines, show the cost of the additional HRS systems and truck distribution needed to distribute the 15% remaining Hydrogen production.

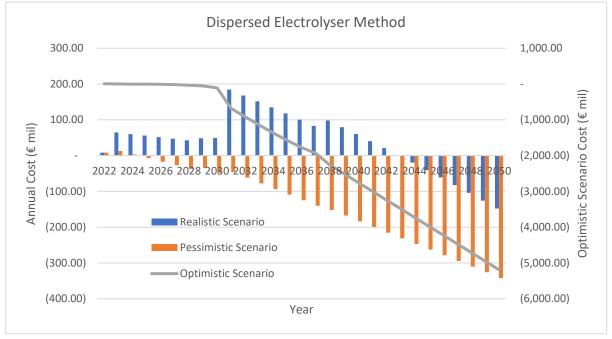
The table 21 represents the final costs of this distribution method at the end of the 29 year period.

Table 21:	Total	Pipeline	Cost

	Base Cost	€ 1,36 billion
Realistic Scenario	Total Cost with HRS and Trucks	€ 6,24 billion
	Final Cost with Production	€ 9,43 billion
Pessimistic Scenario	Total Cost with HRS and Trucks	€ 2,81 billion
	Final Cost with Production	€ 5,07 billion
Optimistic Scenario	Total Cost with HRS and Trucks	€ 10,64 billion
	Final Cost with Production	€ 5,08 billion

Table 21 shows not only the total cost of distribution with the additional HRS and truck costs included, but also shows the final cost of the overall system with the hydrogen production costs included. Upon observation, the optimistic scenario numbers work out to be cheaper than those of the realistic scenario.

This indicates that in the long run, the optimistic scenario will eventually be feasible and hence, should be considered as a viable option.



Hydrogen Dispersed by Small and Large electrolysers

Figure 17: Dispersed Electrolyser Cost

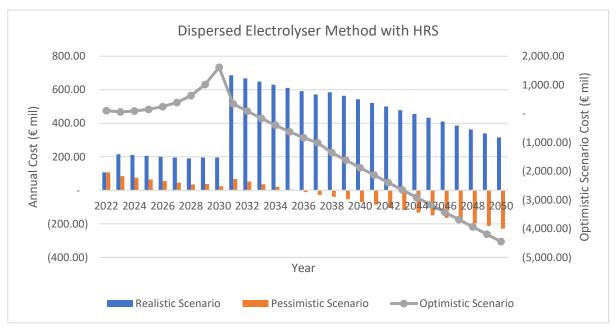


Figure 18: Dispersed Electrolyser Cost with HRS

The two figures 17 and 18 represent the cost of implementing a Dispersed Electrolyser distribution system for all three scenarios. The Optimistic scenario cost is displayed on a secondary axis due to the higher values of the data. The cost shown in the chart corresponds to 100% of the hydrogen produced in each scenario. There is no additional cost associated with the distribution method as the electrolysers being spread out across the country eliminate the need for fuel transportation. Another observation that

is visible that the annual cost is much higher than the previous two methods. This is due to the fact that these calculations cover the production cost of hydrogen as well. Hence, when considering the final cost of the system, the production cost for each scenario will not have to be added to this distribution system. Table 22 below shows the total cost of this distribution method over the 29 year period considered for this study.

Realistic Scenario	Final Cost	€ 1,09 billion
	Final Cost with HRS	€ 12,02 billion
Pessimistic Scenario	Final Cost	-€ 4,01 billion (Profit)
	Final Cost with HRS	-€ 1,06 billion (Profit)
Optimistic Scenario	Final Cost	-€ 58,05 billion (Profit)
	Final Cost with HRS	-€ 36,10 billion (Profit)

Table 22: Total Dispersed Electrolyser Cost

Table 22 shows the results of the third method of distribution. The data suggests that this system has massive potential for economic gain based on the values determined for the Pessimistic and Optimistic Scenario. The values of the optimistic scenario are quite skewed due to the fact that the conditions assumed are quite favourable. The realistic scenario shows promising results as well. Overall, this method suggests that if the conditions for the project are set somewhere between the realistic and optimistic scenarios, there is immense potential to make this study economically viable.

