



Issues on hydrogen vehicles modelling

Instituto de Engenharia Mecânica

Instituto Superior Técnico, Universidade de Lisboa

Authors:

Carla Alexandra Monteiro Silva (coordinator)

João Ribau

Ana Filipa Ferreira

Teresa Batista

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Abbreviations and acronyms

BEV – Battery Electric Vehicles

CCS - Carbon Capture and Storage

CO₂ – Carbon Dioxide

CTG – Cradle-To-Grave

EJ – Exajoule, 1 EJ = 10¹⁸ J

FCV/FCEV - Fuel Cell Vehicles

FCHEV – Fuel Cell Hybrid Electric Vehicle

FCH-JU – Fuel Cell and Hydrogen Joint Undertaking

FCPHEV - Fuel Cell Plug-in Hybrid Electric Vehicle

GHG - Greenhouse Gases

Gt – Gigatonne, 1 Gt = 10⁹ tonne

HEV - Hybrid Electric Vehicle

H₂ HEV – Hydrogen Hybrid Electric Vehicle

ICE-Internal Combustion Engine

IGCC –Integrated Gasification Combined Cycle

LCA – Life Cycle Assessment

LDV – Light-Duty Vehicle

LWP – Lower Warming Potential

MAIP – Multi-Annual Implementation Plan (2008-2013) from Fuel Cell and Hydrogen Joint Undertaking

Mtoe - Million tons of oil equivalent

PJ – Pentajoule, 1 PJ = 10¹⁵ J

PHEV - Plug-in Hybrid Electric Vehicles

R&D – Research and Development

RD&D – Research, Development and Demonstration

RNBC 2050 – Roteiro Nacional Baixo Carbono

SET – Plan - Strategic Energy Technology Plan

SMR – Steam Methane Reforming

SWOT - Strength, Weaknesses, Opportunities and Threats

TTW – Tank-to-Wheel

TOC – Total Ownership Cost

Water Electrolysis - WE

WTT – Well-to-Tank

WTW – Well-to-Wheel

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1. EXECUTIVE SUMMARY

This report refers to the AP2H2 subcontracted study “Estudo de modelação de penetração do Hidrogénio na mobilidade no quadro da ENE 2020/30/50”.

The present report is subdivided into 2 parts. The first part refers to a review of hydrogen roadmaps throughout the world. The second part refers to a review of hydrogen cars life cycle analysis.

1.1. First part: Review of hydrogen roadmaps

For moving to a low carbon economy in 2050, and respect the 2°C maximum temperature rise, the developed countries will need to target a cut of 80-95% of greenhouse gas emissions below 1990 levels by 2050. Knowing that the road transport contribution share for this emission is roughly 20%, this sector has been particularly studied as far as forecasting/ backcasting/ scenarization is concerned. Concerning scenarios in the this review it is noted that the variations are not only due to hydrogen penetration but also different assumptions concerning other technologies, demography, oil dependency, feedstock energy cost and economic growth, between others.

Hydrogen as an energy carrier and its use in passenger transportation through the fuel cell technology is widely considered as part of the solution to help meeting the targets. Hydrogen vehicles may include vehicles with internal combustion engines, but for the longer term fuel cell powered vehicles are expected to prevail. Due to being an in-use zero emission technology, the need for a methodology on how to account for GHG intensity of energy carriers and determining appropriate metrics is essential to make sure that post 2020 targets provide the right incentives to manufacturers and energy suppliers. Therefore some studies consider the hydrogen complete chain, i.e., hydrogen production and use to compute an overall GHG benefit comparing with conventional diesel/gasoline fuel use. This approach is called well-to-wheel (WTW), and is composed by fuel production (well-to-tank, WTT) and fuel use when driving the vehicles (tank-to-wheel, TTW). Some other studies consider only the WTT stage. Concerning energy security, hydrogen is one of

the fuels that become more secure, due to expected increased contributions from renewables.

The following studies were analyzed:

- Global Transports Scenarios [1];
- Technology Map of the European SET-Plan [2];
- Roteiro Nacional Baixo Carbono [3];
- Scenarios for Portugal [4];
- HYRREG for SUDOE [5];
- HyWays for Europe [6];
- Mckinsey for Europe [7];

The following tables summarize the main findings for the studies, on hydrogen production, supply, use, cost and potentially CO₂ reduction for the time periods 2020/2030 and 2050.

Table 1- Studies specifications and CO₂ reduction potential.

Study	Region	Time-frame	Methodology	CO ₂ reduction (-) or increase (+) 2050 vs 1990
Global Transports Scenarios	World	2005-2050	Scenarios forecast	TTW Tollway +72% Freeway +144%
Technology Map of the European SET-Plan	Europe (32 nations)	2010-2020/2030	Plan of the Energy Policy	NA
Roteiro Nacional Baixo Carbono	Portugal	2005-2050	Scenarios backcast	GHG - TTW CASM, CBSM 0% CA60, CB60 -60% CA70, CB70 -70%
Scenarios for Portugal	Portugal	2010-2050	Scenarios forecast	LCA from energy consumed in Portugal BAU +19.50% S5 +6.40% M4 -2.40%
HYRREG for SUDOE	30 regions and cities of Spain, France, Portugal and Gibraltar: 18.2% area of EU-27	2020-2030-2050	Forecast and SWOT analysis	NA
HyWays for Europe	Finland, France, Germany, Greece, Italy, the Netherlands, Norway, Poland, Spain, United Kingdom	2010-2050	Scenarios backcast (starting point: penetration rate of H ₂)	WTW baseline scenario: -10% modest policy + modest learning: -37% high policy + fast learning: -60% very high policy + fast learning: -64%
Mckinsey for Europe	Europe (29 nations)	2010 - 2050	Forecast and backcast	WTW -100% (emissions close to zero in 2050)

Table 2- Hydrogen production pathways.

Study	H ₂ production	H ₂ distribution	H ₂ share in energy
Global Transports Scenarios	NA	NA	(in car fleet) Scenarios 2030 2050 Tollway 1.00% 4.00% Freeway 0.54% 0.62%
Technology Map of the European SET-Plan	(Ton/day) capacity in 2020 centralized (SMR and gasification) + CCS 200 decentralized reforming of biogas 3 electrolysis 50	NA	H ₂ consumption in transports in 2020 0.4 Mt/year
Roteiro Nacional Baixo Carbono	Biomass gasification	NA	(in transports) Scenarios 2050 CASM, CBSM 0.00% CA60 10.71% CB60 0.00% CA70 16.50% CB70 0.07%
Scenarios for Portugal	40% decentralized electrolysis 60% centralized SMR	NA	2050 BAU 0.00% S5 0.45% M4 9.00%
HYRREG for SUDOE	Estimated timeframe 2020 2030 feedstock wind solar PV NG electricity process onsite central electrolysis electrolysis central SMR + CCS onsite SMR	Estimated timeframe 2020 2030 CGH ₂ truck LH ₂ truck pipeline liquid vector	NA
HyWays for Europe	Scenarios Stakeholders (-35% CO ₂) -80% CO ₂ CCS failure (-35% CO ₂) Least cost (-35% CO ₂) Main pathways in 2050 NG, coal nuclear, renewable Wind, NG, coal wind, biomass NG, coal, biomass	2030 low populated + remote areas: onsite supply, LH ₂ transport too low demand + centralized areas: onsite supply large stations in city borders: gaseous from pipeline (pipeline dominates the gaseous transport)	NA

Mckinsey for Europe		Until 2020	2020-2050	2020 Gaseous truck 2030 Gaseous truck + liquid trucks + pipeline 2050 Gaseous truck + pipeline	NA
	Central SMR	40%	30%		
	Distributed SMR	30%	-		
	Central WE	-	15%		
	Distributed WE	30%	15%		
	IGCC	-	30%		
	Coal Gasification	-	10%		

Table 3- Hydrogen cost.

Study	H ₂ cost		FC cost		FCV cost	
Global Transports Scenarios	(\$ ₂₀₀₀ /kg)		(\$ ₂₀₀₀ /kW)		(\$ ₂₀₀₀ /car)	
	Scenarios	2030 2050	Scenarios	2030 2050	Scenarios	2030 2050
	Tollway	3.32 3.21	Tollway	148.02 84.13	Tollway	18200 21900
	Freeway	2.95 3.09	Freeway	250.00 250.00	Freeway	18200 21900
Technology Map of the European SET-Plan	2020	6.6	2020	50 (€/kW)	2020	
	2030	5.0 (€/kg)			<30000 (€/car)	
Roteiro Nacional Baixo Carbono	NA		NA		NA	
Scenarios for Portugal	2020	2.5	NA		(€/car) 2030 2050	
	2050	3.6 (€/kg)			FCHEV	21656.9 22802.3
					FCPHEV	30737.7 32745.8
HYRREG for SUDOE	NA		NA		NA	
HyWays for Europe	2020	4.0	2030	50 (€/kW)	2030 20000-23000 (€/car)	
	2030	3.0 (€/kg)				
Mckinsey for Europe	2030	5.0	2020	43 (€/kW)	2020 31000	
	2050	4.4 (€/kg)			2030 26000 (€/car)	

Table 4- Hydrogen use in road transportation.

Study	H ₂ use	H ₂ vehicles share in fleet
Global Transports Scenarios	Light-duty vehicles	(car fleet) Scenarios 2030 2050 Tollway FCV 2.3% 5.2 % H ₂ HEV 1.0% 1.0% Freeway FCV 0.5% 0.4% H ₂ HEV 1.2% 0.9%
Technology Map of the European SET-Plan	Light-duty vehicles Buses Auxiliary Power Unit (APU) for: Aircraft, heavy-duty and board cruise ships	Number of vehicles in 2020: 0.39 million
Roteiro Nacional Baixo Carbono	Light-duty vehicles Heavy-duty vehicles (more representative)	NA
Scenarios for Portugal	Light-duty vehicles Heavy-duty vehicles	(FCHEV+FCPHEV) Scenarios 2050 BAU 0.0% S5 1.3% M4 22%
HYRREG for SUDOE	Light-duty vehicles	NA
HyWays for Europe	Light-duty vehicles Buses	Scenarios 2030 2050 modest policy + modest learning 3% 26% high policy + modest learning 8% 40% high policy + fast learning 12% 59% very high policy + fast learning 24% 74%
Mckinsey for Europe	Light-duty vehicles (particularly segment C/D)	FCV 2050 25%

1.2. Second part: Hydrogen vehicles life cycle analysis

The main methodology used by the scientific community to compare alternative vehicles with conventional ones is the life cycle assessment (LCA), through a so called energy source life cycle analysis, Well-to-Wheel (WTW) (fuel upstream WTT plus fuel use TTW) and a materials life cycle analysis, the so called materials cradle-to-grave CTG or embodied materials analysis. LCA based methods use, essentially, the global warming potential impact category. Few studies look to acidification potential, human toxicity potential or eutrophication potential. Despite not being recommended in the ISO norms, this studies use the final indicator of the method Eco Indicator to facilitate the technologies comparison. Three case studies were considered for hydrogen end-use: private cars of Portugal, London taxis and Portuguese urban bus fleets.

Regarding private cars [1]:

The main objective was to analyze the impact of the market share increase of hydrogen based road vehicles in terms of energy consumption and CO₂, on today's Portuguese light-duty fleet. Actual yearly values of energy consumption and emissions were estimated using COPERT software: 167112 TJ of fossil fuel energy, 12213 kton of CO₂ emission and 141 kton of CO, 20 kton of HC, 46 kton of NO_x and 3 kton of PM. These values represent 20–40% of countries total emissions. Additionally to base fleet, three scenarios of introduction of 10–30% fuel cell vehicles including plug-in hybrids configurations were analyzed. Considering the scenarios of increasing hydrogen based vehicles penetration, up to 10% life cycle energy consumption reduction can be obtained if hydrogen from centralized natural gas reforming is considered. Full life cycle CO₂ emissions can also be reduced up to 20% in these scenarios, while local pollutants reach up to 85% reductions. For the purpose of estimating road vehicle technologies energy consumption and CO₂ emissions in a full life cycle perspective, fuel cell, conventional full hybrids and hybrid plug-in technologies were considered with diesel, gasoline, hydrogen and biofuel blends. Energy consumption values were estimated in a real road driving cycle and with ADVISOR

software. Materials cradle-to-grave life cycle was estimated using GREET database adapted to Europe electric mix. The main conclusions on CO₂ full life cycle analysis is that light-duty vehicles using fuel cell propulsion technology are highly dependent on hydrogen production pathway. The worst scenario for the current Portuguese and European electric mix is hydrogen produced from on-site electrolysis (in the refueling stations). In this case full life cycle CO₂ is 270 g/km against 190 g/km for conventional Diesel vehicle, for a typical 150,000 km useful life. A brief energy price analysis was presented. We conclude that hydrogen price equivalent to gasoline energy price (€/MJ) is important to the consumer preference of hydrogen based vehicles. It is also possible a fuel cell cost become comparable with internal combustion engine cost if sufficient market penetration and power density increase are attained.

Regarding taxi fleets [2]:

A small fleet of classic London Taxis (Blackcabs) equipped with hydrogen fuel cell power systems was prepared for demonstration during the 2012 London Olympics. This part of the report presents a Life Cycle Analysis for these vehicles in terms of energy consumption and CO₂ emissions, focusing on the impacts of alternative vehicle technologies for the Taxi, combining the fuel life cycle (Tank-to-Wheel and Well-to-Tank) and vehicle materials Cradle-to-Grave. An internal combustion engine diesel taxi was used as the reference vehicle for the currently available technology. This is compared to battery and fuel cell vehicle configurations. Accordingly, the following energy pathways are compared: diesel, electricity and hydrogen (derived from natural gas steam reforming). Full Life Cycle Analysis, using the PCO-CENEX drive cycle, (derived from actual London Taxi drive cycles) shows that the fuel cell powered vehicle configurations have lower energy consumption (4.34 MJ/km) and CO₂ emissions (235 g/km) than both the ICE diesel (9.54 MJ/km and 738 g/km) and the battery electric vehicle (5.81 MJ/km and 269 g/km).

Regarding bus fleets [3]:

Fuel cell powered hybrid electric vehicles (FC-HEV) and plug-in hybrid electric vehicles (FC-PHEV) are being addressed by the automotive industry as improved and more sustainable alternative technologies relatively to conventional vehicles. Nevertheless, hybrid propulsion raises new challenges in designing the vehicle powertrain. This study highlights the significance of the driving conditions and the conflict between the optimization of investment cost, efficiency and life cycle impact (LCA) in powertrain design optimization of these kinds of vehicles. A single-objective (minimization of cost, fuel or LCA CO_{2eq}) and multi-objective genetic algorithms (minimization of the couples cost and fuel, cost and LCA CO_{2eq}, fuel and LCA CO_{2eq}), linked with the vehicle simulation software ADVISOR, are used to optimize the design of powertrain components. The main outcomes of the research are as follows. The optimization of LCA CO_{2eq} emissions and cost are conflicting as well as cost and energy use, what can be observed in the Pareto solutions. The fuel and LCA CO_{2eq} emissions optimization are coupled for pure hybrids but not for plug-in hybrid configurations, due to the electricity consumption. Fuel cell buses can reduce the energy consumption by 58%, and emit 67% less LCA CO_{2eq} than the conventional diesel bus, and achieve compensatory payback of 0.620 \$/km (depending on the hydrogen price). The FC-PHEV configuration shows more potential for achieving higher operation efficiencies, but the FC-HEV shows to have lower life cycle impact and lower cost in general.

2. DOCUMENT ORGANIZATION

The executive summary presents the abstract of the document, containing a brief of the main bottom lines/ findings of each study reviewed, in table format, what allows an easy comparison between them.

The first part of the report contains an introduction which presents the objective of this part of the report, identifies the contribution of the transport sector for the energy consumption and its pollution associated; the future challenges regarding these aspects are also placed. Identifies the H₂ vector as a potential alternative energy for transports and describes its characteristics and possible feedstocks. Describes vehicle technologies running on hydrogen and enumerates existing demonstration programs. Identifies the studies that will be reviewed in the following section and explains the approaches used in them. It follows a review, where it is presented a short description of each analysed study, its objectives, the approach used in each one and main results obtained, considering between other aspects, the H₂ production, supply, use, respective costs and CO₂ emissions. For studies that comprise action plans, it is also presented a brief of that. Finally the conclusions, in this part it is made a comparison between the results obtained in each of the studies revised. Differences and convergences among them are identified. It presents the range of possibilities in the medium and long term concerning the main points. It is also described the barriers to be overcome for the hydrogen introduction and advises measures to be taken in that sense.

The second part of this report deals with life cycle analysis of hydrogen road vehicles and is divided in three main chapters dealing with different hydrogen end-use applications in transportation systems: private cars in Portugal (Chapter 2), taxi in urban London (Chapter 3) and urban buses in Portugal (Chapter 4).

FIRST PART – HYDROGEN ROADMAPS REVIEW

1. INTRODUCTION

This report refers to the point 2.a)1) of the AP2H2 subcontracted study “Estudo de modelação de penetração do Hidrogénio na mobilidade no quadro da ENE 2020/30/50”.

This report presents a review of existing roadmaps worldwide that embrace hydrogen as an energy vector for the transportation sector. It is expected to contribute to draw a roadmap of hydrogen to Portugal, focusing on the road transportation sector, for the period 2015-2050.

The transportation sector is facing challenges in two main areas: the need to reduce energy dependency on petroleum based fuels; and the need to drastically reduce emissions like world greenhouse gases (GHG) and local pollutant emissions.

In 2010, the transportation sector consumed about 2.200 million tons of oil equivalent (mtoe), representing 19% of global energy supplied, 96% from which is coming from oil. In 2010, road transport accounted for 76% of the transportation energy consumption [1].

According to the Global Transport Scenarios, in 2010, the CO₂ emissions from the transport sector were about 23% of global CO₂ emission levels and emissions from cars were about 41% of total transport emissions [1].

In Portugal the transportation sector represented 40% of the countries' energy consumption in 2008, while in EU27 the average was 32%. The same trend happens for CO₂ emissions where the transports emissions share reached 25% in Portugal and 19% in the EU27 in 2008. In Portugal, the road transports consumed 81% of transportation energy; in Europe consumes 85%, in 2008 [8]. For CO₂ emissions, the road transports accounted for 97% in Portugal and 94% in EU27 [9].

Regarding the impact of the transports in the environment, international goals and commitments have been established. The European Commission Climate and Energy policy set in 2007 the "20-20-20" targets, that defines for all individual EU states: 20% reduction in GHG emissions from 1990 levels, 20% renewable energies and 20%

improvement in energy efficiency in 2020 [10]. In 2009 the European Union (EU) and G8 leaders agreed that CO₂ emissions must be cut by 80% by 2050 if atmospheric CO₂ is to stabilize at 450 parts per million and global warming stay below the safe level of 2°C. But 80% global decarbonization by 2050 may require 95% decarbonization of the road transport sector. With the number of passenger cars set to increase to 273 million in Europe and to 2.5 billion worldwide by 2050, this may not be possible only through improvements to the traditional internal combustion engine or alternative fuels. The traditional combustion engine is expected to improve its efficiency by 30%. There is also uncertainty as to whether large amounts of (sustainably produced) biofuels (more than 50% of demand) will be available for passenger cars, given the potential demand from other sectors, such as goods vehicles, aviation, marine, power and heavy industry. Combined with the increasing scarcity and cost of energy resources, it is therefore essential to develop a range of alternatives that will ensure the long-term sustainability of mobility [7].

The main European document regarding the transportation sector, the EU “White Paper, Roadmap to a Single European Transport Area” analyses the developments in the transportation sector, future challenges and the policy initiatives that may be considered. Accordingly, there is necessity of action in: improving the energy efficiency performance of vehicles across all modes and developing and deploying sustainable fuels and alternative propulsion systems; using transport and infrastructure more efficiently through the use of improved traffic management and information systems, advanced logistic and market measures. Regarding GHG, the objective is to achieve a 60% reduction of emissions in the total transportation system for 2050. For that, in the road transports, one of the targets, among others, is to promote alternative vehicle technologies and energy sources by reducing to half the number of conventional vehicles used in urban environment until 2030, and totally remove them from cities by 2050 [11].

Hydrogen appears as an alternative fuel for the transportation sector, it is the most abundant chemical element in the Universe and has the highest energy density. It is an energy carrier like electricity. Hydrogen can be produced from a variety of raw materials

and energy resources with potential zero emissions: nuclear energy, renewable energy (wind and solar), biomass and from fossil fuels considering carbon capture and storage (CCS). As a result hydrogen offers a long term potential for an energy system that produces zero emissions and is based on available domestic resources, improving security of supply [5] [6]. The properties of hydrogen considered in this study are:

H₂ (gaseous):

Lower Heating Value (LHV) - 120MJ/kg

Density - 0.09 kg/m³ (0°C and 1 atm) [12]

H₂ (liquid):

Density - 71 kg/ m³ (-252.8°C and 1 atm) [13]

The use of fuel cells in vehicles, produce electricity using hydrogen and only release water. However, hydrogen is not found naturally in its pure state, what means that it has to go through chemical or biological processes to be extracted. This requires additional energy for the extraction, and atmospheric emissions may be released in these operations. Usually hydrogen is produced from natural gas, using a steam reforming process. Additional hydrogen can be produced from oil, water electrolysis (WE), coal and biomass gasification or biomass fermentation [14]. The production of H₂ can be distributed or centralized, but in this last case, a distribution system is needed.

About 450 billion m³ of hydrogen were produced and consumed worldwide in 2011, but mostly as raw material for the production of chemicals rather than as a fuel itself [15].

Regarding vehicles using hydrogen, several technologies are possible: Fuel Cell Vehicles (FCV), Fuel Cell Hybrid Electric Vehicles (FCHEV), Fuel Cell Plug-in Hybrid Electric Vehicles (FCPHEV) and Internal Combustion Engines (ICE) being this last option possible to combine with hybridization, defined as H₂ HEV.

Mainly demonstration projects are related to the public bus sector, such as the Clean Urban Transport for Europe (CUTE), the Global Hydrogen Bus Platform (HyFLEET:CUTE), the Sustainable Transport Energy Programme (STEP) and the Ecological City Transport System (ECTOS). Some original equipment manufacturers (OEM) of light-duty vehicles have already engaged in alternative powertrain using hydrogen. About those prototypes,

out of more than 20, there are: Mercedes-Benz F600 Hygenius (hybrid), Honda FCX (hybrid), GM Chevy Volt Hydrogen (hybrid plug-in) and Ford Edge with HySeries Drive (hybrid plug-in) [16], [4].

Despite the promising aspects of hydrogen economy, its realization faces multiple challenges, from economic to technological and institutional barriers that arise the need for a coordinated Roadmap with a strategy to overcome these barriers [5].

Several studies address the probable evolution of the world energy sector and in particular of the road transportation sector, presenting different vehicle technology and mobility possible pathways as a result of different policy strategies for medium (2020/2030) or long-term (2050), in which the hydrogen is contemplated.

Scenarios, roadmaps and similar foresight methods are used to cope with uncertainty in areas with long planning horizons, such as energy policy and the future of hydrogen energy in transports. Between the studies reviewed, the following possible approaches were identified:

- Forecasting - use formal quantitative extrapolation and modelling to predict likely futures from current trends, several scenarios can be explored and results over time are observed;
- Backcasting - start with a predetermined end point — a desirable and plausible future and then investigate possible pathways to that target [17];
- Action plans;
- Roadmaps - can be defined as a tool that allows the analysis of alternative paths, according to a table of information and conditions, determined a priori, to achieve a certain goal or vision [3]. A roadmap is frequently based on studies of backcasting and forecasting;
- Scenarios - provide a set of plausible stories about different possible futures, taking into account uncertainties, critical factors, and driving forces.

The following studies were analyzed:

- Global Transports Scenarios [1];
- 2011 Technology Map of the European SET-Plan [2];

- Roteiro Nacional Baixo Carbono [3];
- Scenarios for Portugal [4]
- HYRREG for SUDOE [5];
- HyWays nfor Europe [6];
- Mckinsey for Europe [7];

For each study the main conclusions on the following points are presented, for the time periods 2020/2030 and 2050:

- CO₂ reduction;
- Hydrogen production;
- Hydrogen supply;
- Hydrogen use;
- Cost (H₂, FC and vehicle).

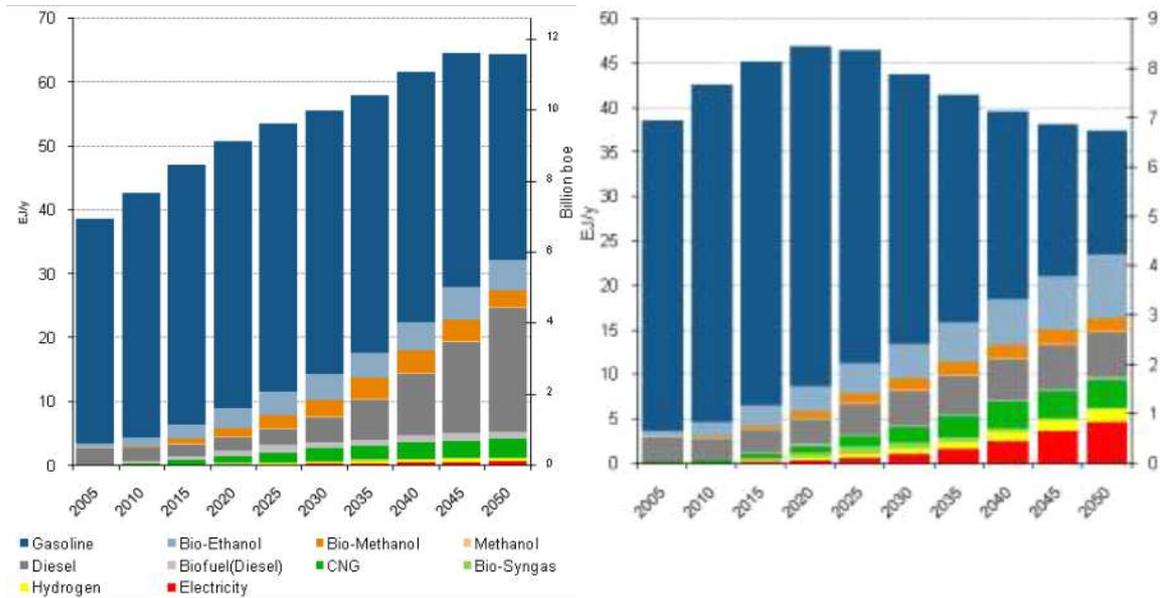
2. REVIEW

2.1. Global Transports Scenarios

The future of the transport and mobility sector is examined by World Energy Council (WEC), building Global Transport Scenarios to 2050. These scenarios describe potential developments in transport fuels, technologies, and mobility systems until 2050 in the world.

Two distinct transport scenarios “Freeway” and “Tollway” are defined, based on the examination and combination of regional inputs on transport policies, existing and potential developments in both fuels and technologies, in addition to major driving forces and critical uncertainties. The main difference between the two scenarios is the degree and kind of government intervention in regulating future transportation markets. The reality will certainly be between these two scenarios with regional differences playing a major role. The “Freeway” scenario foresees a world where pure market forces prevail to create a climate for open global competition. The “Tollway” scenario predicts a more regulated world where governments decide to interfere in markets to promote technology solutions and infrastructure development that set common interests at the forefront. The Freeway and Tollway scenarios describe the extreme ends of the potential future [1].

2.1.1. H₂ consumption



a) Freeway Scenario

b) Tollway Scenario

Figure 1 – Demand for fuel between 2010 and 2050 for Light Duty Vehicles (LDV), (World Energy Council, 2012)

According to Figure 1 the demand for H₂ in light duty vehicles (LDV) will reach in the Tollway scenario 1% of the total fuel consumed by LDV in 2030, increasing to 4% in 2050, when it reaches a total value of 1.50 EJ/year. On the other hand, regarding Freeway scenario, the H₂ consumption represents 0.54% of the consumption in 2030, and 0.62% in 2050, when it reaches a total of 0.4 EJ/year.

2.1.2. Cost

Analyzing the tendencies for H₂ costs, the scenarios converge to values between 3.09 (Freeway) and 3.21 (Tollway) \$₂₀₀₀/kg in 2050, being in 2030 the cost between 2.95 and 3.32 \$₂₀₀₀/kg.

The cost of the FCV also converge in both scenarios, with no variation between 2030 and 2050, it should be about \$₂₀₀₀ 18200 for FCV and 21900 for H₂ HEV (without battery and FC costs). The ICEV is expected to cost between \$₂₀₀₀ 18071 (petrol) and 19971 (diesel) with

no variation considered between 2030 and 2050, so FCV becomes competitive. The fuel cell will remain in 250 \$₂₀₀₀ /kW in the Freeway with no variation between the medium and long term, while for the Tollway, there is a decrease in the cost, 148 \$₂₀₀₀/kW would be the cost in 2030 and 84.13\$₂₀₀₀/kW in 2050.

2.1.3. Fleet

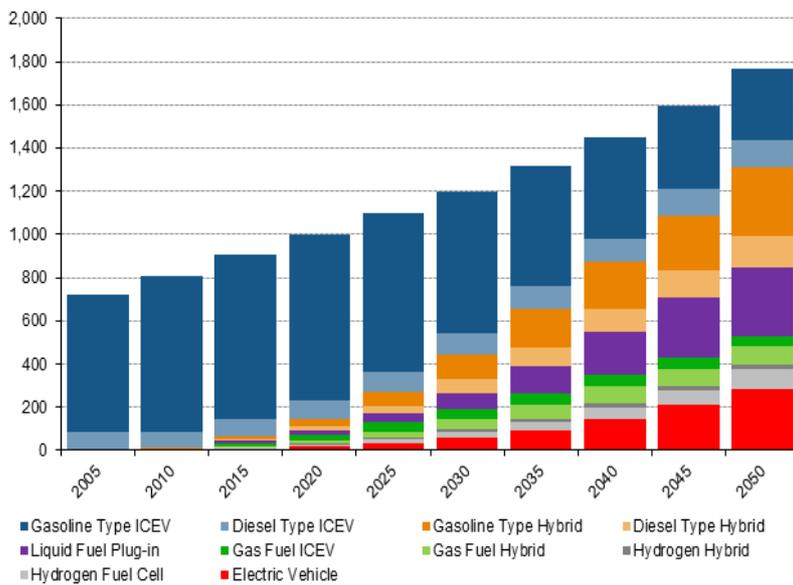
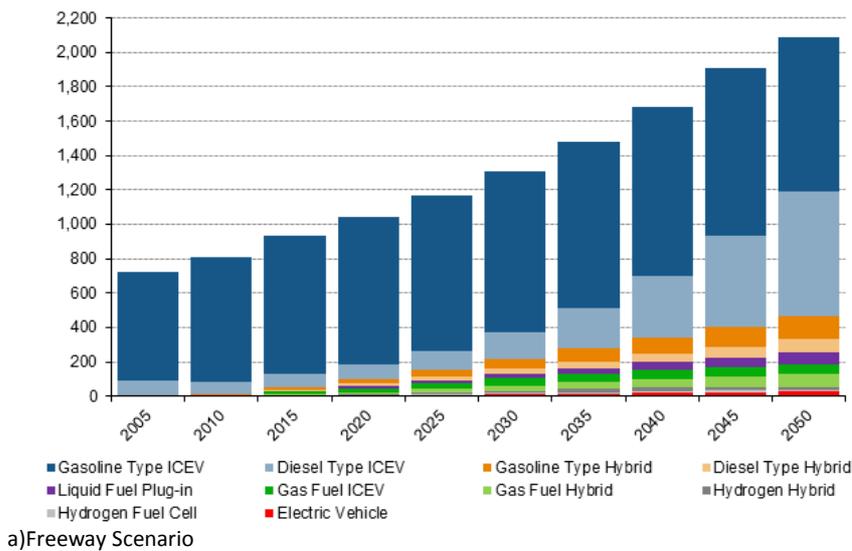


Figure 2 – Technology mix for cars in million vehicles (World Energy Council, 2012)

As it can be seen in Figure 2, the FCV in 2030 is expected to be between 0.5% of the car fleet (Freeway) and 2.3% (Tollway). In 2050 the FCV is projected to share between 0.4% (Freeway) and 5.2% (Tollway) of the car fleet.

The percentage of H₂ HEV in the car fleet does not vary significantly between scenarios, it is forecasted to be about 1% in both whether in 2030 or 2050.

2.1.4. CO₂ emissions

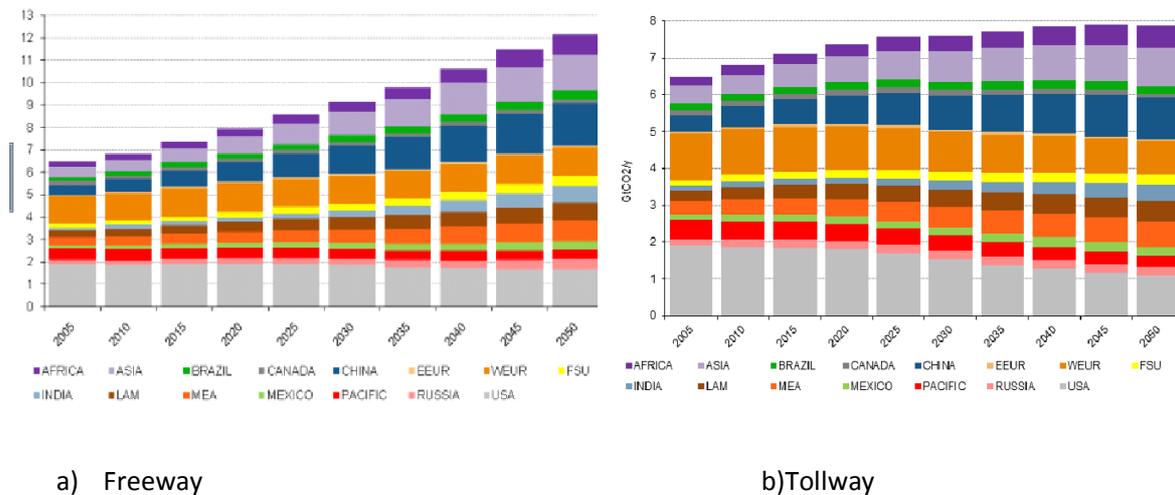


Figure 3 – Total transports CO₂ emissions (Gt CO₂/y), (World Energy Council, 2012)

Concerning the CO₂ emissions (TTW approach) resulting in both scenarios from cars, it can be achieved in 2050 an increase of 144% (Freeway) compared to 1990 value or an increase of 72% (Tollway), see Figure 3.

The scenario with lower emissions corresponds to the one with higher percentage of vehicles running on hydrogen and consequently higher percentage of energy consumption of hydrogen. Anyway there are many variables between these two scenarios that influence the CO₂ emissions results.

2.2. Technology Map of the European SET Plan

The SET-Plan defines an energy technology policy for European Union concerning 32 nations (EU-32). It is a strategic plan to speed up the development and deployment of

cost-effective low carbon technologies. The plan includes measures relating to planning, implementation, resources and international cooperation regarding energy technology. SET Plan is a catalyzer for the creation of necessary condition for the timely market roll-out of low-carbon energy technologies [2]. SETIS is the European Commission's Information System for the SET-Plan, it supports the strategic planning and implementation of the SET-Plan. SETIS provides information and analyses on the technological, market status and the impact of deployment of low-carbon energy technologies, thereby assisting decision makers in identifying future Research & Development, as well as demonstration priorities and identifies corrective measures if needed for the SET-Plan. Between other initiatives, the SET-Plan includes the Fuel Cells and Hydrogen (FCH) Joint Technology Initiative, that designed a Multi-Annual Implementation Plan (MAIP), [2] [18]. This initiative aims to accelerate the development of hydrogen-supply and fuel-cell technologies to enable the industry to take the large-scale commercialization decisions necessary for mass market introduction in the timeframe 2015-2020.

The Technology Map SET-Plan is based on the forecasts and objectives of other studies, including Mckinsey for Europe that is also reviewed on the present document and others such as the “Hydrogen Infrastructure Market Analysis and Global Demand Forecasts for Hydrogen Fuel and Fueling Infrastructure to Support Fuel Cell Cars, Buses, Forklifts, Scooters, and Stationary Power” from the Pike Research Center [19].

2.2.1. H₂ production

According to the objectives defined in the MAIP, in 2020, the hydrogen will be mainly produced from fossil fuels (200t/day), through centralized reforming or gasification, with CCS, followed by electrolysis (50t/day) and decentralized reforming of biogas (3t/day). This study also comprehends the capital cost for each producing way, as well as the efficiency of the production processes [2].

2.2.2. H₂ Distribution

The number of stations for 2020 is targeted to be 2000 in Europe and according to Pike Research the consumption of hydrogen in the world will be around 0.048 EJ/year [19].

2.2.3. H₂ Cost and Consumption

The H₂ cost is expected to be 6.6€/kg in 2020 and 5€/kg in 2030 (without taxes included), the FC about 50€/kW and FCV <30000€. Regarding the number of vehicles, 0.39 million are expected. The consumption of H₂ in 2020 for the FCV is foreseen to be 0.85 kg/100km [2].

2.2.4. Potential of the hydrogen vector and barriers

The hydrogen is identified as storage, enabling time shifting of wind and solar generated electricity to compensate for daily and seasonal variability and ensure a balance between supply and demand. In addition it can help balance generation and load, storage at regional level can also increase network stability. The MAIP targets a 580 ton of total installed storage capacity of hydrogen produced from renewable grid electricity by 2020 [2].

This study also identifies barriers to the development of the large scale deployment of hydrogen and measures to surpass it, such as:

- disruptive nature i.e. need to be phased-in gradually in applications where they perform better than conventional ones);
- increased competition from other zero-emission or near zero-emissions technologies, such as battery electric and plug-in hybrid electric vehicles;
- availability of H₂;
- market position and public acceptance of competing incumbent technologies and systems for which external costs are not included in their overall costing;
- technological improvement performance and durability of fuel cells, energy density of onboard hydrogen storage;

- economical barrier: include cost of fuel cells and hydrogen, lack of cash-flow and of a supply base during the first phase of deployment;
- institutional barrier: difficulties of policy and regulatory frameworks for disruptive technologies;
- social barrier: insufficient coverage of fuel cells and hydrogen technologies in education curricula and the resulting safety perception and low awareness of societal benefits.

SET Plan recognizes that market forces alone cannot overcome existent barriers, so technology-push, as well as regulatory pull measures, including tailored and time-phased policies and incentives for public and private market actors are needed for the transition. In view of the long-term horizon and the high winnings in terms of contribution to European Union policy goals of GHG emissions reduction, security of supply, urban pollution reduction and enhanced competitive base, it is necessary public support to help reduce industry development times and offset first-mover disadvantages. A roadmap for Research and Development activities until 2020 is presented in Figure 4 [2].

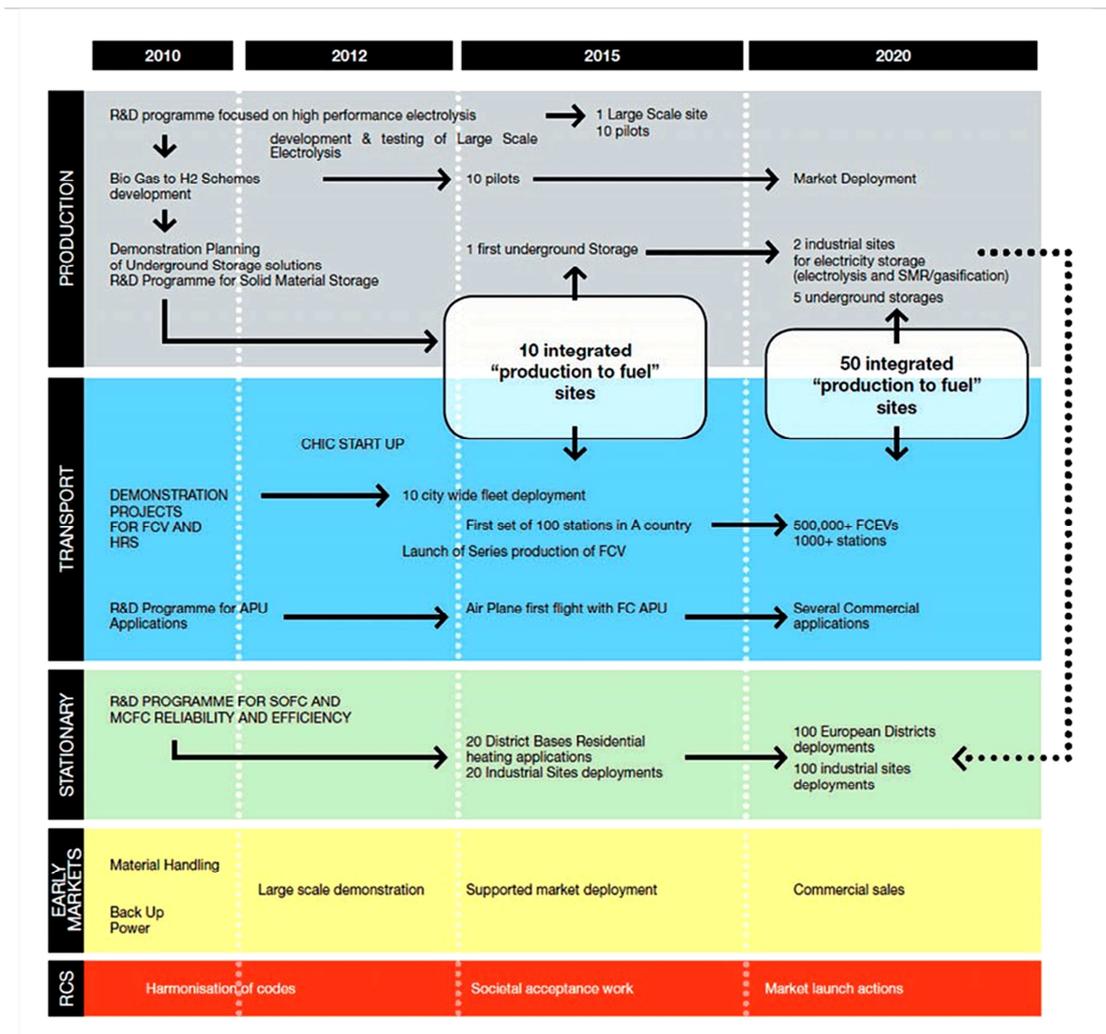


Figure 4 - Schematic roadmap for R&D activities in FCH Technology Map (Joint Research Centre, 2011)

2.3. Roteiro Nacional Baixo Carbono (RNBC 2050)

RNBC 2050 is a roadmap for Portugal that follows the European Commission communication "A Roadmap for moving to a competitive low carbon economy in 2050". The objective is to study technical and economic viability of trajectories of GHG emissions reduction in Portugal until 2050. It makes the evaluation of GHG emission trajectories for different objectives of reduction, supported by socio-economic scenarios and based on the technological evolution and primary energy prices. It contemplates different energy sectors, among them the transports. It is presented the necessity for the European Union

concerning 27 nations (EU-27) to reduce internally its domestic GHG emissions in 80% in 2050 (comparing to 1990 levels) to make the transition to a low carbon economy. According to that, the sectorial evolution in transports is defined as: +20 to -9% (2030) and -54 to -67% (2050) [3].

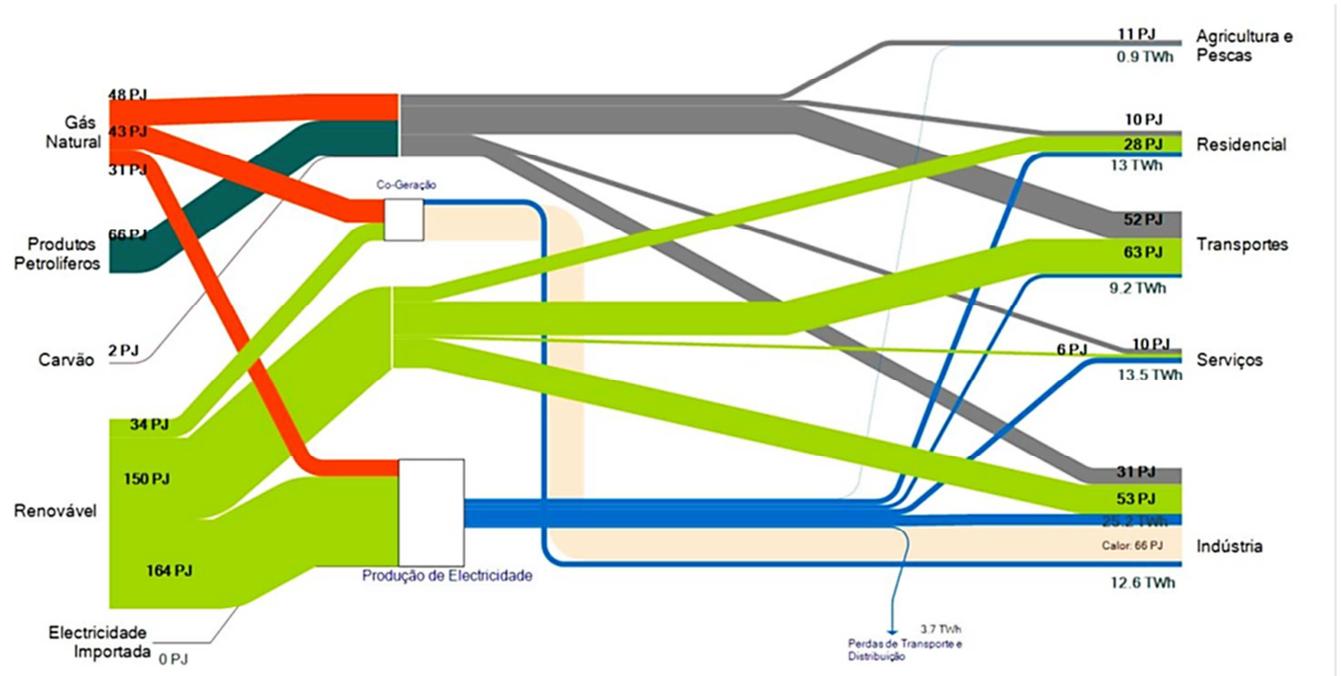
RNBC 2050 uses methods of projection based in scenarios, supporting in two contrasting macro-economic scenarios: high scenario and low scenario, that represent respectively the superior and inferior limits of economic development, to which correspond contrasted standards of energy services needed. Over these scenarios, it is imposed GHG emissions limits, corresponding to reductions of 60% to 70% (compared to 1990 levels), resulting in:

- CBSM - scenario for low economic development and no emissions limits;
- CASM - scenario for high economic development and no emissions limits;
- CB60 - scenario for low economic development and 60% reduction of GHG emissions;
- CB70 - scenario for low economic development and 70% reduction of GHG emissions;
- CA60 - scenario for high economic development and 60% reduction of GHG emissions;
- CA70 - scenario for high economic development and 70% reduction of GHG emissions.

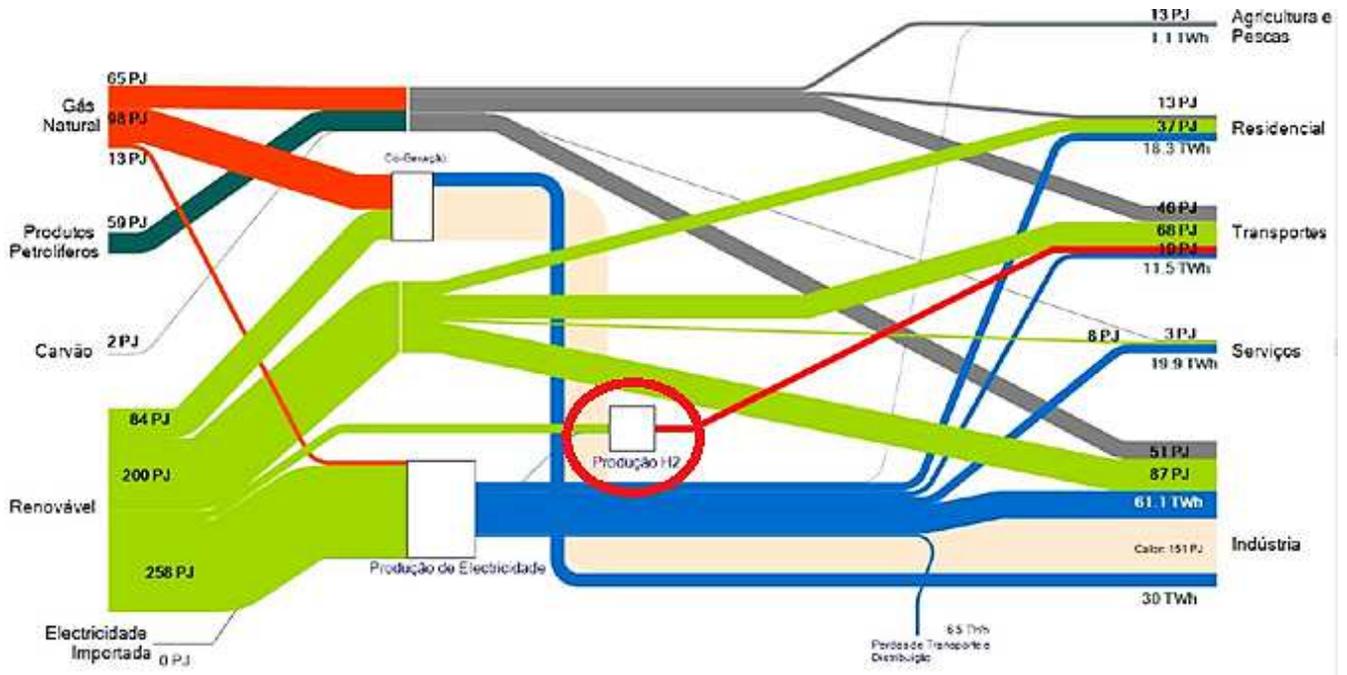
High economic development assumes that gross domestic product increases 3%/year between 2016 and 2050 and population grows; Low economic development assumes that gross domestic product increases 1%/year between 2016 and 2050 and population decreases.

The model used for the simulation is the TIMES_PT, technological based and driven by cost-effectiveness criteria. Models were built taking into account assumptions from the energy and the climate policies.