Finally when comparing all three methods of distribution combined with the production investment values, only the Dispersed Electrolyser method, while including the oxygen benefit, shows promise of successful implementation.

Using equation 2, the LCOH value for this distribution method was determined using the realistic scenario conditions. The LCOH value obtained was \in 4,92/kg of H₂. This value is very promising and is quite close to the ideal LCOH value required for making hydrogen-based mobility competitive.

TCO ANALYSIS FOR EACH TRANSPORTATION MODE



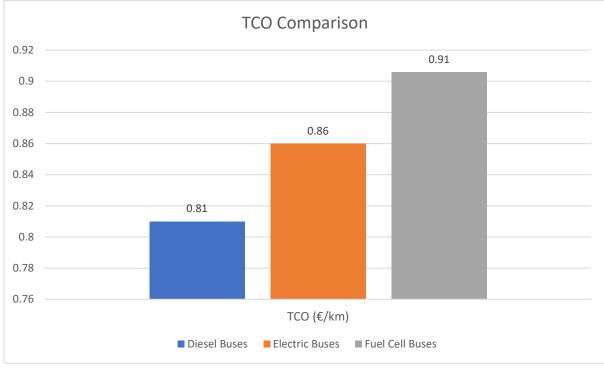


Figure 19: TCO for Buses

In comparison, Figure 19, average TCO values for diesel and electric buses are 0,81 (\notin /km) and 0,86 (\notin /km) respectively. As seen above, Figure 19, fuel cell buses are still considerably 12% more expensive than its diesel and electric counterparts. However, fuel cell costs are projected to drop significantly over the coming years and should help bring down the TCO values.

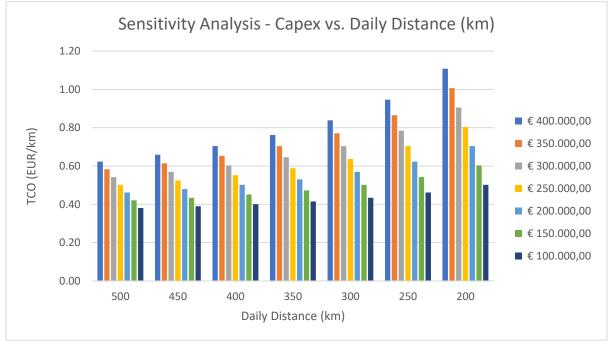
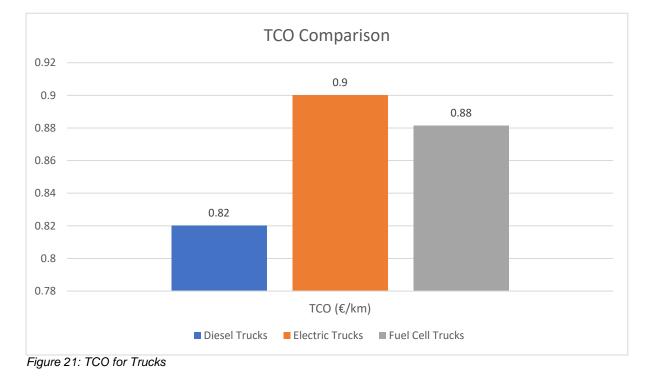