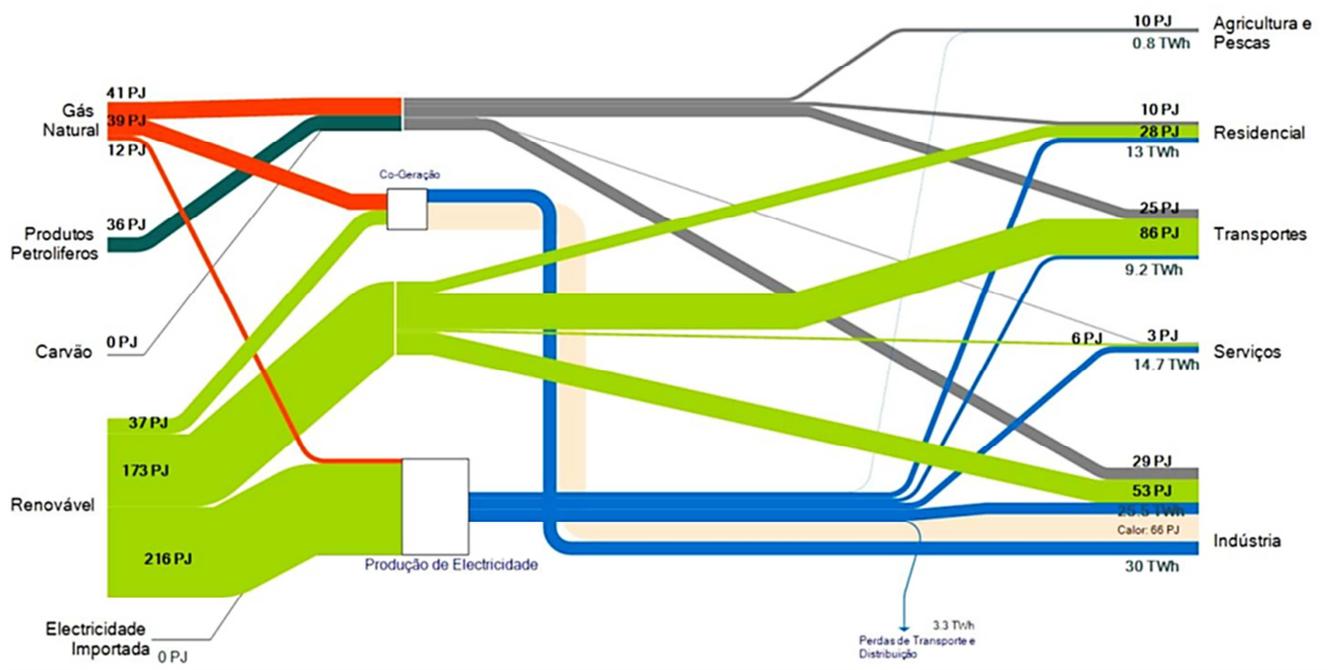
2.3.1. H₂ consumption



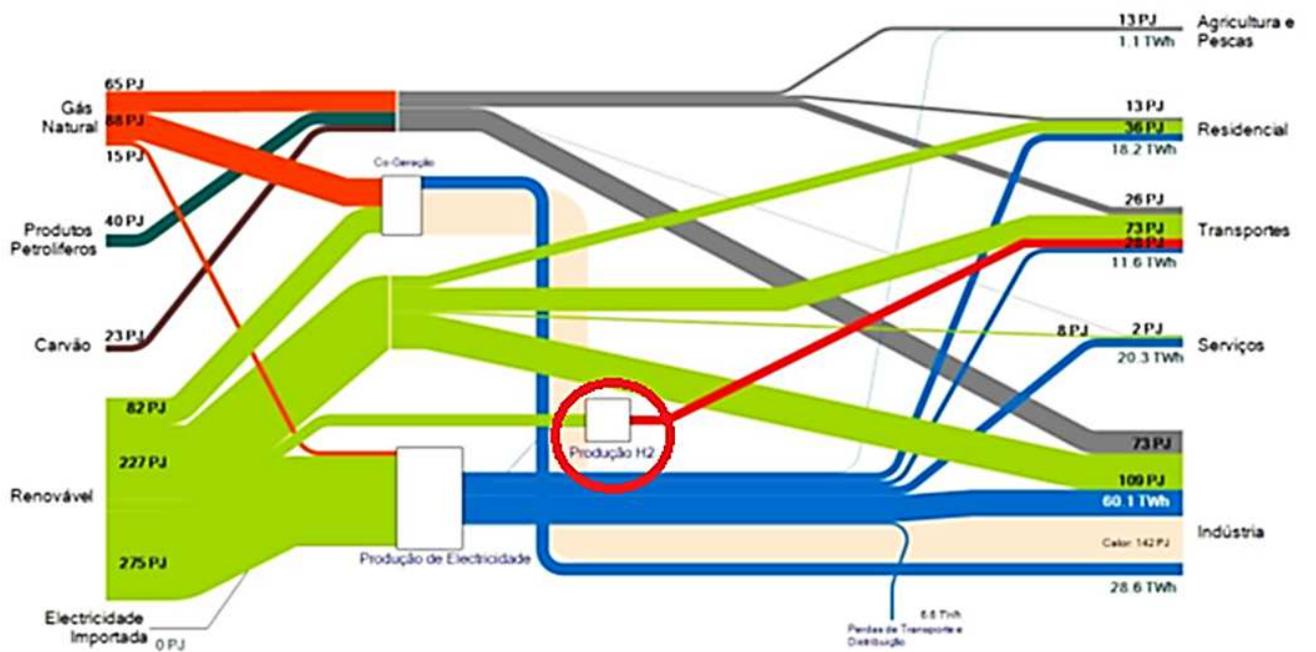
a) CB60 Scenario



b) CA60 Scenario



c) CB70 Scenario



d) CA70 Scenario

Figure 5 – Energetic balance in 2050 [3]

As it can be analyzed in Figure 5 and Figure 6, the hydrogen carrier enters in the energetic system for transports in the high economic development (CA60 and CA70). There is also a slight enter of hydrogen in the CB70, that cannot be seen in the scheme, but represents 0.07% of the energy consumed in transports. In the CA60 the hydrogen use achieves 0.0186EJ in 2050, about 11% of the energy consumed in transports; in the CA70 it achieves 0.0279EJ, about 17% of the total energy consumed in transports. The hydrogen use in transports is forecasted to start only in 2040-2050. FCV will be the option, with H₂ essentially produced by biomass gasification.

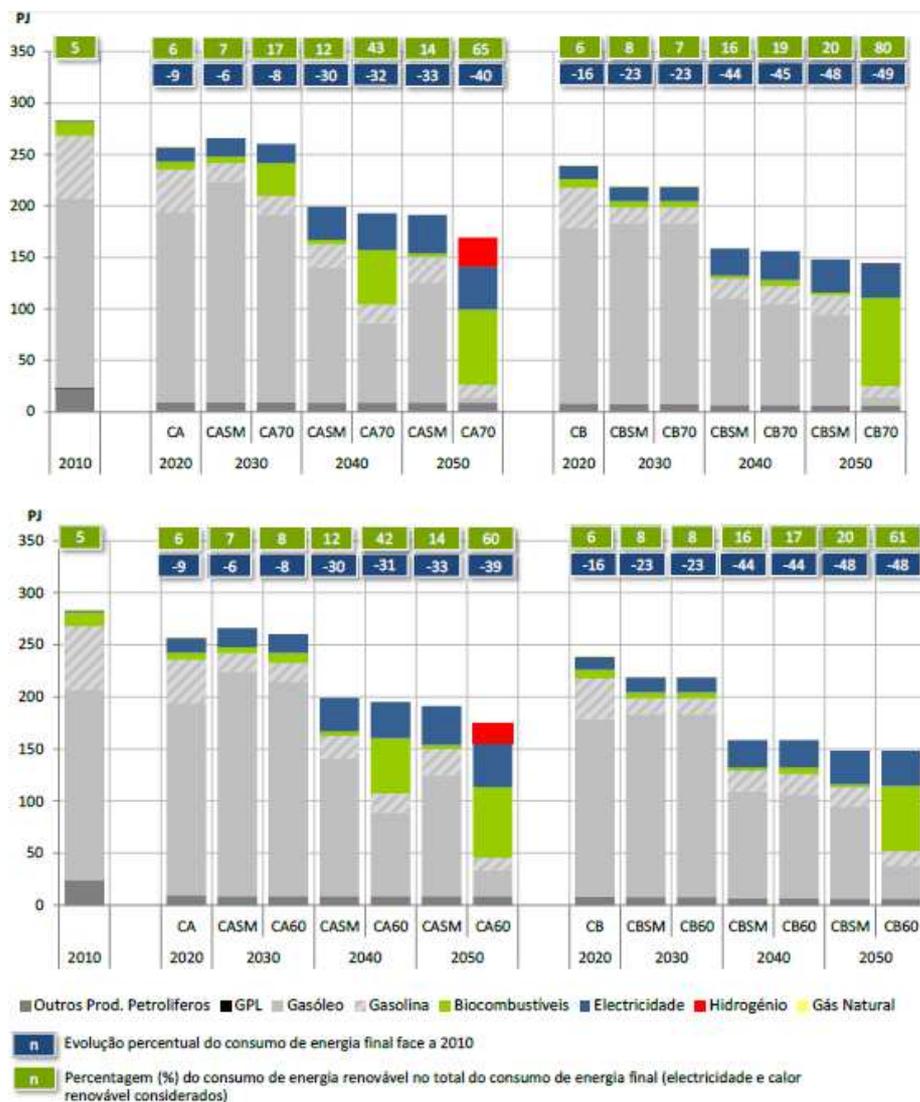


Figure 6- Evolution and structure of the final energy consumption in transports (road, rail, aviation and national navigation) [3]

It is estimated a structural modification in goods mobility, due to the restrictions for those transports to produce emissions in-use. In 2050, higher percentages of hydrogen are consumed in heavy-duty than in light-duty. The higher percentage of hydrogen consumption corresponds to CA70, achieving 16% of the energy consumed in heavy-duty and 1.7% of the energy consumed in light-duty vehicles. Regarding heavy duty ones, the H₂ is responsible for 29% (CA60) and 43% (CA70) of the goods mobility. H₂ buses reach a representativeness of 15% in the scenario of 70% reduction [3].

2.4. Scenarios for Portugal

This thesis focus on the road transportation sector, aiming to evaluate the impacts of introducing different policy options, either in terms of alternative vehicle technology, energy sources, or promoting other types of mobility options in Portugal in 2010-2050. It performs an integrated analysis of the road transportation sector future behavior, in order to understand its dynamics and the impact of our present and future options [4].

It is used a fleet model tool, named Projections for Alternative Transportation Technologies Simulation tool (PATTS) [16]. PATTS is capable of generating scenarios considering different options in terms of introducing alternative vehicle technologies (conventional, hybrid, plug-in hybrid, electric, fuel cell and natural gas), energy source pathways (fossil fuels, biofuels, electricity, hydrogen, etc.), global mobility options, cost of driving, etc. The results assess how road transportation sector (light-duty and heavy-duty vehicles) is affected mainly in terms of primary energy consumption, CO₂ emissions and local pollutants emissions considering a life-cycle approach (LCA). Additionally, the total ownership cost (TOC) for the user is also assessed in the generated scenarios. The inputs are: demography, car stock, mobility, vehicles technology, energy source and cost. The results are for all fleet, in which 50-60% are LDV. Between the existing scenarios, three were chosen to be analyzed in the present report:

- Business-as-usual (BAU) scenario - corresponds to continuing the current trends in terms of fleet, based on a liquid fuel vision, a very low incorporation of alternative vehicle technologies and biofuels;

Liquid fuels based - the road transportation sector remains dependent on liquid fuels and no alternative refueling infrastructure is deployed. The consumer will choose more efficient liquid fuel based vehicle technologies, so more efficient both gasoline and diesel ICE and HEV are considered;

- M4 scenario- combines the medium options concerning demography, car stock, mobility, energy source and cost, and hydrogen powered infrastructure regarding vehicle technology, see Figure 7.

Hydrogen powered vision assumes a wide hydrogen refueling infrastructure is deployed allowing the consumer to fast adopt fuel cell vehicles at a large scale. Storage and cost issues are overcome, see Figure 7. The hydrogen is considered in this study for being produced 40% by electrolysis and 60% SMR. It does not take into account CCS.

- S5 scenario: Industry stakeholders scenario - reflecting the opinion of 9 members of the main Portuguese oil company, GALP Energia, based on a diversified vision regarding vehicle technology.

Diversified vision: a wide diversity of alternative vehicle technology/energy sources penetrates in the road transportation sector; initially the consumer will choose more fuel efficient vehicles HEV but as the electricity recharging infrastructure is available the consumer chooses BEV and increasingly more Plug-in Hybrid Electric Vehicles (PHEV) due to autonomy issues; the acceptance of the electricity recharging infrastructure enables a later introduction of an hydrogen refueling infrastructure and consequently of FCV, see Figure 7.

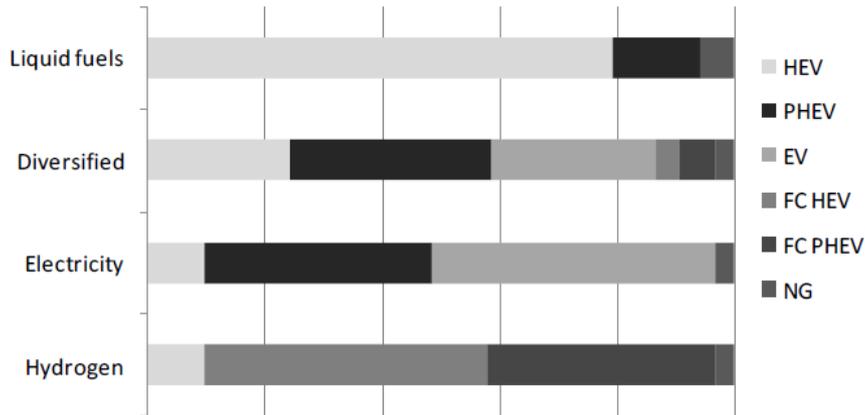


Figure 7 - Relative market share of alternative technologies in vehicle sales [4]

2.4.1. Fleet

The H₂ HEV technology is not evaluated, and only fuel cell vehicles in the hybrid or plug-in hybrid are considered. According to the developed scenarios, see Figure 8, in the medium term timeframe (2020) no hydrogen vehicles will appear in the fleet. In 2050, the number of hydrogen vehicles in the M4 scenario will be 1.44 million, representing a percentage of 22% of the LDV fleet and 0.087 million, representing 1.3% of the LDV fleet in the S5 scenario. In the BAU scenario there are no H₂ vehicles in the fleet.

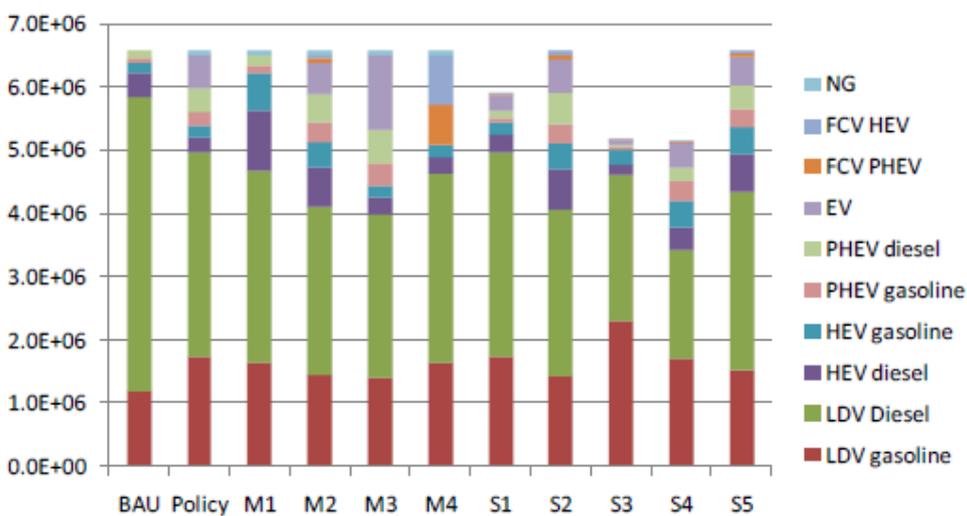


Figure 8 – Number of LDV per vehicle technology in 2050 [4]

2.4.2. CO₂ emissions

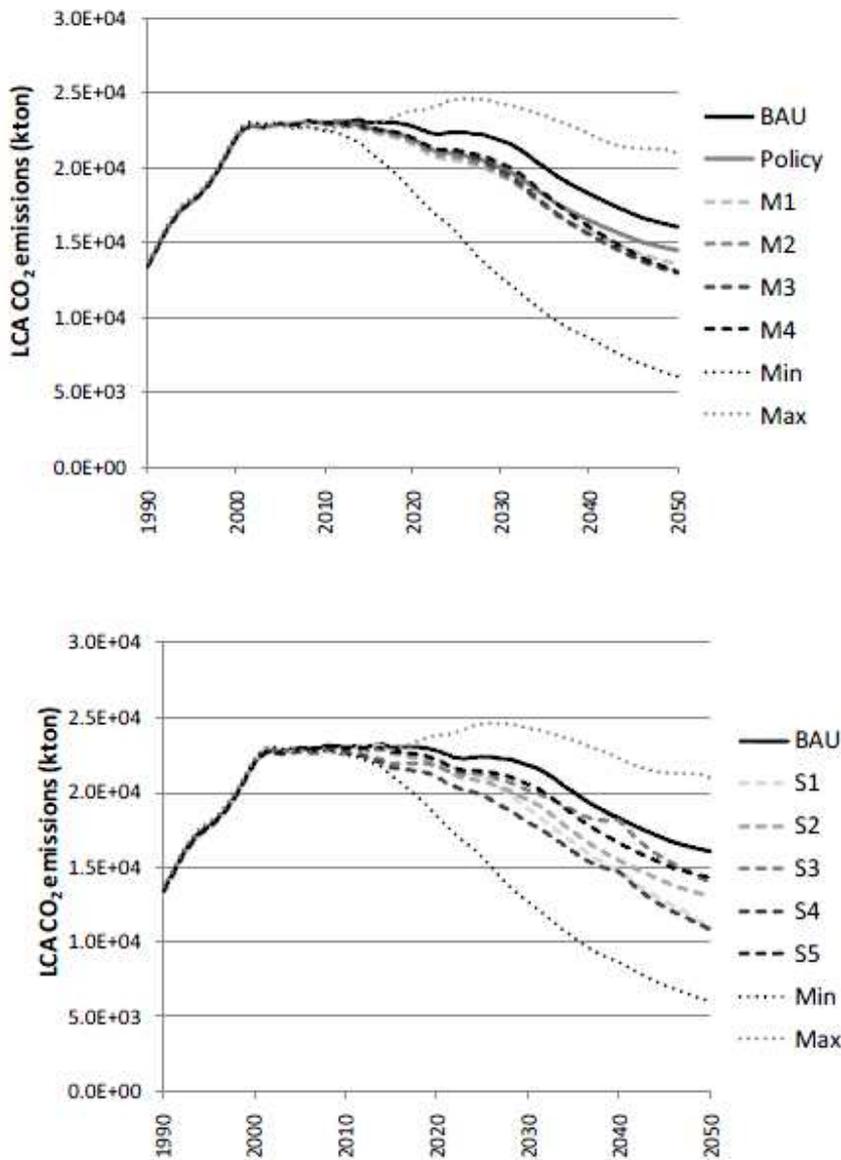


Figure 9- National LCA CO₂ emissions of the fleet in 2050 [4]

The national LCA CO₂ emissions results correspond to the energy consumption and emissions within Portugal, so most part of the Cradle-to-Grave (CTG) is not included, once Portugal is a vehicle importer. As a result all energy consumption and emissions regarding the vehicle manufacturing occurs outside the country. Only the dismantling and recycling

stages of the vehicle are accounted inside Portugal. As it can be analyzed in Figure 9, for both scenarios, BAU and S5, CO₂ emissions increase from 1990 and 2050, respectively 19.5% and 6.4%. In the M4 scenario (the one corresponding to the higher H₂ penetration), there is a slight decrease of -2.4%. It is noted that the CO₂ difference between each scenario is not only due to the difference in the H₂ share, but also all the varied assumptions between the scenarios.

2.4.3. H₂ cost

The H₂ cost considered to calculate the average TOC of the fleet for each scenario was 2.5€/kg in 2020 and 3.6€/kg in 2050 [20]. The average lifetime taken into account for calculations was 150000 km. In 2020 the average fleet TOC does not differ that much between scenarios, corresponding the higher TOC to the BAU (51638 €) and the lower to the S5 (51197 €), M4 TOC is between BAU and S5 (51294 €). In 2050 the higher TOC continues to correspond to BAU (47669 €), the lower to S5 (46492 €) and M4 maintains the middle position (47305 €).

The FCHEV technology is competitive in 2050, being its TOC about 38788 €, so lower than the average fleet for all considered scenarios. FCPHEV on its turn has a TOC much higher than the average, around 65248 €. Regarding the acquisition cost, that is the approach easiest to compare with other studies reviewed, for the FCHEV is about 21656.9 € in 2030 and 22802.3 € in 2050. The FCPHEV is more expensive, being the acquisition cost 30737.7 € in 2030 and 32745.8 € in 2050.

2.5. HYRREG for SUDOE

HYRREG roadmap aims to define the scientific, technological, economic, political and social capabilities and insufficiencies of SUDOE area regarding hydrogen and fuel cells. SUDOE Region is comprised of 30 regions and autonomous cities of Spain, France, Portugal and Gibraltar representing 770 120 km² (18.2% area of EU-27) and 61.3 million inhabitants (12.4% of EU-27). According to HYRREG consortium there is a good basis for supporting the development and introduction of hydrogen-based technologies in the

region especially with respect to the use of hydrogen for storage, as renewable energy sources are growing steadily [5].

2.5.1. Methodology

HYRREG makes a mainly qualitative analysis, it takes into account stakeholders' preferences and country specific conditions such as availability of resources, environmental policies, characteristics of the present and future energy system and profile in relation to the future H₂ economy. The vision of a hydrogen economy in each region is based on the expectation that hydrogen can be produced from different resources, in an economically and environmentally acceptable manner, facilitating the end-use of hydrogen technologies. This enables a significant market share in the near future, thus ensuring a greater degree of energy security and an improved environmental quality for the region. The goal is to select the most appropriate pathways to produce, distribute and use hydrogen in each country and to identify the barriers in its implementation [5].

For the baseline scenario it takes into account the predictions results from previous studies that apply to Europe, than it is defined a starting scenario of a hydrogen economy based on questionnaires concerning hydrogen energy chain: production, storage/distribution, conversation/ final use, and perception/ promotion. It results in a SWOT (Strength, Weaknesses, Opportunities and Threats) matrix of each region regarding the implementation of a hydrogen economy.

2.5.2. Portuguese case

Portugal has already tax incentives to foster energy efficiency, renewable energies and emerging technologies and a number of policy instruments, mostly of short term, to promote the use of hydrogen and fuel cells. According to this study, the Portuguese mix already has a high percentage of renewable energy (14% hydro power + 14% wind power in 2009), arising the need of a storage process, to allow the incorporation of more

renewable energies. The hydrogen chain can be based on a wind and solar combination, once solar radiation varies almost inversely to the wind velocity [5].

The first hydrogen user centers in Portugal would be:

1st: Lisbon and Oporto (a corridor is established between these two main centers to serve the transport sector);

2nd: Braga and Algarve;

3rd: Coimbra and islands.

2.5.3. Production and Distribution

The hydrogen production chains selected for Portugal in the HYRREG are presented in this paragraph. The estimated timeframe for feedstock as wind, natural gas (NG) and electricity is 2020 and for solar photovoltaic is 2030. Concerning the production process, the timeframe for onsite electrolysis and onsite Steam Methane Reforming (SMR) is 2020, while for central electrolysis and central SMR with CCS is 2030. Regarding transport of H₂ in 2020 it starts through Compressed Gas H₂ (CGH₂) truck and pipeline (mixed with NG) and in 2030 Liquefied H₂ (LH₂) truck and conversion to liquid vector (e.g. ammonia) enter. According to the stakeholders, the H₂ will start to be used in road transport by 2030.

2.5.4. SWOT analysis of the feedstock

Regarding Portugal, the study develops a SWOT analysis for four feedstocks: wind, solar photovoltaic, NG and electricity. Main points are the following:

Wind (electrolysis):

- production still needs involvement from the energy companies, financial services and mainly from the specialist hydrogen equipment manufacturers;
- could be the first economical viable renewable system;
- internationally, knowledge about designing and operating renewable electrolysis is growing;
- zero emissions of pollutants and CO₂; impact on noise and biodiversity.

Solar Photovoltaic (electrolysis):

- still too dependent on research, equipment manufacturers and funding;
- as solar energy is disperse and widespread, H₂ can be used to transport energy to the main centers of consumption;
- the cost of H₂ production from solar energy is high compared with fossil fuels or even other renewable energy (hydroelectric, biomass or wind);
- centralized photovoltaic-hydrogen will not be available until 2040, decentralized can be reached by 2035;
- this chain needs higher collaboration and communication levels between academics, laboratories , policymakers and companies;
- there are no noise or emissions in operation, but some components used in the films are toxic and poisonous.

Natural gas:

- NG continue to be imported from countries with political instability, the secure of supply may not be guaranteed;
- NG is one of the cheaper fossil fuel;
- possible to use 20% H₂volume/volume of NG in the actual NG infrastructure reducing relevant implementation costs;
- the distribution infrastructure of NG is oversized, limitations of capacity are not expected in short term;
- the use of NG contribute to more external energy dependency in fossil fuels;
- some studies indicate the possibility of NG reserves in south of Portugal;
- CCS need development and guaranties of success.

Electric Grid (electrolysis)

- Electricity energy is the biggest energy network in the country, hydrogen production will be considered an integral part of this energy system, given its storage characteristics;
- For long-term storage, H₂ offers the advantage of a highly flexible option with the possibility for multiple use, but needs higher conversion efficiency and lower cost.

2.5.5. Action plan

As H₂ and FC are a very innovative technology option that is not compatible with existing systems, barriers have to be surpassed, between them: technical (efficiency and costs) probably the most important, social, political and regulatory. This HYRREG provides an Action Plan for the SUDOE region, a series of actions concerning governments, public administrations, industry, universities, environmental organizations and other H₂ and FC related parts that will help to create a strategy to overcome barriers. New infrastructure and vehicle fleets will have to be built up at the same time, requiring diligent planning and governmental support.

Concerning production, the necessary actions identified are:

- Prioritize the production of hydrogen by renewable energies as a milestone;
- Develop strategies for integrating renewable energies in the H₂ production by electrolysis;
- Optimize of the performance of H₂ production and cost reduction of the process;
- Improve in gasifier's design to increase H₂ ratio;
- Increase the efficiency of CO₂ capture and sequestration process.

Storage and distribution:

- Invest in new materials for H₂ storage;
- Invest in infrastructures for filling stations.

Social level:

- Improve social awareness and win public's trust through the dissemination of H₂ and FC benefits;
- Include in educational programs different levels of training on this technology;
- Dissemination of H₂ impact on the environment, public health and energy security.

Regulatory:

- Speed up the procedures to incorporate hydrogen and FC in the list of technological facilities and create legislation and regulations for them;
- Develop codes and standards for the design, manufacture and operation of H₂ systems;

- Streamline procedures for obtaining building permits for these facilities.

Policy:

- Align the interests of all ministries involved in the introduction of hydrogen into the energy system;
- Establish a specific H₂ and FC Development Energy Plan, to develop projects and the first user centers;
- Provide a hydrogen specific policy support scheme in the short term, to ensure H₂ gradual implementation and make it competitive with alternative option.

Market/ Economic:

- Coordination of private and public institutions to accelerate the introduction of prototypes into the market;
- Demand creation should begin with demonstration continued projects (social and technical impact): vehicles moving from one city to the other, so the experience can be repeated;
- Mechanisms to facilitate the distribution of subsidies to small and medium enterprises;
- Promotion/ incentives for the purchase of fuel cell vehicles;
- CO₂ taxation;
- Free parking in pollutant areas for zero emissions vehicles, like FCV.

2.6. HyWays for Europe

HyWays is an integrated project co-funded by research institutes, industry and the European Commission under the 6th Framework Programme. The objective is to develop a validated and well-accepted roadmap for the introduction of hydrogen in the energy system in Europe. The HyWays project explores and plans the potential of the integration of hydrogen technologies into the energy system and its contribution to the challenges of ensuring that Europe has a secure, environmentally sustainable and economically competitive supply of energy services for the future [6].

Ten countries are considered: Finland, France, Germany, Greece, Italy, the Netherlands, Norway, Poland, Spain and United Kingdom. It ensures a large coverage in land and population, representing the diversity and geographical spread of Europe, increasing the confidence in the validity of the synthesis at European level. It contemplates the use of hydrogen as a transport fuel and, in addition, the stationary end use application. Hydrogen is identified as can as a medium for energy storage to remedy the mismatch between energy demand and supply in a renewable electricity system mainly based on intermittent resources such as wind energy. More detailed information concerning each of the ten countries can be consulted in the “European Hydrogen Roadmap – Member State’s Report” [21].

The HyWays study use stakeholders’ input and with that information creates market scenarios for end-use applications and technological progress. The scenarios consider a combination of two aspects: technical learning and policy support. The technical learning can be modest or fast, while the policy support can be modest, high and very high.



Figure 10 - Hydrogen corridors [6]

In Figure 10 it is presented early user centers and corridors of the ten countries. It was identified 25 000km of early corridors to connect the European user centers by stakeholders to allow commuting within and future linking with individual countries.

2.6.1. Vehicle penetration

HyWays has not performed a simulation, in a sense that the penetration rate is a function of the cost of the hydrogen technology. The aim was to build a roadmap for the introduction of hydrogen in the energy system. Consequently, the penetration of hydrogen applications was the starting point that can be seen in Figure 11 , not the result.

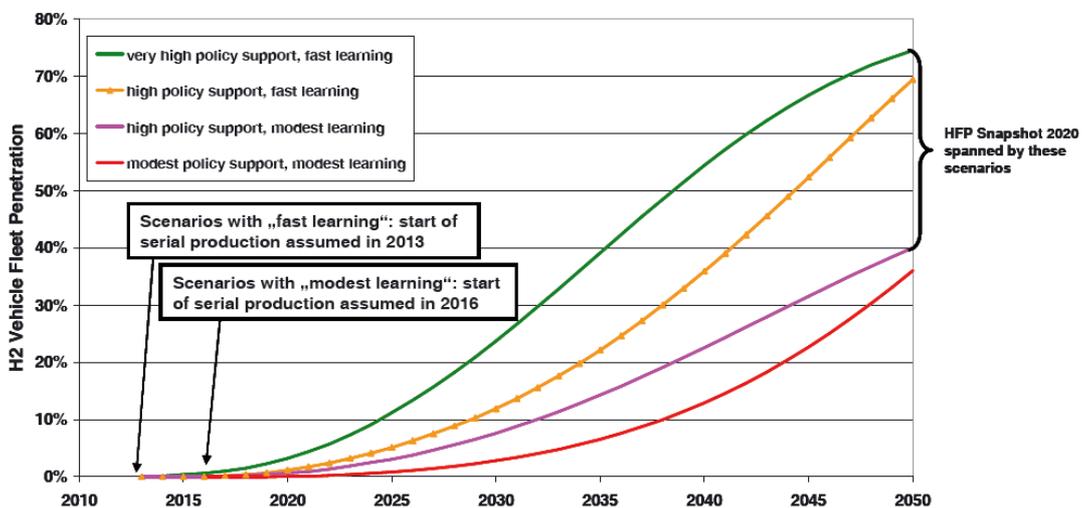


Figure 11 - Development of the penetration rate of hydrogen vehicles for passenger transport [6]

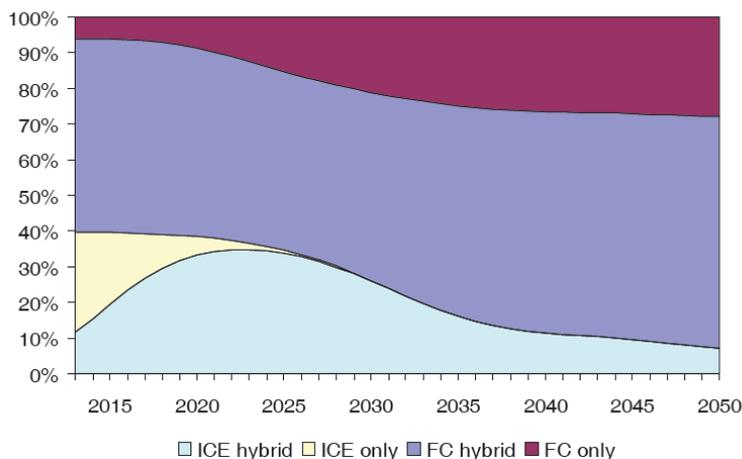


Figure 12 - Distribution of various hydrogen fuelled vehicles: fuel cell vehicles and hydrogen ICE vehicles (hybridized and pure) [6]

The modelling of the vehicle hydrogen demand over time is shown in Figure 12. ICE hybrid percentage decrease over the time, ICE disappears, while the share of FC hybrid (FCHEV) and FCV rise.

2.6.2. H₂ Production

The combination of the production pathways for H₂ is subjected to a sensitivity analysis to: energy prices, availability of CCS technology and CO₂ reduction target. The CO₂ reduction target is essentially achieved by the road transport.

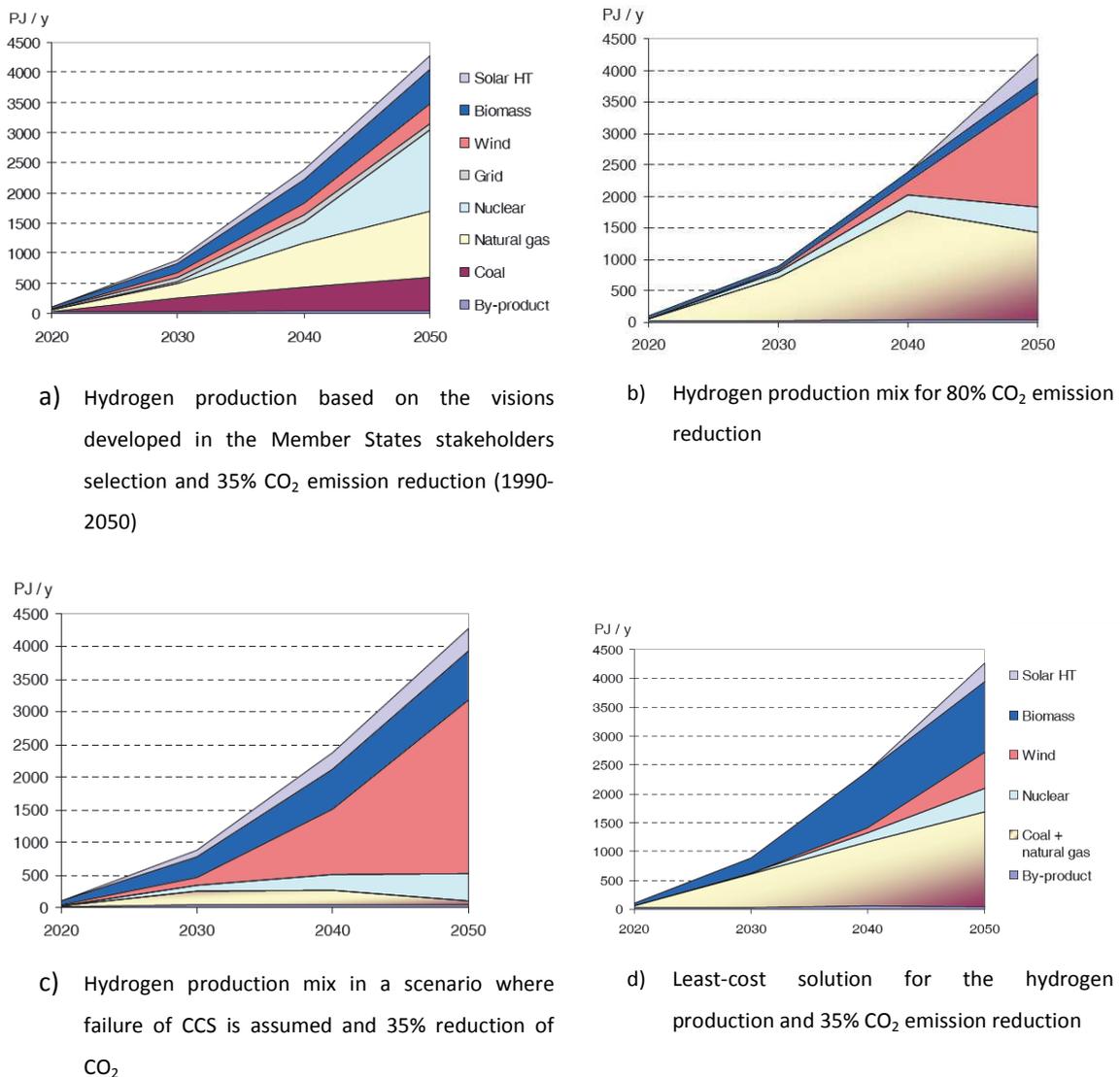


Figure 13 – H₂ production pathways [6]

According to Figure 13, a) scenario, natural gas, biomass and wind energy based pathways have been selected by all member states participating in HyWays. Given the constraints imposed by the member state visions on the development of a future hydrogen system in their country, the share of renewable resources in the production mix is about 1/3 by 2050. Natural gas, coal mainly equipped with CCS and, after 2030, nuclear energy pathways play an important role in the hydrogen production mix.

In the b) scenario the share of natural gas + coal and nuclear energy based pathways in 2050 is about the same of the scenario d). Before 2040, the reduced availability of biomass for hydrogen production is compensated by an increase in the share of coal and natural gas based pathways. After 2040, the hydrogen production pathways based on wind electricity become cost competitive and take over the role of biomass.

The scenario c) shows the hydrogen production mix in case of a failure of CCS. This technology is a key factor for hydrogen production pathways based on fossil fuels, which knowledge has not yet proven its capability at very large scale. A potential failure of CCS not only has an influence on the hydrogen production pathways, it also influences the power sector to a large extent. Since a CO₂ emission constraint of -35% has to be met by 2050, the share of nuclear energy and biomass in the power sector increases severely whilst the share of fossil fuel decreases considerably. Since most biomass resources and the nuclear capacity are utilized by the power sector, hydrogen production from wind energy does become the preferred option. Due to the CO₂ emission reduction constraint, fossil fuel based pathways, in this case without CCS, play a marginal role. The sensitivity analysis shows that in case of a failure of CCS, the energy system can still meet the reduction target, but only by utilizing potentials of carbon free sources to its maximum.

The scenario d) is based on the pathways selected by the member states but ignoring the minimum and maximum shares that were set by them. A sensitivity analysis on energy prices showed that the share of coal vs. natural gas is very sensitive to changes in the relative price of these energy carriers. In comparison to scenario a), the share of renewables in the hydrogen production mix in 2050 is significantly higher and the share of nuclear energy is substantially lower. Wind energy enters somewhat later in the

production mix but reaches a higher share in 2050. This can be explained by the fact that first the price of wind electricity has to drop sufficiently, due to technological learning, before the technology becomes cost competitive. As soon as it reaches this phase, the market share increased quickly.

2.6.3. H₂ Distribution

The hydrogen station location influences the technical solution chosen for hydrogen retailing. For instance, in remote locations, with constant and small demand the best solution is onsite production; for large stations in rural areas, e.g. along motorways, it is better liquid H₂ by truck; for large stations in city borders, liquid H₂ by truck or gaseous from pipeline [6].

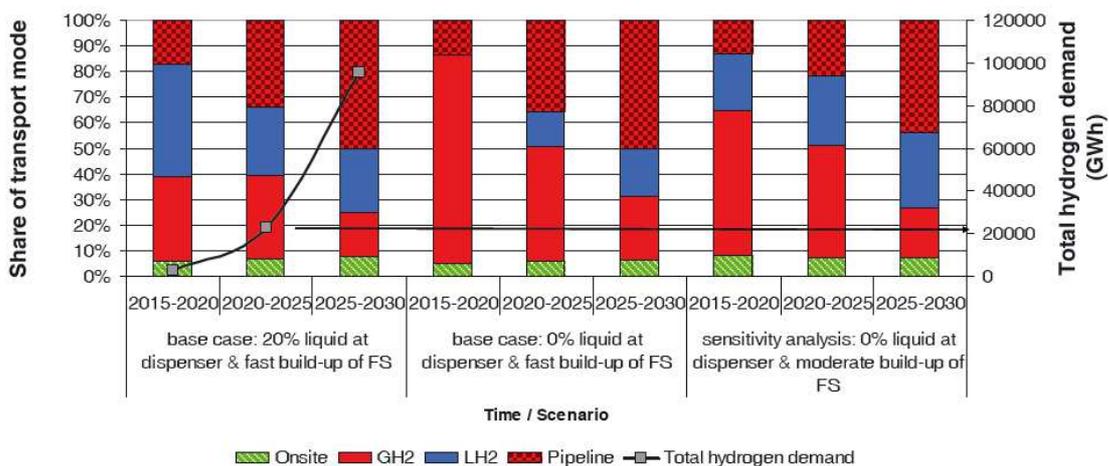


Figure 14 – Share of H₂ transport mode and total hydrogen demand until 2030 [6]

As it can be analyzed in Figure 14, assuming that 20% of all hydrogen demand will be in liquid form, initially hydrogen LH₂ transported by trucks has the highest share, more than 40%. Along with the appearance of decentralized, regional production, compressed gas H₂ truck distribution is a solution for the transition phase towards the pipelines.

Onsite supply methods at the fuelling station from natural gas/biogas or electricity are considered over the whole period studied in areas where there is too low demand for more centralized schemes. The supply of gaseous hydrogen will gradually be dominated

by pipeline. In those less populated and remote areas, onsite supply and LH₂ transport remain the most economical choice. Many hydrogen stations will be placed on already existing conventional refueling stations and the network requires 60-80 km between two adjacent stations. Between 2015 and 2025 it is expected 13000-20000 stations with 4 dispensers and post 2025, the same patterns as today's conventional refueling network, with bigger stations (10 dispensers).

2.6.4. Costs and CO₂ emissions

The impact of hydrogen on CO₂ emission is determined by the penetration rate of hydrogen end-use applications and the way hydrogen is produced as it can be seen in Figure 15 and Figure 16.

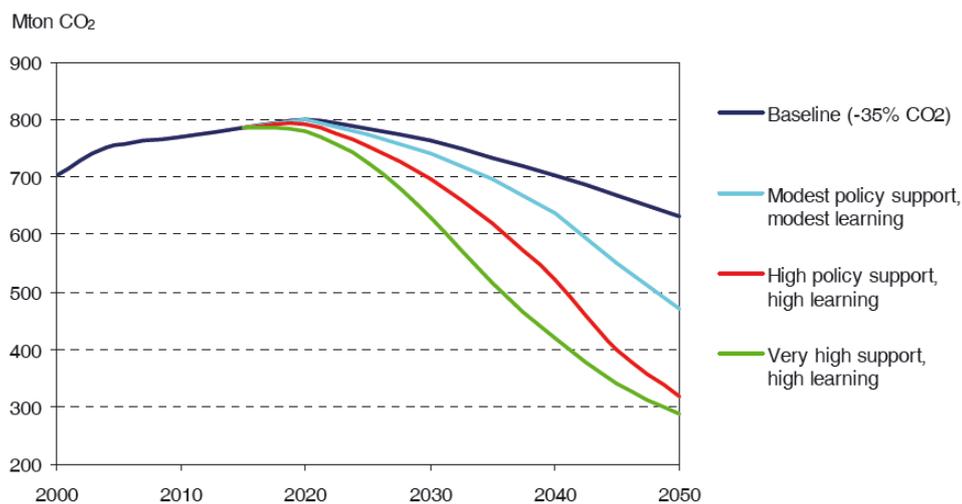


Figure 15 - Development of total CO₂ emission for road transport for the 10 member states [6]

The evolution of CO₂ emissions presented in Figure 15 includes emissions during the production process of hydrogen as well as petrol and diesel (indirect and direct fuel emissions: Well-to-Wheel - WTW). In the baseline scenario, the demand for transport increases substantially explaining the increase in CO₂ emissions until 2020, being the emissions in 2050 only 10% below the emission level of 1990. To achieve the 35% target reduction the modest learning and modest policy is sufficient. The introduction of hydrogen in the high learning scenarios decrease impressively the CO₂ emissions in the

transport, about 55-60% compared to the baseline scenarios or 60-64% compared to the emission level of 1990.

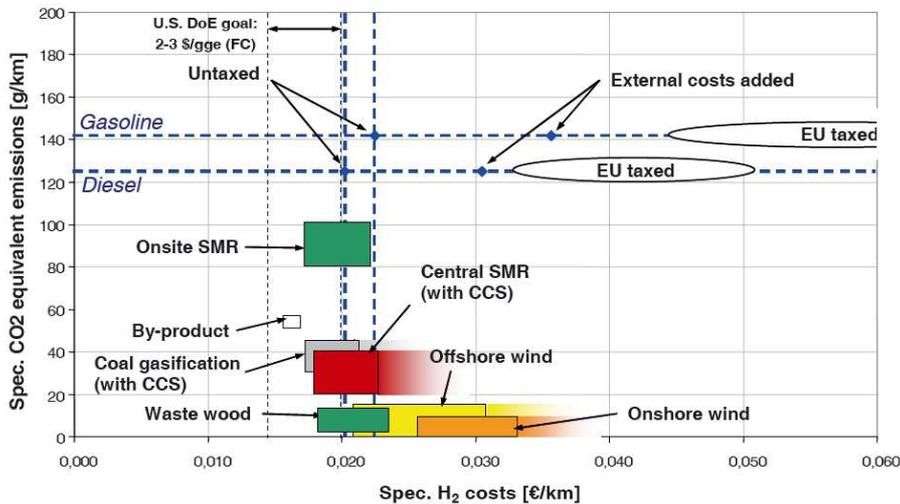


Figure 16 - Portfolio analysis of hydrogen production pathways as selected by the Member States, reference year 2030 (WTW emissions and specific WTW costs), [6]

As it can be analyzed in Figure 16, the specific H₂ pathways costs (0.018 – 0.024 €/km) for the majority of the hydrogen energy chains are in 2030 in the order of the diesel and gasoline reference costs (0.020 – 0.022 €/km). In the action plan it is presented the cost of 3€/kg in 2020 and 4 €/kg in 2030. On its turn the FCV is expected to cost between 23 and 26 k€ in 2020, 20-23 k€ in 2030 and the FC about 50€/kW. This roadmap also presents the cumulative investment necessary for the production, transport, distribution and refueling until 2027.

2.6.5. Potential of hydrogen and Action plan

According to this study, the hydrogen could become one of the solutions for wind and photovoltaic intermittency, as it offers the opportunity to store and transport the energy. Another option combines production of electricity and H₂ with CCS, which improves energy supply security as a result of diversification of fossil feedstock, the main risk lies in the potential failure of permanent underground storage of CO₂.

The main challenge lies in the reduction of the cost for hydrogen end-use applications and in the build-up of a hydrogen infrastructure. Cost reductions can be achieved through both R&D (technological progress) and deployment (economies of scale). A monitoring framework is necessary to ensure that support levels are appropriate and ensuring that R&D and deployment support are in balance in order to reach competitiveness at minimum costs and as early as possible.

Priorities on R&D should focus on demonstrations, component technology development and cost reduction of drive trains and production chains. In more detail, until 2015, focus on pre-commercial applications: system integration, market preparation and continued cost reduction. Components need to be developed, tested in large-scale demonstration projects and integrated in energy systems to a fully commercial level, while creating market demand.

From 2015, focus on commercialization: switch from modified conventional vehicles to purpose-built vehicles, verify hydrogen safety and reliability and develop consumer confidence (marketing experts). In the first phase, incentives need to be provided through a hydrogen specific support scheme, for instance, no tax on hydrogen as a fuel. Substantial investments are needed in infrastructure build-up and public-private partnerships seem the way. For the market penetration, a hydrogen specific deployment support framework needs to be developed, starting with equal total costs (€/km) for the use of a hydrogen vehicle in comparison to a conventional vehicle. Early markets need to be created utilizing the advantages offered by hydrogen applications. Examples are city center access regulations or procurement of zero emission vehicles within governmental services. Education and training are also necessary to facilitate the large employment shifts.

The internalization of the external costs should be also studied in more detail: non-CO₂ emissions, short-term relevance of local pollution abatement, decentralized energy supply schemes and load management of the power sector. Another point explored on the HyWays is the cost effectiveness of CO₂ emissions reduction, if hydrogen is introduced into the energy system, the cost to reduce one unit of CO₂ decreases 4% in 2030 and 15%

in 2050, implying that hydrogen is a cost effective option for the reduction of CO₂. This allows lowering the cost of meeting future CO₂ emission reduction targets.

2.7. Mckinsey for Europe

Regarding the commitment assumed of cutting 80% the CO₂ emissions by 2050 if atmospheric CO₂ is to stabilize at 450 parts per million² – and global warming stay below the safe level of 2°C, the question according to this study is: 80% decarbonization overall by 2050 may require 95% decarbonization of the road transport sector. With the number of passenger cars expected to rise to 273 million in Europe, and to 2.5 billion worldwide by 2050, this may not be achievable only through improvements on the internal combustion engine or alternative fuels: the traditional combustion engine is expected to improve by 30%, so achieving full decarbonization is not possible through efficiency alone. There are uncertainties about whether large amounts of (sustainably produced) biofuels will be available for passenger cars, given the potential demand from other sectors, such as goods vehicles, aviation, marine, power and heavy industry. This study was undertaken in order to compare the performance and costs of alternative power-trains for passenger cars FCV, BEV and PHEV, with conventional ICE vehicles. This included a factual evaluation of the economics, sustainability and performance of every step of the value chain, a well-to-wheel approach.

It was used a combined forecasting and backcasting approach to maximize accuracy: from 2010 to 2020, all cost and performance projections are based on proprietary industry data; after 2020, on projected learning and annual improvement rates. It is based on a share of 25% FCVs, 35% BEVs, 35% PHEVs and 5% ICEs in the EU by 2050. Some results consider different segments: A/B (small cars), C/D (medium) and J (larger). Economic comparison between power-trains is based on the TOC. The TOC takes into account the purchase price and the running cost, the lifetime considered is 180 000 km [7].

2.7.1. H₂ Production

About the production mix scenario, the study examined two hydrogen production mixes: a balanced and economically driven production mix with CCS; the other without CCS, representing 100% electrolysis with 80% renewable energy by 2050. They both lead to CO₂-free hydrogen by 2050, as it is shown in Figure 17. While the production of hydrogen from SMR with CCS remains the lowest-cost scenario, 100% electrolysis production mix only increases the TOC of FCVs (C/D segment) by 5% in 2030 and 3.5% in 2050.