Figure 20: Sensitivity Analysis for TCO Bus

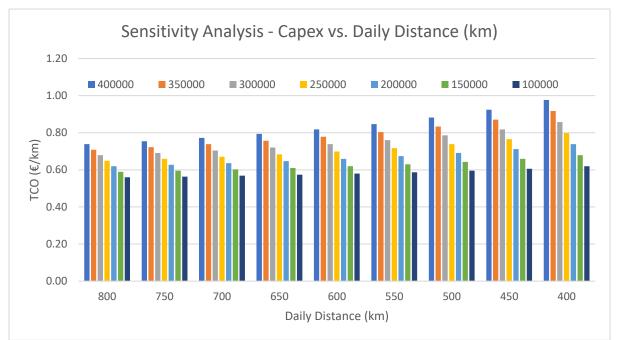
In order to fully understand the relation of TCO with Capex cost and vehicle mileage, a sensitivity analysis was conducted. Based on figure 20, the daily distance driven plays a much larger role in deciding the TCO than the Capex cost, where the TCO ranges from 0,38 (\in /km) to 1,11 (\in /km).

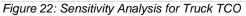
To make hydrogen-based heavy transport a success, the TCO costs need to be controlled and fixed at a point equal or lower to its counter parts. In the case of buses, this would mean bringing down the Capex cost. The lower capex will automatically drive the daily distance in the right direction causing a further decrease in TCO values in the long term.



Trucks

As seen above, Figure 21:, the cost of fuel cell trucks is already lower than that of electric trucks. This is due to the lighter weight fuel solution that occupies lesser space in the vehicle. However, there is still room for improvement in cost as the diesel trucks are a mature market with lower TCO values.





In order to fully understand the relation of TCO with Capex cost and vehicle mileage, a sensitivity analysis was conducted. Based on figure X, the daily distance driven plays a much larger role in deciding the TCO than the Capex cost, where the TCO ranges from 0,56 (\in /km) to 0,98 (\in /km).

In the case of trucks, this would mean bringing down the Capex cost. The lower capex will automatically drive the daily distance in the right direction causing a further decrease in TCO values in the long term.





Figure 23: TCO for Trains

In comparison, average TCO values for diesel and electric trucks are 8,0 (\in /km) and 6,6 (\in /km) respectively. As seen above, the cost of fuel cell trains is slightly lower than that of electric trucks. This is due to the lighter fuel solution that occupies lesser space in the vehicle. However, there is still room for improvement in cost as the diesel trains are a mature market with lower TCO values.

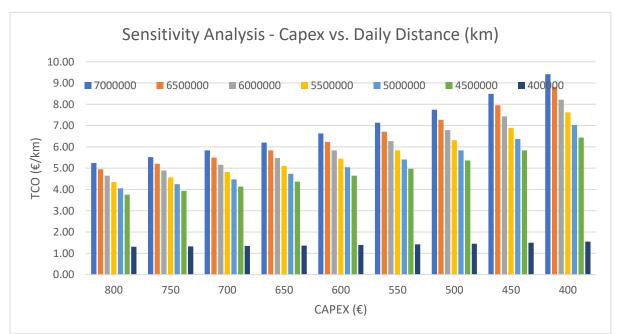


Figure 24: Sensitivity Analysis for TCO Train

In order to fully understand the relation of TCO with Capex cost and vehicle mileage, a sensitivity analysis was conducted. Based on figure 24, the daily distance driven plays a much larger role in deciding the TCO than the Capex cost, where the TCO ranges from 1,31 (\in /km) to 9,42 (\in /km).

LCOH SENSITIVITY

MIBEL allows for trading night-time renewable power and low-price power during periods of low demand. This would allow for the curtailed electricity to be utilized for hydrogen production.

Portugal has plans to increase the solar energy contribution to the country's energy portfolio from the current 2% to 14-15% by 2030. So, along with certain government incentives, it should be fairly easy to sign PPAs with solar parks and wind farms to have direct access to renewable power at a low price.

In order to analyse the response of cheaper electricity and more operational hours, an LCOH sensitivity analysis was conducted on a 1MW AEC system. The results obtained can be observed in the figures below. The base value for the LCOH obtained was \in 9,11/kg of H₂.