As total hydrogen demand for FCVs is low before 2020, a conventional production mix is assumed, utilizing excess hydrogen from existing assets: central SMR has 40%, distributed SMR and distributed WE each have 30% share of production. After 2020, when hydrogen demand for FCVs increases rapidly, a balanced and economically driven scenario is assumed, reflecting the diversity of resources available in different parts of Europe and including new sources of clean hydrogen: central SMR and Integrated Gasification Combined Cycle (IGCC) each have 30%, coal gasification has 10% and central WE and distributed WE account with 15% share of new production, each one, see Figure 17. It is assumed that CCS is applied to all new central SMR, IGCC and coal gasification capacity starting in 2020 [7].

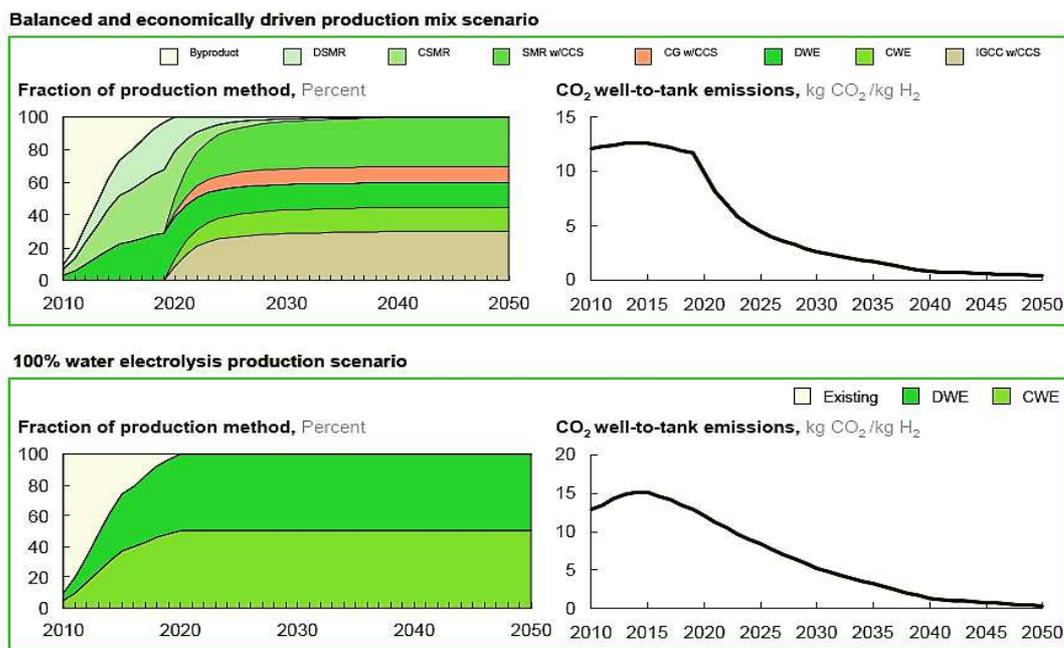


Figure 17 – H₂ production mixes until 2050 [7]

According to Figure 18, the most economic midterm future production methods use existing technologies – SMR and coal gasification, but their cost will increase in the future due to increasing fuel prices and costs of CCS. While that, cost of water electrolyzers reduces due to efficiency improvements.

CCS is identified as an important solution for reducing CO₂ emissions, while the technology is being developed to decrease the CO₂ footprint of power generation, an additional benefit is that pre-combustion CO₂ capture technology also allows the production of large volumes of CO₂-free hydrogen. This is important to the economic assumptions of the study, as in the balanced and economically driven hydrogen production scenario, 70% of hydrogen is assumed to be produced using CCS [7].

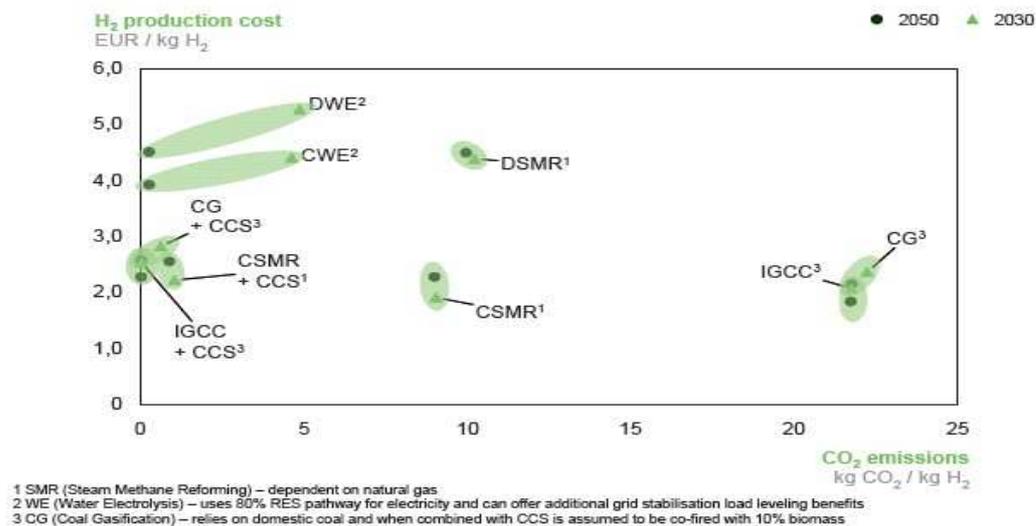


Figure 18 - Future cost levels of available technologies to produce hydrogen and respective CO₂ emissions [7]

2.7.2. H₂ cost

The cost of hydrogen reduces by 70% in 2025 and after that stays relatively flat (excluding taxes and incentives), see Figure 19. The retail cost decreases considerably, while the production and distribution do not vary that much. In order to persuade current gasoline/ diesel station owners to start providing hydrogen, it will be necessary not to tax H₂ and dealers will require subsidy [7].

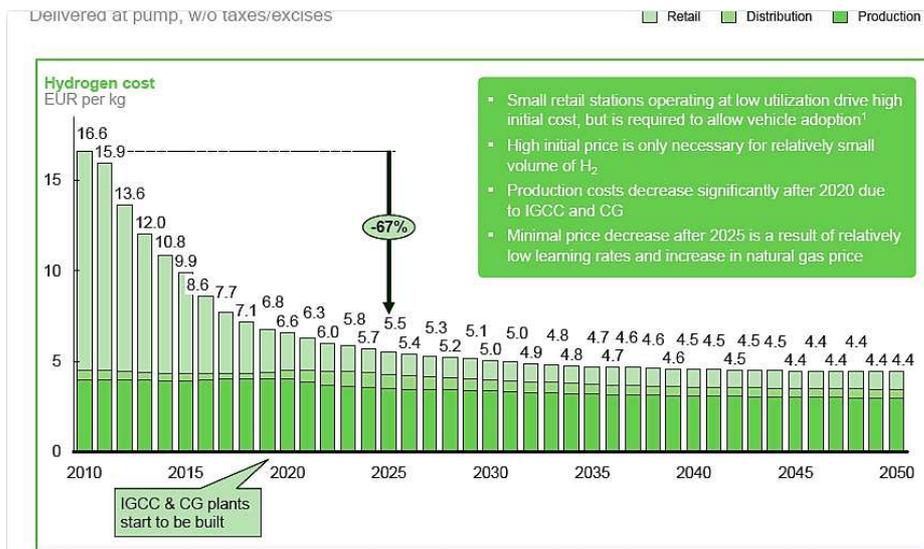


Figure 19 - Hydrogen cost evolution [7]

About the cost of the vehicles by 2020, the purchase costs of BEVs, FCVs and PHEVs is several thousand more euros than ICEs, what can be offset by tax exemptions.

Beyond 2030, FCV have a TOC advantage over BEVs and PHEVs in the largest car segments and by 2050, FCVs are more economic than ICEs for larger cars and fully competitive for medium-sized cars. For A/B segment they are not competitive. Regarding C/D segment the FCV acquisition cost is expected to be about 31000€ in 2020 and 26000€ in 2030. If hydrogen is not taxed like gasoline and diesel in the ramp-up phase, infrastructure and fuel costs for FCVs can become cost-competitive with ICEs as early as 2020 [7].

2.7.3. H₂ Distribution

At the initial stage of the introduction of the technology the transportation will be essentially of compressed gas H₂ by truck, followed by a transition phase towards transport by pipelines, where liquid H₂ by trucks will be used, see Figure 20. The use of pipelines will result in a reduction of both the cost of hydrogen and in the CO₂ emissions.

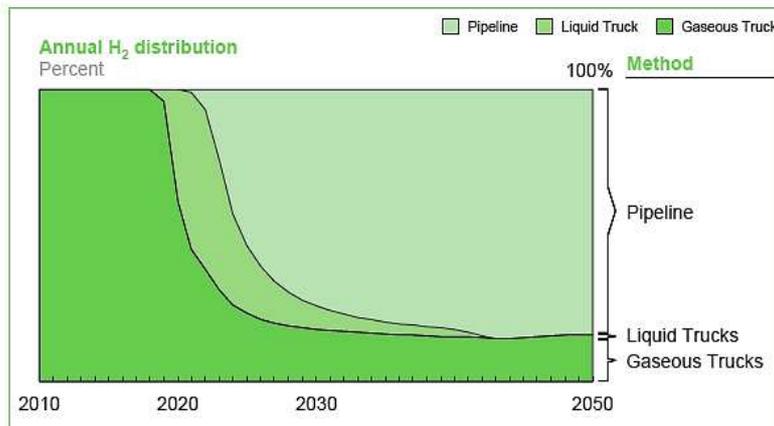


Figure 20 - H₂ distribution systems forecast [7]

The refueling stations size will depend on the demand and the area to be covered. In the early stages, when the demand increase is lower than the application area, H₂ refueling stations will have small size, while at following stages, when demand increases faster than the area, refueling stations size will be larger, see Figure 21 and Table 5.

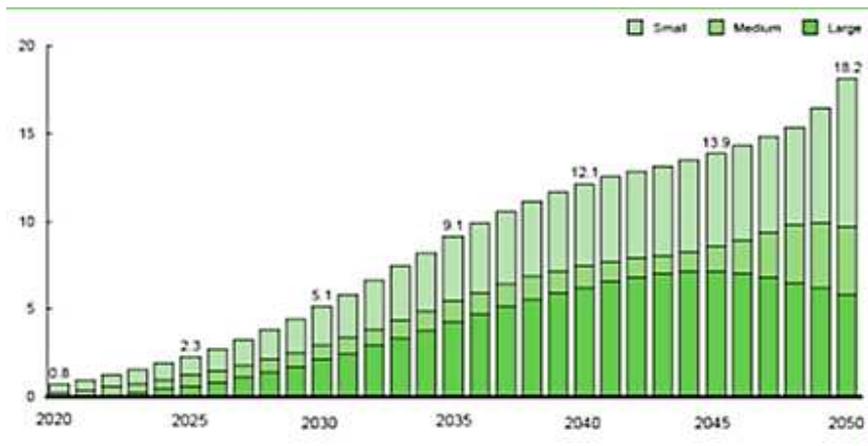


Figure 21 - The number of hydrogen retail stations from 2020 to 2050 (Thousand retail stations in EU29), [7]

Table 5 - Retail stations: size and capacity.

Small station (70-100 cars per day)	2 dispensers, 0.4 tonnes of hydrogen/day
Medium station (150-250 cars per day)	4 dispensers, 1 tonne of hydrogen/day
Large station (450-600 cars per day)	10 dispensers, 2.5 tonnes of hydrogen/day

2.7.4. CO₂ emissions

Despite improvements in fuel economy, the capacity of ICE vehicles to reduce CO₂ is considerably less than that of BEVs and FCVs, which can achieve close to zero CO₂ emissions (well-to-wheel), see Figure 17 and Figure 22. As the range of BEVs is limited for medium sized cars, they are ideally suited to smaller cars and shorter trips. Medium/larger cars segment account for 50% of all cars and 75% of CO₂ emissions because they generally cover longer distances. Replacing the ICE vehicles in these segments with FCV therefore potentially achieves a significant CO₂ reduction. As FCVs also have a clear TOC advantage over BEVs and PHEVs for medium/larger cars and longer trips, FCVs represent the lowest-carbon solution for a large proportion of the car fleet, based on current mobility patterns [7].

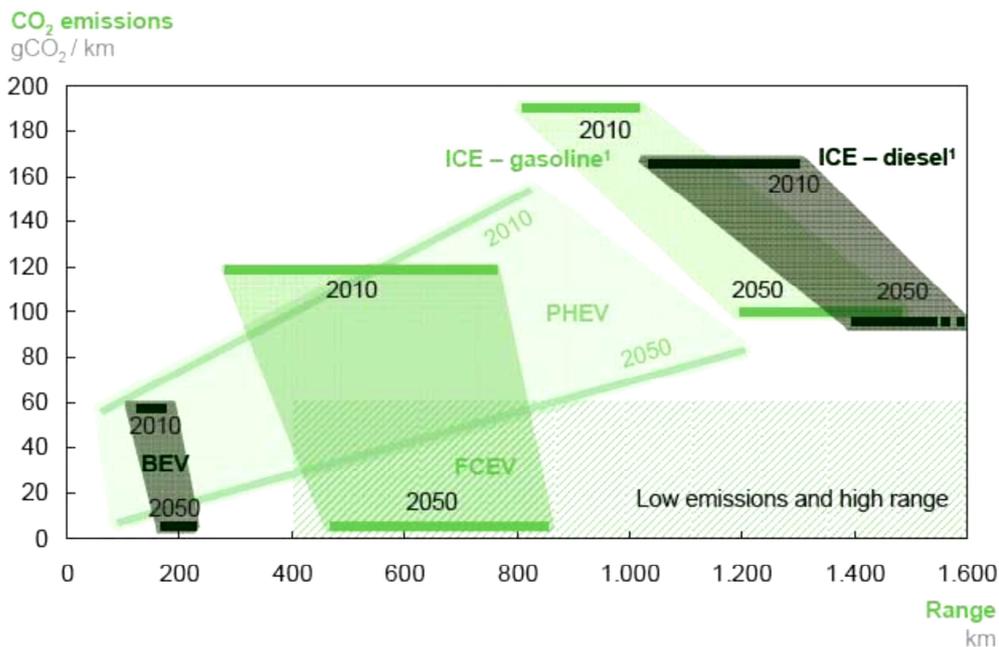


Figure 22 – CO₂ Emissions (WTW) and range comparative for different kind of vehicles [7]

2.7.5. Infrastructure building

This study underlines the necessity of close value chain synchronization for the FCV market and external stimulus in order to overcome the first-mover risk of building hydrogen retail infrastructure. The risk is high and therefore greatly reduced if many companies commit on the investment, coordinated by governments and supported by dedicated legislation and funds incentives. With the market established, subsequent investment (2020-30) will present a significantly reduced risk and by 2030 any potentially remaining economic gap is expected to be directly supported by the consumer.

The attractiveness of the business case for FCVs is affected by the additional costs required for distribution and retail. In other words, if FCVs make commercial sense, as demonstrated by this study, building dedicated hydrogen infrastructure can be justified. This study also presents the investment required for that.

3. CONCLUSIONS

Conclusions will be made for the main items hydrogen production, supply, use, hydrogen technology and fuel cost. It is noteworthy that in the reviewed studies hydrogen is considered as part of the solution to reduce CO₂ emissions and oil dependency but always integrated with other energy carriers/vehicle technologies.

Concerning the production of H₂, it is identified a tendency to consider the production in the short-medium term (2020-2030) by SMR and electrolysis, this last one essentially in decentralized mode. The CCS appears as a new technology, which development will play a key role in the chosen feedstock and production process. In the long term there is a trend for more centralized production, gasification of coal and biomass entering in the mix. It is expected that H₂ is produced from a diversity of resources, depending on the endogenous resources available in each region. In Roteiro Nacional de Baixo Carbono, that is specific for Portugal it is presented the H₂ production mainly from biomass gasification [3]. HyWays for Europe [6] and the HYRREG for SUDOE [5], present the electrolysis essentially from renewable sources, being the wind the preferred feedstock, solar photovoltaic also appears in the second study as a potential source after 2030, in Portugal. The endogenous energy resources of each region can determine which one to use for the electrolysis process. The level of population and geographic conditions also influence the most cost-effective (centralized or decentralized) way to produce the H₂ in each area.

The hydrogen distribution is expected to be in the short-medium term by truck (gaseous or liquid), and in the long term it will be mainly by pipelines, remaining the other ways an option for less populated or remote areas. Concerning refueling stations, there is a forecast that they will be in the early stages small (2 dispensers, 0.4 tonnes of hydrogen/day), than medium (4 dispensers, 1 tonne of hydrogen/day) and large stations (10 dispensers, 2.5 tonnes of hydrogen/day) take place.

About the use of H₂ in the transports, it will be made essentially by means of the fuel cell technology in hybrid configurations of passenger cars. For studies that only take into account the midterm, like [2] and [6], the consumption could be respectively between the order of 10 and 10⁻⁴ PJ. The Global Transports Scenarios [1], forecasts a total

consumption of H₂ between 0.1 and 1 EJ for cars in 2050, what means, depending on the scenario, 0.62 to 4% of the total energy consumed in that sector. It does not consider the use of hydrogen in other transports. For the specific case of Portugal, in Roteiro Nacional de Baixo Carbono [3], the consumption in 2050 can reach 0.01EJ, corresponding to a percentage between 0 and 16.5% in of the total energy consumption in transports; in the Scenarios for Portugal [4] the percentage of hydrogen consumption in Portugal in 2050 will reach a maximum of 9% in the fleet, corresponding to 10 PJ.

Regarding the fleet penetration, the Global Transports Scenarios [1], preview the penetration of hydrogen vehicles between about 1.6 and 3.3% (FCV+H₂ HEV) in 2030, while in 2050 the percentage can vary among 1.25 and 6.17%. Studies for Europe are more optimistic concerning the penetration of hydrogen vehicles, in the scenarios of HyWays for Europe [6], the percentage reaches 3 to 24% in 2030, while in 2050 it varies from 26 to 74%. The Mckinsey for Europe [7] considers a penetration of 25% of hydrogen vehicles in 2050. The Scenarios for Portugal [4], depending on the scenarios shows an entering that can vary from 0 to 22% in 2050.

Analyzing the cost of the H₂ for the midterm 2020-2030, the range of values from the different studies goes from a minimum of 2.5€/kg [4] to 6.6€/kg [19]. In 2050 the value varies between 3.09 \$/kg [1] and 4€/kg [7]. Concerning the Fuel Cell cost, it is forecasted for the midterm the cost between 148 and 250\$/kW [1], while the European studies for the same timeframe consider the cost in the order of dozens. For 2050, only in [1] it is expected a value, that can vary among 84 and 250 \$/kW. The FCV acquisition cost in the midterm (2020-2030) is among \$18200 [1] and 31000€ [7]. In the long term (2050) the cost can vary between 21900 [1] and 22802 € [4].

The level of CO₂ emissions from the H₂ production depend on the process and the feedstocks used. Anyway, according to the assumptions assumed (variations also in the demography, economic, other technologies used, energy cost, between others), the scenarios considering the introduction of hydrogen in the energy used in transports result in a considerable decrease in the CO₂ emissions. According to [7], FCV can achieve in 2050 zero CO₂ WTW emissions. There is a univocal opinion between the revised studies that

technological developments are necessary for the envisaged hydrogen economies to be low-carbon: abundant and competitive renewable electricity or carbon sequestration. While fossil fuels are seen by most studies as transitional, some envisage a long-term role for fossil fuels based on CCS. In cases of CCS technology failure, a high percentage of renewables is the option for low-carbon H₂ production.

The studies reviewed identify the H₂ as an energy vector that will play an important role in the in the transport sector. Nevertheless, the introduction of hydrogen into the energy system does not happen autonomously. Substantial barriers have to be overcome, ranging from economic, technological, institutional, social and infrastructural barriers. An interchange between national and local policy makers, manufacturers, consumers and producers will be essential if we are to meet the introduction of H₂ in the transportation system.

Regarding the social part, it is necessary to inform consumers about the benefits of the hydrogen over other vehicles. Subsidies and public support are necessary to encourage both: private and public sector to invest in this technology. It is indispensable a diligent planning and government support in parallel with build infrastructure/ stations and vehicle fleets. It is also necessary to develop legislation and certification standards for material, hydrogen storage and distribution systems. As FCV are very innovative energy technology it is necessary to improve the system efficiency. The infrastructure net needs to be built, with a big investment necessary, the partnerships between the public and private institutions are indicated as a solution. To build the distribution infrastructure there is a high risk and therefore greatly reduced if many companies commit on the investment.

Amidst a range of factors that can define the future of hydrogen, the policy drivers evident in the literature are climate change (international commitments assumed), energy security and reducing fossil fuels dependence.

H₂ and FC implementation in the transportation sector in Portugal has the potential to decrease foreign energy dependency, being an energy storage system and reducing

pollutant and CO₂ emissions. It is also a way of store the excess energy from renewable energies, allowing for an easier management of these resources.

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SECOND PART – HYDROGEN VEHICLES LIFE CYCLE ANALYSIS

1. INTRODUCTION

Regarding road transportation fuel, hydrogen is seen as a potential option. The main barrier to the widespread use of this energy carrier among private vehicle owners is its refueling infrastructure. For this reason, the majority of demonstration projects so far are related to the public bus sector, such as the Clean Urban Transport for Europe (CUTE), the Global Hydrogen Bus Platform (HyFLEET:CUTE), the Sustainable Transport Energy Programme (STEP) and the Ecological City Transport System (ECTOS). However, some original equipment manufacturers (OEM) of light-duty vehicles have already engaged prototype developing. Some of those prototypes, out of more than 20, are: Mercedes-Benz F600 Hygenius (hybrid), Honda FCX (hybrid), GM Chevy Volt Hydrogen (plug-in hybrid) and Ford Edge with HySeries Drive (plug-in hybrid).

The main methodology used by the scientific community to compare alternative vehicles with conventional ones is the life cycle assessment (LCA), through a so called energy source life cycle analysis, Well-to-Wheel (WTW) (fuel upstream WTT plus fuel use TTW) and a materials life cycle analysis, the so called materials cradle-to-grave, CTG, or embodied materials analysis. LCA based methods use, essentially, the global warming potential impact category. Few studies look to acidification potential, human toxicity potential or eutrophication potential. Despite not being recommended in the ISO norms, this studies use the final indicator of the method Eco Indicator to facilitate the technologies comparison.

2. PRIVATE CARS

This study [1] intends to exploit the benefits of introducing fuel cell technology in today's light-duty vehicle market for the Portuguese light-duty fleet. Two options for producing hydrogen were considered: on-site electrolysis (at the refueling station) and centralized natural gas reforming. An extensive life cycle analysis is applied to both individual vehicle technologies (covering conventional, hybrid, hybrid plug-in, electric) and to the complete light-duty vehicle fleet. Life cycle analysis include both fuel and materials layers.

2.1. Portuguese light-duty fleet characterization consumption and emissions

The Portuguese fleet characterization in terms of diesel/gasoline distribution, weight and engine displacement vehicles' distribution is presented in Table 6[7]. To estimate the Portuguese fleet energy consumption and derived emissions COPERT 4 [8] was used, which is an European tool for estimating the emissions and energy consumption of specific fleets (with conventional vehicle technologies). A typical annual and daily mileage of respectively 12800 and 35 km was assumed [7]. For COPERT a mix of urban (24% of total distance), rural (57% of total distance) and highway (19% of total distance) driving was considered. The results obtained for the conventional fleet energy consumption and annual emissions of carbon dioxide (CO₂), carbon monoxide (CO), hydrocarbons (HC), nitrogen oxides (NOx) and particulate matter (PM) are presented in Table 2, according to the categories of vehicle considered. Table 7 shows the results of energy consumption and emissions at vehicle usage stage (tank-to-wheel, TTW).

Table 6- LDV fleet characterization in terms of fuel distribution and engine displacement (year 2005).

Displacement	# vehicles	Fuel	% Total LDV fleet	
<1.4 l	2336655	Gasoline	43%	53%
1.4 - 2.0 l	469837		9%	
>2.0 l	52187		1%	
<2.0 l	1801273	Diesel	33%	46%
>2.0 l	699510		13%	
>2.0 l	22440	LPG	0.42%	
# Total vehicles	5381902		100%	

Table 7- Annual TTW characterization for the Portuguese light-duty fleet in terms of energy consumption and emissions.

Vehicle category	Energy consumption		Emissions (kton)				
	l/100km	TJ	CO ₂	CO	HC	NO _x	PM
Gasoline <1,4 l	6.9	56163	4058	112	15.7	16.0	0.0
Gasoline 1,4-2,0 l	8.2	15223	1100	18	2.5	2.6	0.0
Gasoline >2,0 l	10.3	2150	155	1.2	0.14	0.15	0.0
Diesel <2,0 l	6.1	63989	4724	5.8	0.94	20.0	2.1
Diesel >2,0 l	7.9	28651	2115	2.9	0.83	7.1	1.0
LPG	2.9 ^a	936	61	1.1	0.17	0.18	0.0
Total	7.2^b	167112	12213	141	20	46	3

^a in m³ of liquid propane gas per 100 km. ^b gasoline equivalent.

Summarizing, the Portuguese light-duty conventional road transport sector consumes 167112 TJ of fossil fuel energy and is responsible for a global annual CO₂ emission of 12213 kton and for a local emission of 141 kton of CO, 20 kton of HC, 46 kton of NO_x and 3 kton of PM.

2.2. Fuel cell vehicle penetration scenarios

For assessing the impact of fuel cell hybrid and hybrid plug-in vehicles on the light-duty fleet energy consumption and emissions the following fuel cell representative vehicles were considered [9]:

- Hybrid (FC-HEV) : fuel cell vehicle with a 75 kW electric motor, Li-ion 6 Ah 267 V battery, 50 kW fuel cell and a total weight of 1388 kg;
- Plug-in hybrid (FC-PHEV): lightweight materials, plug-in series hybrid with fuel cell. Fuel cell stack 50 kW, electric motor 75 kW, battery Ni-MH 45 Ah 335 V and a total weight of 1315 kg.

These vehicles have a total power-to-weight ratio of 55 W/kg since this is representative of the top sales of new vehicles sold in Portugal, with whom these new technologies will compete when they start entering the market. Additionally, it guarantees that similar vehicle performances are being compared.

The designed scenarios for the hybrid and hybrid plug-in fuel cell vehicles are indicated in Table 8.

Table 8- Designed scenarios for the penetration of fuel cell vehicles.

Scenarios	Vehicle penetration (%)		
	Total fleet replacement	HEV	PHEV
Base	0	0	0
Scenario 1	10	5	5
Scenario 2	30	10	20
Scenario 3	50	15	35

Additionally, two different hydrogen production pathways were considered as indicated in Table 9.

The base scenario corresponds to the present situation that was described earlier. For scenarios 1, 2 and 3 the number of electric vehicles continuously increases. Regarding air quality pollutants, the amount of new vehicles in the fleet that substitute the conventional ones had zero local emissions instead of those that came out in the tailpipe of the vehicles in base scenario. Concerning energy consumption, since COPERT 4 does not include any of the new vehicle technology considered, for simulating the daily commuting journeys of these new vehicle technologies ADVISOR vehicle simulation software [10] was used. ADVISOR is a micro-simulating tool to estimate the performance and fuel economy of conventional and advanced new vehicle technologies.

Table 9- Percentages for the hydrogen origin, considering each scenario.

Scenarios	Centralized natural gas reforming (A)	On-site Electrolysis (B)
Base	0	0
Scenario 1	0	100%
Scenario 2	50%	50%
Scenario 3	100%	0

A real measured driving cycle was used, representing a mix of urban (24% of km, speed below 50 km/h), rural (57% of km, speed between 50 and 90 km/h), and highway (19% of km, speed higher than 90 km/h) driving. Figure 1 shows the journey driving cycle.

2.3. Full life cycle of individual vehicle technologies

To better understand how road vehicle technologies energy consumption and CO₂ emissions compare with the fuel cell vehicles, a full life cycle perspective is used. This full life cycle comprises the fuel life cycle and materials cradle-to-grave life cycle.

For this analysis the two fuel cell configurations described above were compared with the following vehicles/fuels with similar power to weight ratios (55 W/kg) [11]:

- ICEV (Gasoline, E10, E85, E100): internal combustion engine vehicle that can run with gasoline and blends of gasoline and ethanol E10, E85 and E100, with a four cylinder explosion engine with 63 kW of power and total weight of 1139 kg;
- ICEV (Diesel, B10, B20, B100): internal combustion engine vehicle that can run with diesel and blends of diesel and biodiesel B10, B20 and B100, with a four cylinder Diesel engine with 67 kW of power and total weight of 1210 kg;
- PHEV (Gasoline, E10, E85, E100): plug-in hybrid electric vehicle that can work with gasoline and blends of gasoline and ethanol E10, E85, E100 and electricity. 53 kW internal explosion combustion engine/generator, 75 kW electric motor, Ni-MH 45 Ah 335 V battery , series technology with a total weight of 1323 kg;
- PHEV (Diesel, B10, B20, B100): plug-in hybrid electric vehicle that can work with diesel and blends of diesel and biodiesel B10, B20, B100 and electricity. 53 kW internal Diesel combustion engine/generator, 75 kW electric motor, Ni-MH 45 Ah 335 V battery, series technology with a total weight of 1323 kg;
- HEV FULL (Gasoline): hybrid electric vehicle with parallel and series technology, 43 kW internal explosion combustion engine, 31 kW electric motor, Ni-MH 6.5 Ah 308 V battery, 15 kW generator and 1332 kg;
- EV (100% Electricity): pure electric vehicle with a 75 kW electric motor, Ni-MH 90 Ah 268 V battery, and a total weight of 1389 kg.

The program ADVISOR [10] was used to simulate the energy consumption and emissions of each vehicle in the specified driving cycle (see Figure 23).

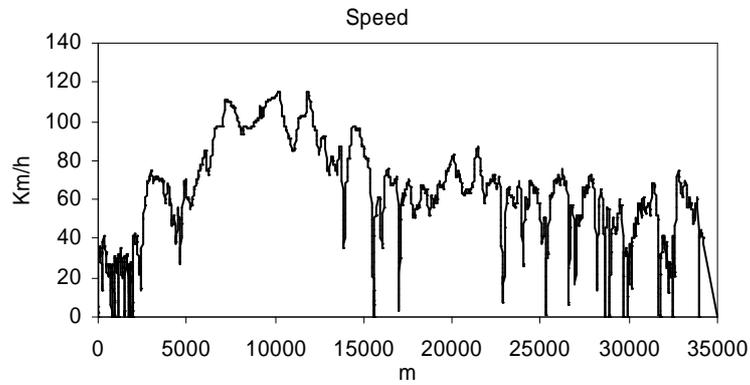


Figure 23- Drive cycle. Average speed 40 km/h, distance 33 km.

Table 10 shows the in-use energy consumption and CO₂ emissions (Tank-to-Wheel part of the fuel life cycle).

Table 10- Fuel life cycle energy and CO₂ WTT and TTW results for pure electric, fuel cell hybrid and hybrid plug-in, gasoline full hybrid, conventional and hybrids plug-in diesel and gasoline with biofuels blends.

Vehicle	WTT		TTW	
	Energy (MJ/km)	CO ₂ (g/km)	Energy (MJ/km)	CO ₂ (g/km)
EV (Electricity)	1.06	72.9	0.57	0.0
FC-HEV (A)	0.62	95.4	1.08	0.0
FC-HEV (B)	3.89	223.3	1.08	0.0
FC-PHEV (A)	0.31	56.7	0.55	0.0
FC-PHEV (B)	1.97	96.4	0.55	0.0
HEV Gasoline	0.26	23.2	1.85	135.0
ICEV B10 (A)	0.43	28.5	1.63	110.7
ICEV B10 (B)	0.40	24.9	1.63	110.7
ICEV B100 (A)	1.90	74.3	1.60	0.0
ICEV B100 (B)	1.57	39.5	1.60	0.0
ICEV B20 (A)	0.59	33.6	1.62	98.8
ICEV B20 (B)	0.53	26.5	1.62	98.8
ICEV Diesel	0.27	23.7	1.67	124.4
ICEV E10 (A)	0.50	27.9	1.96	133.3
ICEV E10 (B)	0.61	33.4	1.96	133.3
ICEV E100 (A)	2.56	58.5	1.97	0.0
ICEV E100 (B)	3.66	113.3	1.97	0.0
ICEV E85 (A)	2.22	53.4	1.97	30.4
ICEV E85 (B)	3.15	99.9	1.97	30.4
ICEV Gasoline	0.27	24.5	1.96	143.0
PHEV B10 (A)	0.70	47.8	1.31	73.6
PHEV B10 (B)	0.68	45.4	1.31	73.6
PHEV B100 (A)	1.82	83.5	1.40	0.0
PHEV B100 (B)	1.57	57.8	1.40	0.0
PHEV B20 (A)	0.77	51.4	1.32	65.7
PHEV B20 (B)	1.31	46.6	1.32	65.7
PHEV Diesel	0.60	44.6	1.34	82.8
PHEV E10 (A)	0.65	41.6	1.13	61.3
PHEV E10 (B)	0.70	44.1	1.13	61.3
PHEV E100 (A)	1.65	56.9	1.17	0.0
PHEV E100 (B)	1.83	83.2	1.17	0.0
PHEV E85 (A)	1.50	54.9	1.18	14.8
PHEV E85 (B)	1.96	77.5	1.18	14.8
PHEV Gasoline	0.55	40.1	1.13	65.7

For the fuels production and distribution stage part of its life cycle “Well-to-Tank” analysis WTT, a database [12][13] was used for the calculation of the energy spent and CO₂ emissions for different fuels and different pathways. The fuel cycle has been defined as

the energy spent to bring the fuel to the vehicle, not including the energy of the fuel itself. For each type of fuel a path was defined since its acquisition or production until it is available for use in the vehicles. The fuels used were gasoline, diesel, ethanol from sugar beet, pulp to heat (ethanol A), ethanol from sugar beet, animal feed export (ethanol B), biodiesel from rapeseed (biodiesel A), biodiesel from sunflower (biodiesel B), electricity, hydrogen from central natural gas reforming plants with steam co-generation (hydrogen A) and hydrogen produced in refuelling stations via onsite electrolysis generation (hydrogen B). Table 10 shows results for complete fuel life cycle.

For the study of the materials life cycle (cradle-to-grave) the program GREET was used. The program consists of a worksheet that was developed in open-source [14] (that deals with the materials cycle since the extraction, assembling till the dismantling and recycling). The electric mix of the database was adapted to European reality [11]. Table 11 shows the materials life cycle (“cradle-to-grave”) results including tire, battery and fluids maintenance throughout 150000 km useful life.

Figure 24 and Figure 25 shows the combination of tank-to-wheel with well-to-tank for the fuel life cycle with the materials cradle-to-grave for selected vehicles. For the total life cycle only the combustion of fossil fuels is considered to produce CO₂. The combustion of biofuels is considered to produce zero CO₂ emissions because the same amount of CO₂ is captured by the plants that produce the biofuel itself.

Table 11- Materials energy and CO₂ cradle-to-grave for pure electric, fuel cell hybrid and hybrid plug-in, gasoline full hybrid, conventional diesel and gasoline, and hybrid plug-in diesel and gasoline vehicles.

Vehicle	Energy (MJ/km)	CO ₂ (g/km)
EV	0.77	47.8
FC-HEV	0.73	48.4
FC-PHEV	0.77	49.5
HEV	0.58	37.7
ICEV Diesel	0.50	32.0
ICEV Gasoline	0.48	30.7
PHEV Diesel	0.70	43.8
PHEV Gasoline	0.70	43.7

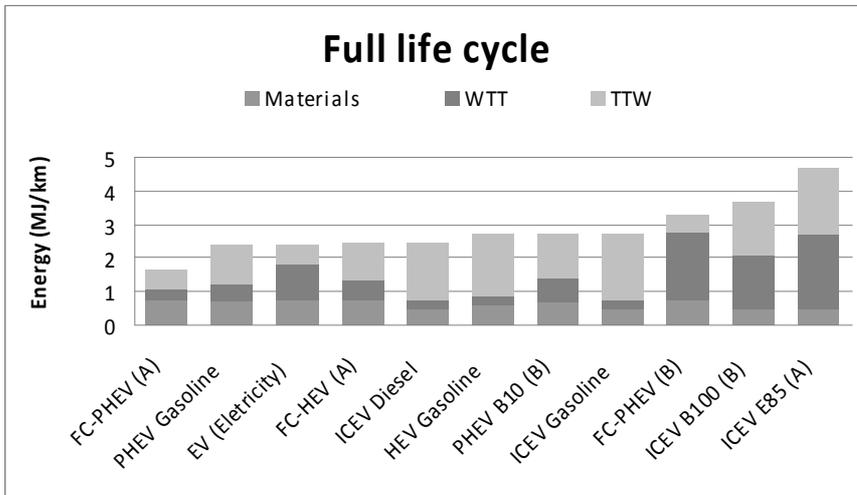


Figure 24- Full life cycle energy for selected vehicles (fuel cell hybrid plug-in, gasoline hybrid plug-in, pure electric, fuel cell hybrid, conventional diesel, gasoline full hybrid, B10 plug-in hybrid, conventional gasoline, conventional B100 and E85).

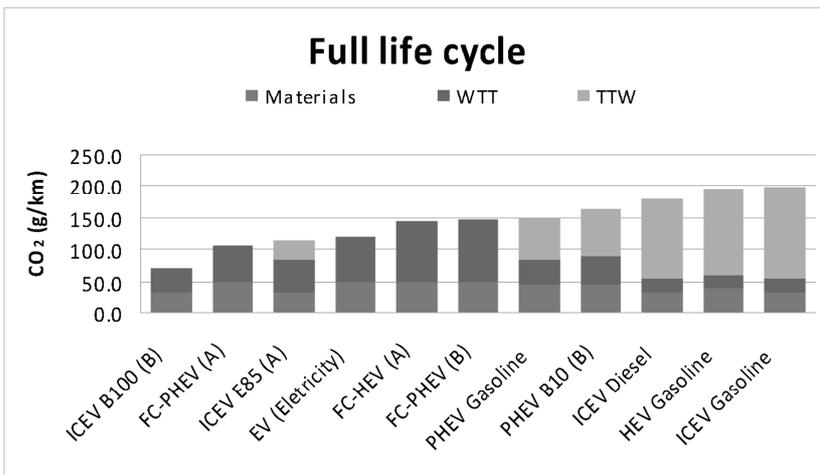


Figure 25- Full life cycle CO₂ for selected vehicles (same vehicles as fig.2).

2.4. Full life cycle of the light-duty fleet

For the TTW stage, the Portuguese fleet's annual energy consumption according to the vehicle type and the considered scenarios is presented in Table 12.

Table 12- Annual TTW disaggregated total fleet energy consumption (TJ) for the three scenarios.

Vehicle	Energy source	Scenarios (TTW)		
		1	2	3
Conventional	Gasoline/Diesel/LPG	155247	127506	93583
FC-PHEV	Hydrogen	2308	9231	16154
	Electricity	1447	5787	10127
FC-HEV	Hydrogen	3720	7440	11160
Total		162721	149964	131024

As expected, the conventional fuels consumption decreases along the three scenarios (from 7 to 44%) while the hydrogen and electricity consumption increases.

By analyzing Table 13, it is possible to conclude that the replacement of older vehicles by less polluting ones allows a significant reduction in terms of local pollution, with 27-77% reductions for CO, 35-85% for HC, 17-56% for NO_x and 17-60% for PM.

Table 13- Annual TTW local pollutants emissions for the considered scenarios.

Scenarios	CO (ton)	HC (ton)	NO _x (ton)	PM (ton)
Basecase	141	20	46	3
1	102	13	38	3
2	57	7	28	2
3	32	3	20	1

After combining the materials cradle-to-grave with the fuel TTW and WTT, the following energy and CO₂ emissions distributions were obtained (see Figure 26 and Figure 27).

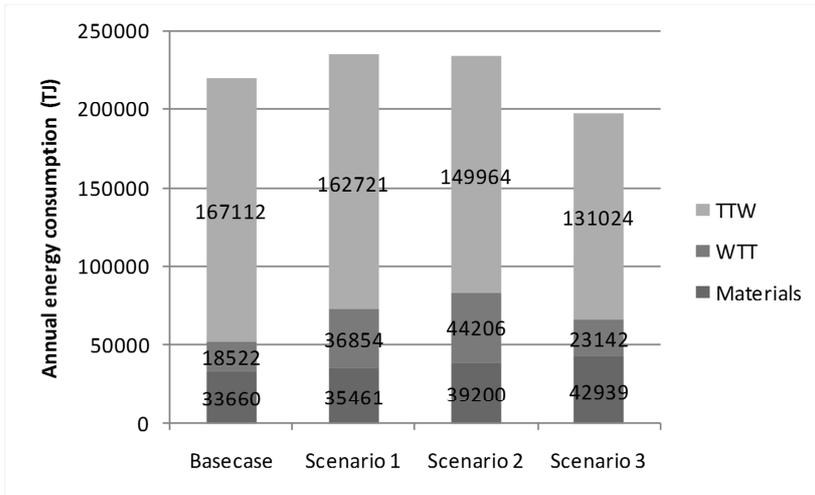


Figure 26- Annual fleet's life cycle results for materials, WTT and TTW regarding energy consumption in the considered scenarios.

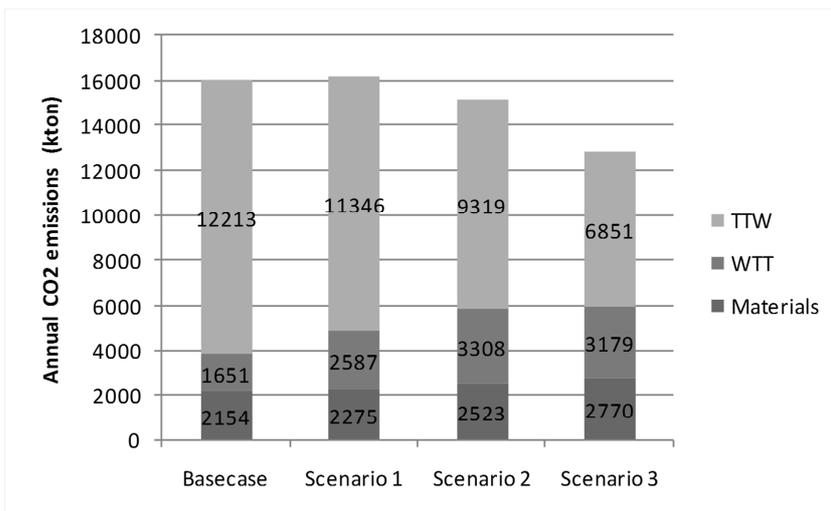


Figure 27- Annual fleet's life cycle results for materials, WTT and TTW regarding CO₂ emissions in the considered scenarios.

A clear shift from the magnitude of TTW to the WTT results is observed with the increasing penetration of hydrogen and electricity based vehicles. Additionally, as the number of these vehicles increases the materials stage also gains importance, since fuel cell vehicles manufacturing is more energy intensive.

In terms of the annual energy consumption it is clearly observed that scenarios 1 and 3, where on-site electrolysis is considered, present a 7 and 6% increase in the full life cycle analysis, while scenario 3 (based on centralized natural gas reforming) presents a 10% reduction. For CO₂ emissions, scenario 1 presents a 1% increase, while scenarios 2 and 3 present a 5 and 20% decrease correspondingly.

2.5. Energy and technology prices

Energy price evolution according to DGEG (Portuguese Energy Agency) [15] is as presented in Figure 28.

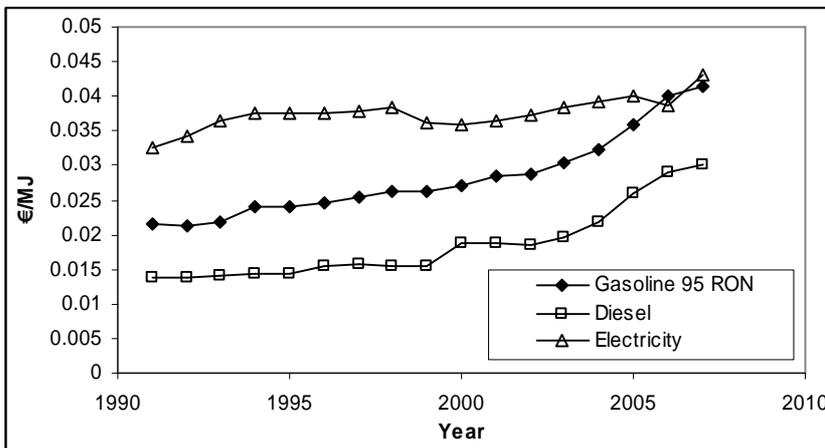


Figure 28- Energy price evolution (including all taxes, electricity is average domestic).

Regarding the average energy price in 2007, the expenses per travelled km (discarding maintenance costs) can be estimated as a function of hydrogen price. From Figure 29, assuming that the infrastructure is ready, it can be observed that a hydrogen price below 0.07 €/MJ is attractive comparatively to gasoline use. A hydrogen price below 0.05 €/MJ is attractive comparatively with diesel use and below 0.03 €/MJ is attractive even for gasoline hybrid plug-in users and pure electric vehicle users.

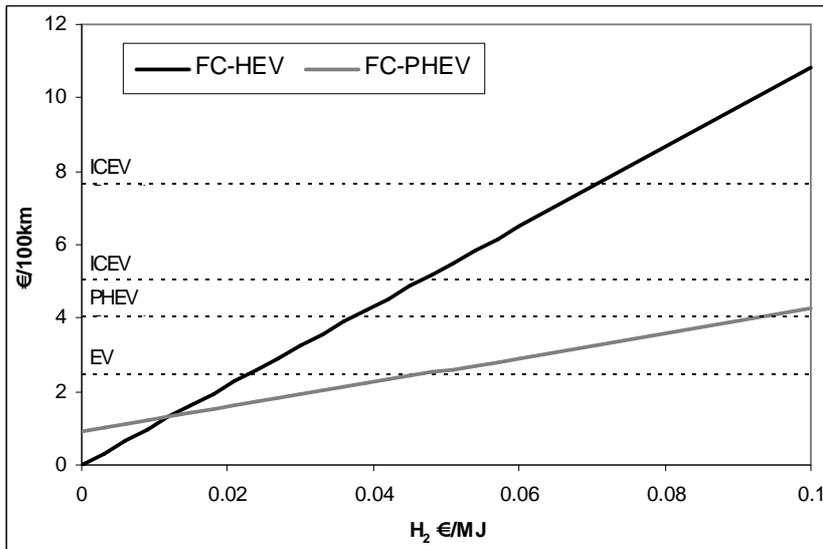


Figure 29- Refuelling cost evolution for fuel cell road vehicles as a function of hydrogen cost.

Other key aspect regarding user preference for fuel cell technology, besides fuel availability and price, is the acquisition cost. This reflects directly the manufacturing costs. Table 14 shows cost differences having ICEV gasoline as the base case, assuming the cost of 18600 € for the ICEV gasoline vehicle (base case) [12], a cost of 30 €/kW for engine plus transmission, a cost of 300 € for gasoline exhaust aftertreatment and 700 € for diesel with particle filter, a cost of 462 €/kWh [16] for the NiMH battery, a cost of 600 €/kWh for the Li-ion battery, a cost of 105 €/kW for the fuel cell stack, a cost of 27 €/kW for the electric motor plus controller and 1500 € for diesel direct injection system. To have a sense of how many km vehicles must be driven to compensate for initial purchase cost it were assumed the 2007 average energy prices and hydrogen price of 0.04 €/MJ. It is important to note that it is possible that a fuel cell cost will be comparable with internal combustion engine cost if sufficient market penetration and power density increase are attained [17].

Table 14- Cost differences in comparison with ICEV gasoline.

Vehicle	Cost difference (%)	km for breakthrough
ICEV Gasoline	0	0
ICEV Diesel	11	76593
FC-HEV	33	175989
PHEV Gasoline	45	228065
EV	59	209408
FC-PHEV	65	220900

This means that the fuel cell, hybrid plug-in and pure electric vehicles compensate in terms of cost only if long distances are driven (higher than 200000 km). This fact is important when calculating eventual tax incentives to purchase these kinds of technologies, having in mind that the final consumer is extremely sensitive to the “km for breakthrough”.

2.6. Conclusions

An extensive full life cycle vehicle technologies study was performed. The main focus was on fuel cell propulsion technology which is highly dependent on the hydrogen production pathway. The required energy and CO₂ emissions resulting from fuel cell production / assembly / dismantling / recycling are, respectively, 100 GJ and 6 ton (about 2 times higher than a conventional vehicle) and represent about 30% of total life cycle in 150000 km life. Concerning hydrogen production, on site electrolysis from European electric grid is the worst energy and CO₂ case scenario. In full life cycle analysis fuel cell vehicles with hydrogen from centralized reforming (series hybrid and plug-in series hybrid versions) emit less 20-40% CO₂ emissions than conventional vehicles.

Regarding the environmental impacts, hydrogen based vehicles fleet penetration have a clear advantage in terms of local air quality (up to 85% emission reductions of HC, CO, NO_x and PM). In terms of global environment impact (full life cycle of vehicle fleet), CO₂ emissions can be reduced by up to 44% when running the vehicles, but this percentage is only 20% if a full cradle-to-grave analysis is accounted for.

A hydrogen price below 0.07 €/MJ is attractive comparatively to gasoline use. A hydrogen price below 0.05 €/MJ is attractive comparatively with diesel use and below 0.03 €/MJ is attractive even for gasoline hybrid plug-in users and pure electric vehicle users. Fuel cell, hybrid plug-in and pure electric vehicles compensate in terms of cost only if long distances are driven (higher than 200000 km) unless exist tax incentives to purchase these kinds of technologies.

2.7. Abbreviations

TTW	Tank-to-Wheel part of fuel life cycle (use in the vehicle)
WTT station)	Weel-to-Tank part of fuel life cycle (production/distribution/storage at refuelling
CTG	Cradle-to-Grave materials life cycle (manufacturing/assembling/dismantling/recycling)
EV	pure electric Vehicle (runs only on electricity)
FC-HEV	Fuel Cell Hybrid Electric Vehicle
FC-PHEV	Fuel Cell Plug-in Hybrid Electric Vehicle
HEV	Hybrid electric vehicle
ICEV	Internal Combustion Engine Vehicle
B100	100% biodiesel
B20	mixture of 20% biodiesel and 80% diesel fuel
E10	mixture of 10% ethanol and 90%
E100	100% ethanol fuel
E85	mixture of 85% ethanol fuel with 15% gasoline fuel
PHEV	Plug-in Hybrid Electric Vehicle

2.8. Acknowledgements

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3. TAXI

3.1. Introduction

Over the last few years the idea of electrifying the transport sector has developed, mainly due to the possible penetration in the market of electrically powered vehicles such as hybrid electric vehicles (HEV), plug-in hybrid electric vehicles (PHEV) and full electric vehicles (EV).