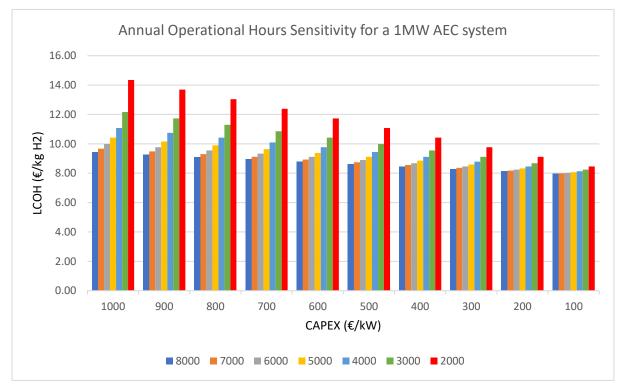


Figure 25: Sensitivity Analysis LCOH - Annual Operational Hours

Based on figure 25, it is quite clear that there is a directly proportional relationship between the LCOH and CAPEX values. Furthermore, the LCOH values are the lowest at 8000 annual operational hours. This confirms the fact that the more the electrolyser is used, the cheaper it is to operate.

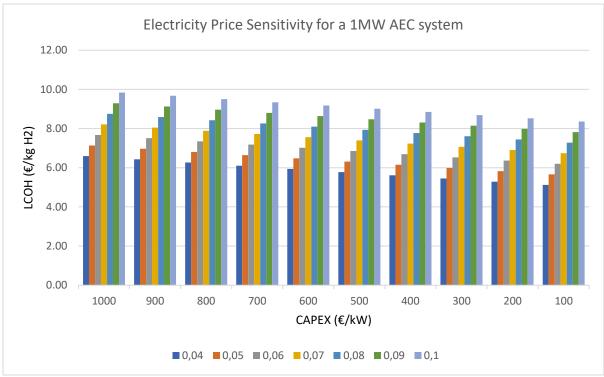


Figure 26: Sensitivity Analysis LCOH – Electricity Price

Figure 26 represents the relationship between electricity price and LCOH values. As it can be observed here, the lower the electricity price, the better the LCOH values are. The capex relationship once again shows a directly proportional reaction to the LCOH values. However, the electricity price seems to have a more significant impact of the LCOH values.

CONCLUSIONS AND FUTURE WORK

This thesis was conducted in order to understand the possible outcomes of implementing a hydrogenbased transportation system for heavy vehicles. Three different scenarios were created to assess the possible conditions that may exist when attempting to implement such a network in real life. These scenarios helped guide the study to decide how much of the transport sector could be powered using hydrogen. The next step of the study explored different distribution techniques to make the produced hydrogen fuel available across the country. This step experimented with three different methods in order to determine the most feasible way forward. Another part of this study was to look at the current TCO values of owning and operating a hydrogen-powered vehicle. Using a direct comparison with electric and diesel powered vehicles, the TCO value was examined for all three vehicle types. Furthermore, a sensitivity analysis was conducted to examine the effect of varying CAPEX and Daily Distance driven. This allowed for a better understanding of the TCO value can be improved going forward. Next, the LCOH value was analysed for a basic AEC 1MW system which was found to be € 9,11/kg of H₂. The effect of the electricity price and the CAPEX on the LCOH value was explored using a sensitivity analysis. Both the parameters were found to have directly proportional relations with the LCOH. However, it was observed that the electricity price had a larger impact on the value. Finally, the study was concluded by deciding that the Dispersed Electrolysis method of distribution combined with a realistic scenario had the best feasibility for a hydrogen-powered transport network. The LCOH value obtained from this particular pathway was \in 4,92/kg of H₂. This particular value is very promising and should encourage the adoption of hydrogen-based mobility.

The next steps for a study such as this one would be to explore the commercial and personal vehicle sector for hydrogen conversion. Cars and ships would be the ideal modes of transportation to analyse. Furthermore, ways to reduce hydrogen storage and dispensing costs should be looked at as the refuelling stations make up a significant portion of the investment expenditure.

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