The use of hydrogen allied to these solutions is also being considered. These technologies could provide solutions to reduce the dependency on fossil energy and to decrease CO₂ emissions [1]. This is especially true with the introduction of renewable sources in electricity generation and hydrogen production.

The methodology used to compare these different vehicle technologies analyzes the product's flows during its lifetime. That is to say that the LCA of a certain vehicle technology powered by a specific fuel must include in the fuel analysis not only its utilization stage related to driving the vehicle, Tank-to-Wheel (TTW), but also its production stage, Well-to-Tank (WTT), as well as the manufacturing, maintenance and recycling for the vehicle itself.

EV are defined as only being powered by a battery pack. Electrical energy is stored in the battery is discharged providing power to the electrical motor that then converts the electrical power into torque which in turn drives the vehicle wheels. On deceleration events typically 10% of rear braking energy is recovered (or 40% if front braking) and stored in the battery. The battery is depleted until it reaches a minimum state-of-charge (SOC), usually 20% to ensure correct battery functionality [4]. The TTW atmospheric pollutants can be considered to be zero.

HEV are powered by at least two sources, the primary power source is usually an internal combustion engine or a fuel cell and the secondary source is typically an energy storage device such as a battery.

PHEV are similar to the HEV but have the capability to recharge the battery from an external source. PHEVs are normally designed to use a charge depleting strategy for the battery (CD mode), discharging the battery until it reaches a minimum state-of-charge (SOC) that can be 30–45% [4] depending on battery and powertrain configuration. After reaching this minimum SOC, a charge sustaining strategy of the battery (CS mode) is employed. The additional power source is used to provide both propulsion and extend the range of the vehicle compared to an equivalent EV.

Regarding the battery packs for both PHEV and EV, the tendency is to use lithium based batteries[5]. In terms of braking energy, there is potential for a 10% recuperation of energy through rear braking or 40% with front braking.

In terms of energy source, if electricity powered vehicles are to succeed, a recharging infrastructure will have to be deployed. For hydrogen refueling, stations are required. Electricity and hydrogen are not a primary energy sources, but are energy carriers or vectors since they are produced using other primary energy resources. This results in global emissions associated to their production.

This work looks in detail at the application of a hydrogen fuel cell power system applied to the classic London Taxis. The project is being led by fuel cell developer Intelligent Energy (IE). This niche application in urban environments may be the starting point for a more widespread utilization of these types of alternative technologies. In this study, an ICE diesel vehicle, a plug-in hybrid electric fuel cell vehicle (PHEV-FC), a hybrid electric fuel cell vehicle (HEV-FC) and an EV are compared in terms of energy and emissions impacts. These are considered more efficient alternatives for this kind of fleet [6]. The results are also validated, qualitatively, with other studies in reference to different vehicle characteristics and emissions.

It is reasonable to assume that in the short to medium term, vehicles with alternative powertrains (PHEV-FC, PHEV, EV, HEV) will be more expensive than conventional ICE designs, although this cost difference would be expected to reduce as volumes increase and supply chains become more established

As an example, according to Concawe [7], fuel cell vehicles may present a 39% increase in the 2010 purchase price compared to conventional diesel vehicles if 2010 vehicle technologies are considered. As for EV (pure battery), in comparison to conventional ICE vehicles this difference may be even higher, reaching approximately 64%.

If future evolution is considered, based on mass production and expected learning curves, the price increase in 2030 may be reduced to around 40% for fuel cell vehicles and 17% for electric vehicles compared to the conventional diesel[8]. In terms of anticipated fuel costs, conventional diesel vehicles are likely to require higher running costs due to the link with the increasing price of crude oil. These values can be reduced in 2030 if fuel cell vehicles or electric vehicles are considered, by approximately 34% or 75%, respectively [8,9]. Similar results on the fuel cell vehicle and electric vehicle comparison were obtained by Thomas[10]. The expected future trend in the total ownership cost points to a convergence of these alternative technologies[11].

3.2. Methodology

3.2.1. Tank-to-Wheel

For simulating the daily commuting journeys of conventional and alternative vehicle technologies, ADVISOR vehicle simulation software [12] was used. Drive cycle specifications (see Figure 30 and Table 15) and vehicle specifications (Table 16) represent the principle inputs used. As a means to validate the simulation model, a simulation of the conventional ICE taxi over the NEDC emissions cycle was compared with Vehicle Certification Agency (VCA) Data.

For the hydrogen powered versions of the Taxi, the main technology of interest, due to the lack of experimental data and due to the specifications of the powertrain energy management, the software package Road Vehicle Simulation (RVS) [13] was also used for comparison purposes. RVS is an enhanced derivative of EcoGest [14] and is similar to ADVISOR. However, a database of input variables are globally available thus for example

facilitating ease of selection of alternative fuels (biodiesel, ethanol, natural gas, hydrogen, LPG), and providing generation of engine fuel consumption and emissions maps as required [15]. The main advantage is improved controllability and ease of programming new powertrain configurations and strategies. The uncertainty associated with these TTW simulation tools is typically less than 10% (on average 5%) for fuel consumption and CO₂ emissions of ICE vehicles [16,17] and less than 5% for electric and fuel cell vehicles[13].

In terms of the Taxi mobility characterization, the Taxi annual kilometers traveled considered is around 90000 km with an average passenger occupancy of 1.48 [18]. The driving conditions correspond to the PCO-CENEX London Taxi Drive Cycle [19] with zero gradient at an ambient temperature of 16°C and A/C off. PCO-CENEX London Taxi driving cycle (see Figure 30) was considered as a representation of the London Taxis’ driving conditions. It is composed of three distinct phases with different durations and average speeds, also including a key off period.

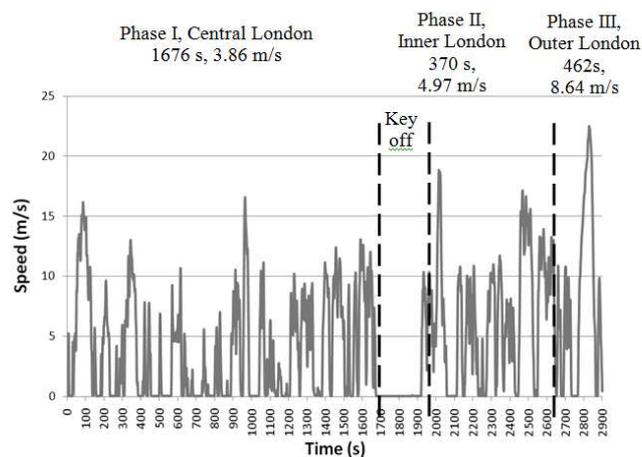


Figure 30 – Speed profile for the PCO-CENEX London Taxi driving cycle.

Table 15 shows the main drive cycle characteristics both for one cycle and for a daily usage pattern of around 251 km (according the annual typical Taxi usage).

Table 15 – Drive cycle main characteristics.

Driving Cycle	1 Cycle		Daily usage		Avg. Speed (km/h)	Abs. Avg. Accel. (m/s ²)	Additional load (kg)
	Time (s)	Distance (km)	Time (hours)	Distance (km)			
PCO-CENEX London	2900	13.3	15.0	251.6	16.5	0.53	150

Table 16 shows general vehicle characteristics. For the PHEV-FC, a daily recharging pattern is considered for electricity before the 15 hours of typical daily usage according to the PCO-CENEX cycle. For the electric battery discharging strategy of the hydrogen powered vehicles, three strategy options were studied, according to Figure 31.

Table 16 – Vehicle main specifications.

Vehicle	Data
Frontal area (m ²)	2.78
Drag coefficient	0.46
Tyre rolling radius (m)	0.325
Rolling coefficient	0.014 (Bosch, 2007)
Accessory Power [W]	1000
ICE Diesel Taxi	
weight (kg)	1895
ICE engine	
Peak power (kW) @rpm	75 kW @ 4000 RPM
Maximum Torque [N.m] @rpm	240 Nm @ 1800 RPM
Peak Efficiency %	41
Transmission	gear ratios: 3.00, 1.67, 1.0, 0.75, 0.67 final drive 4.1
Fuel cell Taxi	
Weight (kg)	2060
Hydrogen storage (kg)	3.73
Storage pressure (MPa)	35
Fuel cell	
Peak power (kW)	32
Limit of response (W/s)	±10000
Peak efficiency	61.6% @ 2.7 kW
Brushless PM Motor/Generator	
Peak power	100 kW @ 2000 to 4500 rpm
Motor continuous (kW)	100
Maximum Torque	550 Nm @ 0 to 1500 rpm
Peak efficiency (%)	92.5
Inverter/Controller (coupled)	
Standby power consumption (kW)	17
Peak efficiency (%)	97
Li-Polymer battery	
N ^{er} of modules	95
Capacity per module (Ah)	40
Nominal voltage per module (V)	3.7
Energy density (Wh/kg)	148
Coulombic efficiency	0.98

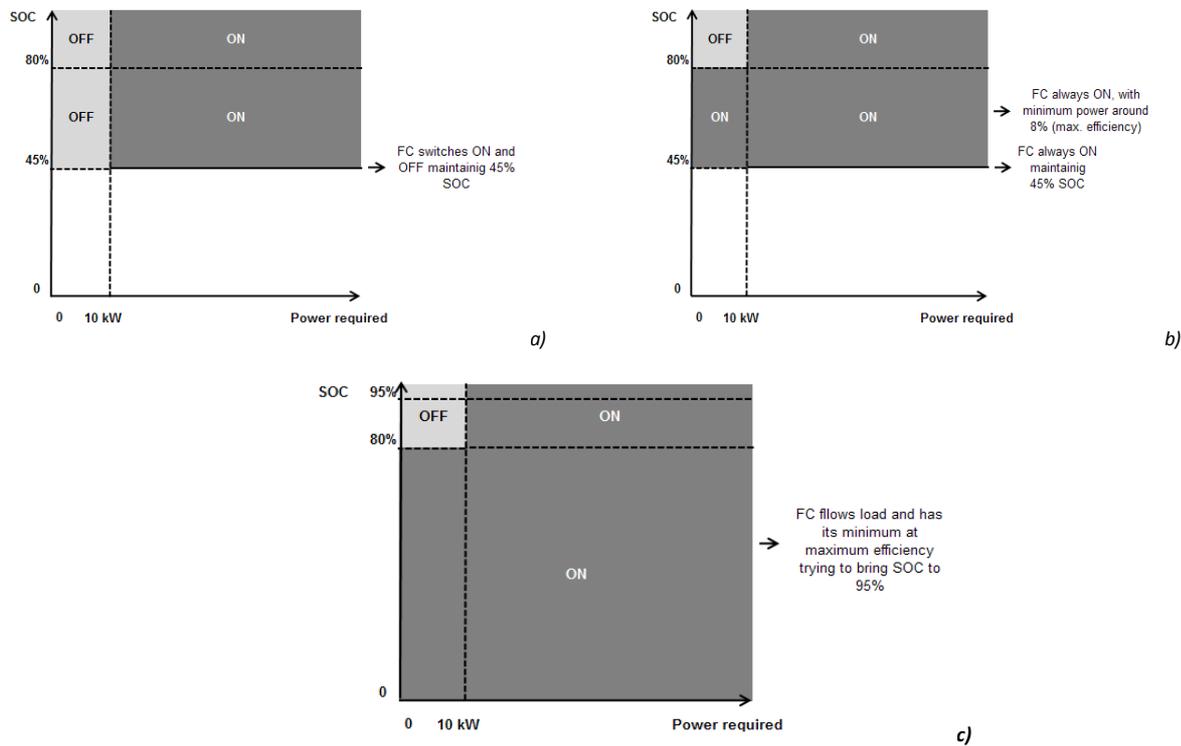


Figure 31 – Fuel cell discharging strategy: Strategy 1 (a), Strategy 2 (b) and Strategy 3 (c).

Strategy 1 considers the vehicle as a PHEV-FC. The fuel cell is OFF when the required power of the electrical motor is below 10 kW and ON above 10kW; when SOC reaches 45%, the fuel cell switches ON and OFF as required by the road load in order to maintain the minimum SOC (CS mode). This strategy was run with ADVISOR (PHEV-FC St. 1).

For Strategy 2 (also considering the PHEV-FC option), the fuel cell is only OFF above the 80% SOC and below the 10 kW power required; for other power and SOC combinations the FC is ON following load and in the maximum efficiency point (2.6 kW point, see Figure 31 b). Strategy 2 was run using both ADVISOR (PHEV-FC ADVISOR St. 2) and RVS (PHEV-FC RVS St. 2). The use of both software tools enabled the consideration of a different battery discharge algorithm (faster discharge), a different fuel cell delay in response (instantaneous versus a 3 second delay in ADVISOR) and slightly different transmission efficiency. With this procedure the influence of different strategies in output results can be observed.

Additionally, Strategy 3 considers the vehicle as a HEV-FC (see Figure 31 c), where the plug-in option is not available. The fuel cell is OFF above the 80% SOC and below the 10 kW power required, and in other situations the fuel cell follows the road load. The minimum operating point of the fuel cell is selected as its maximum efficiency point in order to minimise fuel use as the battery is charged at low road loads. This strategy was implemented with RVS software (HEV-FC RVS St. 3).

The energy storage information for the Fuel Cell Taxi is of 3.73 kg of stored hydrogen capacity at a pressure of 35 MPa.

In order to fulfill the 250 km of daily use, the EV has a 155.9 kWh lithium battery pack and a curb weight of 2834 kg. This configuration discharges the battery up to 20% SOC at the 250 km range of daily use and a recharging of the battery is considered necessary after a day of use. Additional electrical motor and battery pack specifications are as for the FC vehicle.

3.2.2. Well-to-Tank

Data from the UK Department of Energy and Climate Change [20], from the Eurostat [21] and from the Institute for Environment and Sustainability of the European Commission Joint Research Centre [7] was used for the well to tank analysis. The total energy of the WTT pathways (MJ_{ex}) does not include the energy content of the produced fuel, so WTT only includes the energy used to provide the fuel to the vehicle tank.

For the diesel vehicle (defined as D) a reference value for the WTT for Europe was assumed [7]. The diesel WTT accounts for: crude extraction and processing, crude transport, refining, distribution and dispensing (see Table 17).

Table 17 – Fuel pathways with uncertainty range in brackets.

Fuel	Pathways designation	Process	Energy (MJ _{ex} /MJ _{fuel})	CO ₂ (g/MJ _{fuel})
Diesel [17]	D	Extraction & Processing	0.03	3.7
		Transport	0.01	0.9
		Refining	0.10	8.6
		Distribution & Dispensing	0.02	1.0
		Total pathway	0.16 (0.14-0.18)	14.2 (12.6-16.0)
Electricity UK	E (A)	UK-mix power generation	1.69	149.4
		Distribution	0.08	0
		Total pathway	1.77	149.4
Electricity EU	E (B)	UK-mix power generation	1.84	120.8
		Distribution	0.03	0
		Total pathway	1.87	120.8
Gaseous hydrogen	NG (A)	Extraction & Processing	0.04	1.6
		Transport 1000 km-4000 km pipeline	0.08	4.0
		Distribution	0.01	0.7
		Central Reforming	0.32	73.7
		Gaseous H ₂ distribution & compression	0.22	8.5
		Extraction & Processing	0.04	1.6
		Total pathway	0.67 (0.62-0.71)	88.7 (85.0-91.9)
Liquid hydrogen	NG (B)	Extraction & Processing	0.04	1.6
		Transport 1000 km-4000 km pipeline	0.08	4.0
		Distribution	0.01	0.7
		Central Reforming	0.32	73.7
		H ₂ Liquefaction	0.67	37.4
		Liquid H ₂ distribution & delivery	0.04	2.8
		Extraction & Processing	0.04	1.6
		Total pathway	1.16 (0.88-1.35)	120.4 (91.1-139.4)

The WTT analysis was performed for electricity using 2008 UK data [20] (defined as E(A)) and for reference, values for Europe [7] (defined as E(B)). For UK specific data, the grid distribution losses, the electricity generation efficiencies and generated CO₂ were included in the analysis [20]. The grid distribution losses are on average 7.6% [20]. CO₂ emissions in 2008 are reported to be 497 t/GWh [20]. The final energy and CO₂ emissions WTT factors for the UK are as presented in Table 17.

Assuming implementation of the UK's proposed strategy for increasing renewable energy sources in its electricity generation mix, the energy and CO₂ emissions WTT factors for electricity will decrease in the foreseeable future. UK goals aim at achieving 32% of

renewable energy sources in 2020 in their electricity generation mix compared to the present 5%. This translates to an expected reduction of 44% of CO₂ emissions from electricity generation in 2020 compared to 2008 (300 g/kWh in 2020 compared to 540 g/kWh in 2008) with this increasing to 90% in 2030 (50 g/kWh instead of 540 g/kWh) [22].

For the hydrogen energy pathway, centralized natural gas reforming is assumed since this is the expected hydrogen pathway for the London Taxi demonstration project. As a hydrogen infrastructure develops, other solutions may be widely deployed such as integrating the use of renewable energy resources in electrolysis processes, reducing consequently the WTT energy needs and emissions associated with the hydrogen production [7].

Specific data for UK concerning natural gas origin (considering 99% share of compressed natural gas, CNG, via pipeline and 1% liquefied natural gas, LNG, via ship in UK [20] and reference values for Europe were considered [7].

Two pathways were designed, one considering gaseous hydrogen (CH₂) using a local pipeline network (50 km average distance) and compression to 88 MPa at the refueling station, named NG(A), and another considering liquid hydrogen (LH₂) where liquid hydrogen is transported to the refueling station by road tanker, designated NG(B) (see Table 17).

Minimum and maximum values for each process of WTT were considered from [7]. Table 17 shows the final values for WTT and respective uncertainty.

3.2.3. Materials Cradle-to-Grave

The Materials Cradle-to-Grave (CTG) life-cycle analysis refers to the full life cycle of the vehicle. It includes the vehicle assembling, the maintenance during its lifetime and finally the dismantling and recycling processes of the vehicle. The materials life-cycle energy consumption and emissions are spread along the vehicle expected lifetime. For this study, the GREET software [23] from the US Argonne National Laboratory was used. This software has two units, one dealing with the fuel life cycle (GREET 1.7) and the other

dealing with the materials life cycle (GREET 2.7). This latter was adapted for applicability in Europe, with this then used for the UK case.

Data from the GREET software [24] of the US Argonne National Laboratory was used in addition to data from IEA [25]. The total energy and CO₂ emissions of the Materials Cradle-to-Grave pathways were distributed along the vehicles' lifetime kilometers travelled. GREET 1.7 has as an input the electricity generation mix accordingly to the European reality, dominated in 2008 by coal (27.4%), followed by nuclear (25.3%), natural gas (21.7%) and others (25.6%)[25]. This electricity mix is used in GREET 2.7 calculations for the energy use and pollutant emissions related to materials used in the manufacture of the vehicle. Due to a significant UK import rate of the different components of the vehicle, the European electricity generation mix can be considered appropriate.

The vehicle's powertrain system and weight and other information on fluids and vehicle composition and the desired lifecycle (see Table 18 and Table 19) were used in the enhanced GREET 2.7 in order to obtain the energy consumed and the pollutants emissions for the considered life cycle.

Table 18 – Weight (kg) of components for the three vehicle technologies considered.

Components	Vehicle technology		
	ICEV	FCV	EV
Total Vehicle Weight (kg)	1895	2060	2834
Vehicle Components Weight, kilos (excluding battery, fluids, and fuel) (kg)	1851	1917	1746
Battery Weight (kg)	Lead-Acid	12	10
	Li-Ion	-	108

Table 19 – Vehicle Components Composition (% by wt) for the three vehicle technologies considered.

Vehicle Components Composition (% by wt)	Vehicle technology		
	ICEV	FCV	EV
Powertrain System	12.7%	4.2%	0.0%
Transmission System	5.9%	2.6%	2.9%
Chassis (w/o battery)	28.7%	30.5%	32.1%
Traction Motor	0%	2.7%	3.0%
Generator	0%	0.0%	0.0%
Electronic Controller	0%	2.4%	2.6%
Fuel Cell Auxiliary System	0%	4.7%	0.0%
Body: including BIW, interior, exterior, and glass	52.8%	52.9%	59.4%

One important aspect concerning materials cradle-to-grave is the average period between exchange for several vehicle components and consumables. The chosen values in agreement with the lifetime of the vehicles are presented in Table 20. Around 563250 km (350000 miles) was assumed for the Taxi lifetime which corresponds to an average of around 90000 km (56000 miles) per year.

Most of the values used for the servicing intervals were an average between maximum and minimum values recommended by certified car brands [26,27] for similar powertrains. Fuel cell system related servicing periods are recommended by IE and the Lead-Acid and Li-ion batteries by the respective manufacturers. In terms of maintenance, the same components were considered between the different vehicles with the exception of engine oil (only used in ICEV), powertrain coolant (ICE and FC), and Li-ion battery (used only in FCV and EV). As for the specific fuel cell characteristics, the fuel cell stack powertrain systems weights 80 kg while the fuel cell auxiliary systems weights 90 kg.

The Materials CTG uncertainty is mainly due to variance of the inputs concerning the replacements of the consumables of the vehicle. A tire replacement period of 25000 miles (40234 km) and 40000 miles (64374 km) for front and rear tires respectively was assumed. However, if the front tire can be used in the rear after the 40234 km range, the number of pneumatics replacement decreases to 9 for the consider life of the vehicle.. For the lead-acid batteries considered, minimum and maximum values of 500 to 1000 charge/discharge cycles were assumed [5]. Li-ion batteries have a maximum lifecycle of near 2000 cycles based on an average value from several commercial brands [28] and a minimum value of 1000 cycles [4]. The lifetime of fuel cell stacks, according to Ballard, varies from 5000 hours for passenger vehicles to 20000 hours for buses. For the taxi application, an average value of 11220 hours (2 substitutions), with a minimum of 8415 hours (3 substitutions) and a maximum of 16830 hours (1 substitution), was assumed. The replacement of the remaining consumables relies on the servicing schedule as defined by a similar powertrain. Maximum and minimum values recommended for maintenance are listed below in Table 20.

Table 20 – Range of the number of replacements and corresponding kilometers in brackets.

Components	Vehicle technology		
	ICEV	FC	EV
Pneumatics	9-14 (24140-37551)		
Lead-acid battery	2-4 (187757-112654)		
Engine oil	70-116 (4828-8047)	-	-
Transmission oil	5-11 (93878-48280)		
Brakes oil	3-5 (140818-93878)		
Wind shield fluid	10-30 (51206-18170)		
Powertrain Coolant	3-5 (140818-93878)		-
Li-ion battery	-	1-2 (281635-187756)	
FC	-	1-3 (281635-140818)	-

3.3. Results

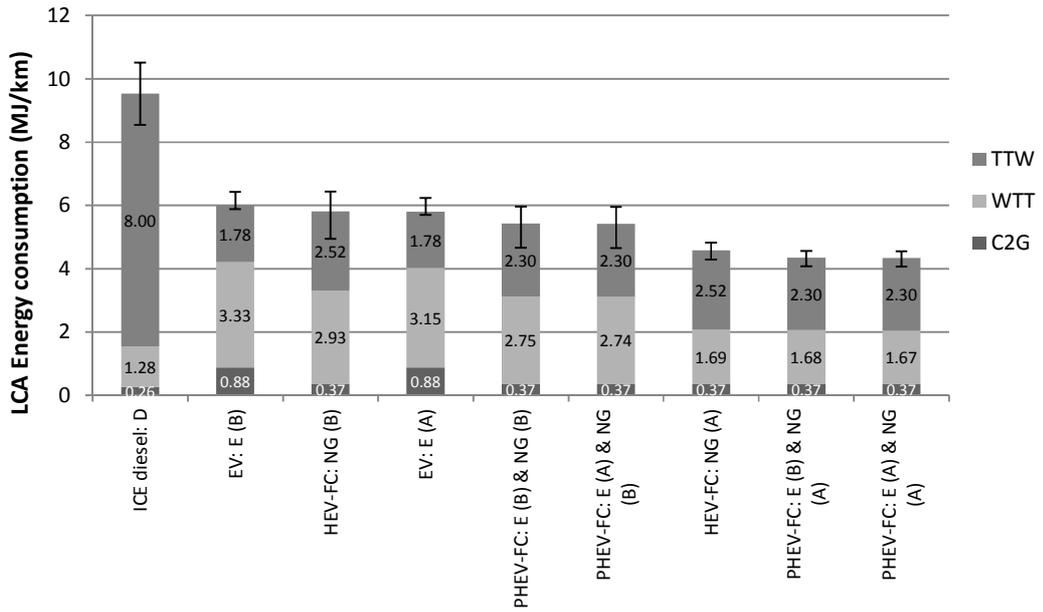
All the TTW, WTT and CTG results were combined in order to obtain the full Life-Cycle results for the selected technologies. Table 21, Table 22 and Figure 32 present the energy consumption and CO₂ emissions results for the LCA analysis in the PCO-CENEX London driving cycle.

Table 21 – Summary of energy consumption results in a full Life-Cycle analysis in the PCO-CENEX London driving cycle.

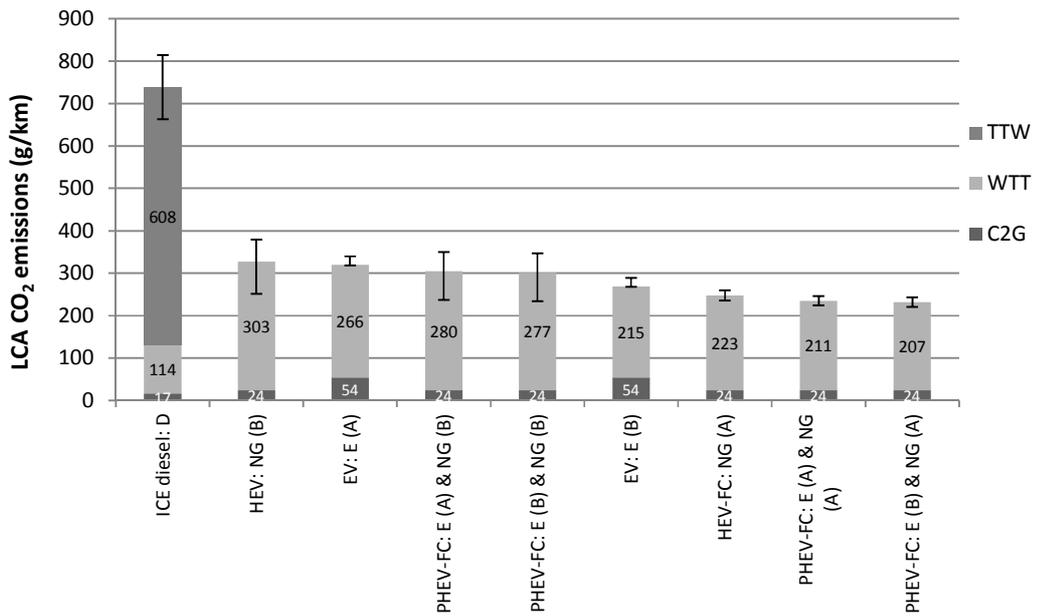
Taxi		Energy source pathway	TTW Energy consumption (MJ/km)			WTT Energy expended (MJ _{expended} / km)			CTG Energy consumption (MJ/km)			Full LCA Energy consumption (MJ/km)		
			av.	min.	max.	av.	min.	max.	av.	min.	max.	av.	min.	max.
Diesel		D	8.00	7.20	8.80	1.28	1.12	1.44	0.26	0.23	0.27	9.54	8.55	10.51
Fuel Cell	PHEV-FC Advisor St. 1	E (A) & NG (A)	2.52	2.39	2.65	1.81	1.68	1.90	0.37	0.34	0.39	4.70	4.41	4.94
		E (A) & NG (B)				2.99	2.31	3.44	0.37	0.34	0.39	5.88	5.04	6.48
		E (B) & NG (A)				1.82	1.69	1.91	0.37	0.34	0.39	4.71	4.42	4.95
		E (B) & NG (B)				3.01	2.32	3.45	0.37	0.34	0.39	5.90	5.05	6.49
	PHEV-FC Advisor St. 2	E (A) & NG (A)	2.52	2.39	2.65	1.81	1.68	1.90	0.37	0.34	0.39	4.70	4.41	4.94
		E (A) & NG (B)				2.99	2.31	3.44	0.37	0.34	0.39	5.88	5.04	6.48
		E (B) & NG (A)				1.82	1.69	1.91	0.37	0.34	0.39	4.71	4.42	4.95
		E (B) & NG (B)				3.01	2.32	3.45	0.37	0.34	0.39	5.90	5.05	6.49
	PHEV-FC RVS St. 2	E (A) & NG (A)	2.30	2.19	2.42	1.67	1.54	1.74	0.37	0.34	0.39	4.34	4.07	4.55
		E (A) & NG (B)				2.74	2.12	3.14	0.37	0.34	0.39	5.41	4.65	5.95
		E (B) & NG (A)				1.68	1.55	1.75	0.37	0.34	0.39	4.35	4.08	4.56
		E (B) & NG (B)				2.75	2.13	3.15	0.37	0.34	0.39	5.42	4.66	5.96
HEV-FC RVS St. 3	NG (A)	2.52	2.39	2.65	1.69	1.55	1.78	0.37	0.34	0.39	4.58	4.28	4.82	
	NG (B)				2.93	2.21	3.39	0.37	0.34	0.39	5.82	4.94	6.43	
Electric Vehicle		E (A)	1.78	1.69	1.87	3.15	3.15	3.15	0.88	0.86	1.22	5.81	5.70	6.24
		E (B)				3.33	3.33	3.33	0.88	0.86	1.22	5.99	5.88	6.42

Table 22 – Summary of CO₂ emissions results in a full Life-Cycle analysis in the PCO-CENEX London driving cycle.

Taxi		Energy source pathway	TTW CO ₂ emissions (g CO ₂ /km)			WTT CO ₂ emissions (g CO ₂ / km)			CTG CO ₂ emissions (g CO ₂ / km)			Full LCA CO ₂ emissions (g CO ₂ / km)		
			av.	min.	max.	av.	min.	max.	av.	min.	max.	av.	min.	max.
Diesel		D	608.0	547.2	668.8	113.6	100.8	128.0	17.0	15.2	18.0	738.6	663.2	814.8
Fuel Cell	PHEV-FC Advisor St. 1	E (A) & NG (A)	0	0	0	230.1	221.2	238.0	24.3	21.4	28.3	254.4	242.6	266.3
		E (A) & NG (B)				306.5	236.0	352.4	24.3	21.4	28.3	330.8	257.4	380.7
		E (B) & NG (A)				226.9	218.0	234.8	24.3	21.4	28.3	251.2	239.4	263.1
		E (B) & NG (B)				303.3	232.8	349.3	24.3	21.4	28.3	327.6	254.2	377.6
	PHEV-FC Advisor St. 2	E (A) & NG (A)	0	0	0	230.1	221.2	238.0	24.3	21.4	28.3	254.4	242.6	266.3
		E (A) & NG (B)				306.5	236.0	352.4	24.3	21.4	28.3	330.8	257.4	380.7
		E (B) & NG (A)				226.9	218.0	234.8	24.3	21.4	28.3	251.2	239.4	263.1
		E (B) & NG (B)				303.3	232.8	349.3	24.3	21.4	28.3	327.6	254.2	377.6
	PHEV-FC RVS St. 2	E (A) & NG (A)	0	0	0	210.6	202.5	217.7	24.3	21.4	28.3	234.9	223.9	246.0
		E (A) & NG (B)				280.0	215.9	321.8	24.3	21.4	28.3	304.3	237.3	350.1
		E (B) & NG (A)				207.4	199.3	214.6	24.3	21.4	28.3	231.7	220.7	242.9
	HEV-FC RVS St. 3	E (B) & NG (B)	0	0	0	276.9	212.8	318.6	24.3	21.4	28.3	301.2	234.2	346.9
NG (A)		223.4				214.1	231.6	24.3	21.4	28.3	247.7	235.5	259.9	
NG (B)		303.3				229.5	351.3	24.3	21.4	28.3	327.6	250.9	379.6	
Electric Vehicle		E (A)	0	0	0	265.9	265.9	265.9	53.9	52.7	74.1	319.7	318.5	339.9
		E (B)				215.0	215.0	215.0	53.9	52.7	74.1	268.9	267.7	289.1



a)



b)

Figure 32 – Summary of full LCA energy consumption a) and CO2 emissions b) for the ICE diesel, PHEV-FC RVS, HEV-FC RVS and EV vehicles technologies in the PCO-CENEX London Taxi driving cycle.

The PCO-CENEX London driving cycle is a very aggressive driving cycle resulting in the highest TTW energy consumption value per kilometer for the ICE diesel (22.8 L/ 100 km or 8.00 MJ/km). By introducing the PHEV-FC technology, the London Taxi TTW energy consumption can be reduced up to 3 to 4 times and local (TTW) CO₂ emissions can be eliminated.

For the Fuel Cell Taxi case, all strategies present very similar results both in terms of hydrogen and electricity consumption in MJ/km (2.30 or 2.52 MJ/km). The representation of the SOC along the PHEV-FC Taxi daily usage for the PCO-CENEX London driving cycle is presented in Figure 33a. For the PHEV-FC Taxi, ADVISOR with Strategy 2 leads to a faster SOC depletion, while ADVISOR Strategy 1 allows a slower SOC depletion. RVS using Strategy 2 reveals a slower SOC depletion. As expected HEV-FC Taxi option (HEV-FC St. 3) maintains the SOC at approximately 80%.

The same analysis along the PCO-CENEX London driving cycle was performed comparing the accumulated fuel cell hydrogen consumption for the three strategies (see Figure 33 b), where naturally the HEV-FC Taxi produces a steeper consumption gradient than the PHEV-FC options.

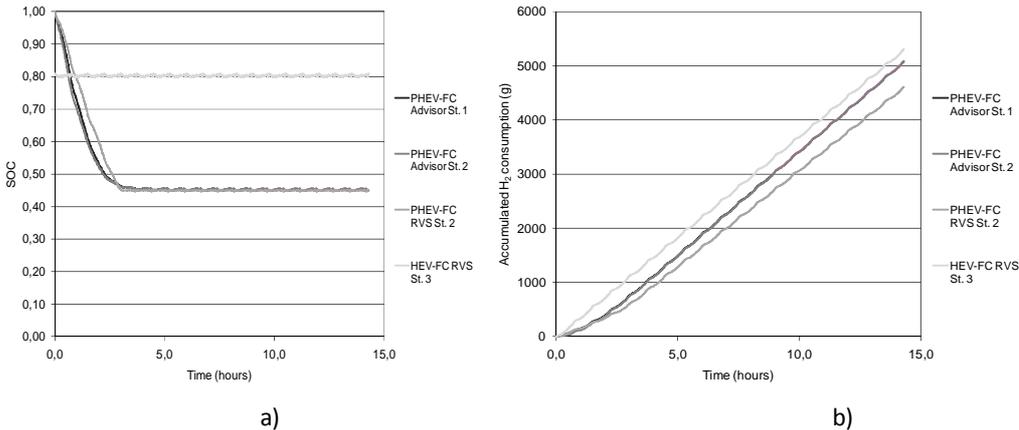


Figure 33 – a) SOC evolution and b) accumulated hydrogen energy consumption for the three tested fuel cell discharging strategies along the 250 daily km.

Considering the derived hydrogen consumption data and the Taxi hydrogen storage capacity (see section 3.2.1), the vehicle is usually required to refill once a day during its typical utilization. Additionally, for the PHEV-FC, the electricity recharging time for the different discharging strategies varies from 2.8 to 3.2 hours.

A considerable amount of weight and volume must be added to the vehicle if an EV version of the Taxi is to be considered (c.a. 38% weight addition) in order to maintain the daily usage patterns of the vehicle and a final battery SOC of 20%, to minimise excessive battery degradation. Even with this increased weight, the EV TTW energy consumption shows favorable results due to its high efficiency (average efficiency for EV is 77% compared to 40% for the PHEV-FC). However, one point of note is that the vehicle requires a charging point of 14 kVA in order to recharge the battery in under 9 hours (a charge time of greater than 9 hours exceeds the 24h per day of combined driving and charging).

Analysing the WTT results, the ICE diesel vehicle has the lower energy and CO₂ emission per km, followed by fuel cell technologies and, finally, by the EV. The fuel pathway energy efficiency is on average 86% for diesel, 53% for hydrogen and 35% for electricity. The WTT element of the vehicle fuel life-cycle represents 14-54% of total WTW energy consumption.

When the TTW results are combined with WTT in order to provide WTW results, the diesel vehicle technology has the highest energy and CO₂ emissions values. Both fuel cell Taxi technologies with compressed hydrogen from centralized natural gas reforming have a combination of lowest energy and CO₂ values. The EV vehicle WTW has similar results to the Fuel Cell options

The PHEV-FC vehicle technology using compressed hydrogen presents the lowest combined WTW results both for energy and CO₂ emissions. Using liquefied hydrogen, independently of the vehicle technology, presents higher energy and CO₂ emissions WTW results. It is interesting to note that CO₂ emissions of fuel cell technologies have the best WTW scores, around 207 to 210 g/km, despite having zero local CO₂ emissions.

As for the Materials CTG, vehicle components and fluids have the most significant contributions to the ICE diesel Materials CTG energy consumption (70 and 17% for each

respectively). If a FC vehicle is considered, a shift from fluids to batteries is observed with the vehicle components maintaining the 70% proportion of energy expenditure and batteries increasing to 24%. In the case of the EV Taxi, a complete shift is observed with batteries being responsible for around 74% and vehicle components decreasing to 23%. Comparatively, the ICE diesel presents the lower CTG result closely followed by the FC vehicle. As for the EV Taxi the inclusion of a large battery pack has negative consequences for both CTG energy consumption and CO₂ emissions results, with the resulting impact much worse than the other two vehicle technologies. The uncertainty of CTG was obtained mainly due to variance of the inputs concerning the replacement of vehicles consumables. The EV Taxi presents a larger variance due to the fact that when doubling the battery replacement another battery is included, which greatly increases the maximum possible value.

Considering a full LCA analysis, combining TTW, WTT and Materials CTG, the hydrogen powered vehicle configurations have lower results both for energy and CO₂ emissions. Compared to the ICE Diesel, both the FC vehicle and the EV present the potential of reducing the full LCA by around 37-55% and 55-69% for energy consumption and CO₂ emissions respectively. Globally, the Fuel Cell vehicle powered by compressed hydrogen presents lower results (4.34 to 4.71 MJ per km and 235 to 254 g per km for energy and CO₂ in a full LCA). Comparing the PHEV-FC and the HEV-FC, these present very similar results with the HEV version slightly higher (4.58 MJ per km and 248 g per km for energy and CO₂ in a full LCA).

If the 2020-2030 trend on decarbonization of UK electricity power sector is considered, a shift from natural gas reforming to electrolysis to produce hydrogen is appropriate, in order to converge to a more efficient and sustainable pathway. In this scenario of decarbonization, the full LCA CO₂ emissions of each technology would be reduced to 82 to 94 g/km for fuel cell vehicles and to 77 to 99 g/km for the EV in 2030. These considerations confirm that the hydrogen option for the Taxi is a valid alternative solution to be used in urban environments in

the near future, particularly when considering the rapid refuelling capability which may prove imperative for some applications

Analyzing the disaggregated results between TTW, WTT and CTG the shifts in energy consumption and emissions are clear. The ICE Diesel TTW accounts for 84% and 82% energy and CO₂ emissions respectively of the full LCA, hence choosing a FC vehicle Taxi reduces the importance of TTW to 54%/0% (energy/CO₂) and in case of an EV to 56%/0% (energy/CO₂). The WTT importance in the ICE Diesel LCA shifts to higher values in the alternative powertrains, from 13%/15% to 51%/94% (energy/CO₂) for the FC vehicle and 56%/83% (energy/CO₂) for the EV, since the energy consumption is transferred from the transportation sector to hydrogen or electricity production sectors. In terms of Materials CTG, the ICE Diesel CTG is only accountable for 3%/2% (energy/CO₂), while in the FC vehicle and EV those values rise to 7%/8% and 15%/20% (energy/CO₂) respectively.

WTW results of the comparison between diesel vehicle and hybrid fuel cell vehicle are qualitatively in accordance with European studies [7,29]. The LCA, including the CTG, is qualitatively in accordance with the Greet 2.7 report results [23]

3.4. Conclusions

A full Life Cycle Analysis of possible alternative vehicle technologies for the traditional London Taxi was performed regarding its energy consumption and CO₂. A plug-in hybrid electric fuel cell vehicle, a hybrid electric fuel cell vehicle and an EV were considered as alternatives to the traditional ICE diesel London Taxi.

The PHEV-FC Taxi resulted in the lowest LCA energy consumption and CO₂ emissions values with a reduction of 55% and 69% respectively when compared to the original ICE diesel Taxi. The HEV-FC achieved reductions of 52% and 39% respectively of energy consumption and the EV Taxi achieved reductions of 67% and 64% of CO₂ emissions..

In the TTW stage, the PHEV-FC and the HEV-FC vehicle found to be 71% and 69% more efficient than the ICE diesel Taxi, whilst the EV achieved the lowest TTW energy consumption with a reduction of 78% compared to the ICE diesel Taxi variant. In terms of the WTT stage, the hydrogen production pathway accounts for 30% more energy than the

Diesel pathway whilst the electricity production was responsible for the highest energy consumption (more than double that of the diesel pathway).

It is worth highlighting the importance of the hydrogen and electricity production pathways. If increased renewable energy resources are included in the electricity generation mix or alternative processes using renewable energy resources are used for hydrogen production, the WTT factors and consequently the LCA results may be improved.

Considering the obtained energy consumption and the daily Taxi service requirements, the HEV-FC is required to refill once a day, the PHEV-FC requires an additional 2.8 hour electricity recharge time, and the EV Taxi needs 9 hour recharge time due to its large battery pack (155.9 kWh) or alternatively requires a 14 kVA charging point.

The results demonstrate that a hydrogen powered solution for the conventional London Taxis, can be a sustainable alternative in a full life-cycle framework with further improvement potential if the UK decarbonisation trend is followed. If this demonstration project proves to be successful, it could be a first step to a more widespread use in urban environments of these alternative vehicle technologies and energy sources.

3.5. Abbreviations

CD	Charge depleting
CH ₂	Compressed hydrogen
CNG	Compressed Natural Gas
LH ₂	Liquefied hydrogen
LNG	Liquefied Natural Gas
CS	Charge Sustaining
CTG	Cradle-to-Grave
EV	Full Electric vehicle (Battery vehicle)
FC	Fuel Cell

FCV	Fuel Cell Vehicle
ICE	Internal Combustion Engine
ICEV	Internal Combustion Engine vehicle
IE	Intelligent Energy
LCA	Life Cycle Analysis
MJ _{ex}	Energy expended in a process discounting the energy of final fuel
OEM	Original equipment manufacturers
PCO-CENEX	London Taxi driving cycle
PHEV	Plug-in Hybrid Electric Vehicle
HEV	Hybrid Electric Vehicle
PHEV-FC	Plug-in Hybrid Electric Fuel Cell vehicle
HEV-FC	Hybrid Electric Fuel Cell vehicle
RVS	Road Vehicle Simulator
SOC	State-of-Charge of the battery
TTW	Tank-to-Wheel
VCA	Vehicle Certification Agency
WTT	Well-to-Tank
WTW	Well-to-Wheel

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4. BUS

4.1. Introduction

Fossil fuels remain the dominant sources of primary energy worldwide. Since 2010 more than a third of the primary energy was derived from oil, and around 62% of the final energy consumption is associated to the transportation sector [1]. In Europe, in the European Union member countries (EU-27) in particular, the transport sector represented approximately 33% of the total energy consumption and was responsible for about 24% of CO₂ emissions in 2011 [2]. Environmental and sustainability issues associated to the oil extraction and use, including the growing economic and political disputes surrounding this energy source, has warned the international community to the importance of the research for new solutions to the mobility sector. Given that, governments have been introducing a large number of policies and measures across all modes in an effort to improve efficiency of energy use. European decision makers have established political goals in order to address these complex issues. Kyoto protocol, 2003/30/EC European, 20-20-20 targets [3] are some examples of a global trend to diminish emissions from the transportation sector that is under effect.

4.1.1. Hybrid and Plug-In vehicles

In order to comply with the established targets, to reduce the energy consumption and CO₂ emissions, new fuels as well as the respective production pathways improvement and new vehicle technologies become extremely important to study. Some solutions regard technology improvements like hybrid electric vehicles (HEV), plug-in hybrid electric vehicles (PHEV), pure battery electric vehicles (BEV) and fuel cell vehicles, and new energy sources like biofuels (e.g. ethanol, biodiesel, and methanol), natural gas, biogas, electricity and hydrogen. In this framework, with the growing importance of sustainability policies, the automotive industry is experiencing the gradual penetration of alternative technologies and fuels. Vehicle electrification enables the improvement of urban air quality (no local emissions), the diversification of primary energy sources (electricity can be generated from a wider range of sources, not necessarily with fossil origin), and allows the use of technologies that may improve energy-efficiency (such as regenerative braking and low consumption electric driven components). The BEV is a full electric vehicle which has a rechargeable battery providing its power and energy. A problem with the BEV

is its short range (all-electric range, AER). The HEV uses energy provided by a combustion engine or by a fuel cell, in addition with an energy storage system (usually the battery). The battery in a HEV is used to better control the energy flow and is usually useful in improving the vehicle's efficiency when compared to the majority of the conventional powertrains. However, most of the efficiency gains in hybridizing a vehicle are modest and rivals with some of today's state-of-the-art diesel technologies.

The PHEV combines HEV with a BEV configuration, since it is possible to use the battery energy in a pure electric locomotion, and when needed it uses the fuel converter to achieve higher power or to extend the vehicle range (and then working like an HEV). In the PHEV the batteries can be recharged directly from the fuel converter or from an external electric supply [4], [5].

Goncalves G. et al. [6] monitored and simulated a fuel cell transit bus. In Wipke K. et al. [7] one of the most used vehicle simulators is presented, the ADVISOR, which is capable to model different types of conventional and alternative powertrains in specific driving conditions. Using this software, Ribau J. et al. [8] analyzed different kinds of FC-PHEVs and BEVs, namely, motorcycles, buses, and light duty vehicles. The performance of several battery types in hybrid vehicles is of great importance and was studied by Burke A. et al. [9]. Moreover, the environmental impact of the battery production was addressed by McManus M. C. [10]. Additionally, the different fuel converters for HEVs were also studied by Ribau J. et al. [5].

The implementation of new technologies for road vehicles such as HEVs and PHEVs depend not only on the public acceptance, but also on the involved logistics for energy distribution. Petrol and diesel logistics problems are solved, but not for electricity supply, required by the PHEVs and BEVs (that need an electricity socket to charge the battery) nor alternative fuels like hydrogen (for fuel cell vehicles). Therefore, a way to boost the alternative vehicle penetration in the transportation sector is to develop fleet implementation projects, since in a fleet (like a taxi fleet or a post fleet) the travelling routes and the infrastructures are better defined than in a personal vehicle. Moreover, the initial investment for alternative technologies can be directly transformed in energy savings (and pollutant emissions reduction), and more important in cost reductions in fuel for the fleet owner.

Fuel cell and plug-in hybrid public transit buses can take advantage of well-defined duty cycles and a fixed fuel and maintenance infrastructure that facilitates the working schedule and refueling of the bus. Buses also allow more space for propulsion system and fuel storage. An example of the

implementation of fuel cell buses was explicit in the Project Clean Urban Transport for Europe (CUTE) [11].

Additional advantages of the PHEV powertrains were studied by Al-Alawi and Bradley [12]. They calculated the relative value that PHEVs can have in reducing an automaker's costs for CAFE compliance.

4.1.2. Optimization of alternative vehicles

In a hybrid powertrain, component sizing and energy management strategy significantly affects vehicle performance, cost and fuel economy. The ability to integrate the optimization of the energy management control system with the sizing of key hybrid powertrain components presents a significant area of research, since optimizing the vehicle's powertrain design can greatly improve the vehicle efficiency and cost. In some cases, when companies acquire their vehicles (e.g. postal fleets, public transportation, services fleets), little efforts are made to adopt optimized vehicle powertrains resulting in the use of vehicles that are usually oversized regarding the real purpose and requirements. In order to minimize the CO₂ emissions produced in the vehicle operation or indirectly by the fuel supply, Stockar S. et al. [13] developed an optimal supervisory control for the energy management of a PHEV using the Pontryagin's minimum principle. In [14] a real-time power splitting method for a FC-PHEV was also developed addressing different driving conditions and aiming to minimize the fuel consumption and to preserve the battery life. Light-duty vehicles are generally the main object of the optimization, however bus optimization can be found in Gao D. et al. [15] which optimized a FC-HEV regarding its energy management strategy aiming to minimize the fuel consumption. Also with the same optimization purpose Desai C. et al. [16] and Ribau J. et al. [17] optimized an HEV bus, however, besides the energy management strategy the component sizing optimization was also performed. In Ribau J. et al. [17], besides fuel consumption, the powertrain cost minimization was also an objective for optimizing a FC-HEV, in real and synthetic driving cycles. Regarding also both component design and energy management strategy optimization in FC-HEVs, stochastic dynamic programming algorithm can be an option to perform the sizing of the fuel cell and battery aiming to minimize the fuel consumption [18]. Also to optimize a FC-HEV Sorrentino M. et al. [19] used parametric and heuristic methods coupled with cost and components weight models. In [20] the effect of the battery size and optimal power split policies are analysed in order to quantify the energy losses and the hydrogen consumption a FC-HEV.

Focusing on the powertrain sizing, many optimal design algorithms have been used to design the powertrain of different vehicle topologies (series, parallel, series/parallel). However the majority of those techniques rely on parametric design optimization. The design variables can be the nominal power of components, number of energy storage cells, or even design characteristics of the transmission or final drive, that are optimized between a given range of options. Aiming to minimize the fuel consumption of a HEV Gao W. et al. [21] optimized the number of battery cells, fuel converter and electric motor nominal power, and final drive ratio using four different methods, genetic algorithm (GA), DIRECT, particle swarm optimization (PSO), and simulated annealing algorithms. Similarly Xudong L. et al. [22] implemented a hybrid method using quadratic programming and GA to optimize the fuel converter power, generator, electric motor torque, and the battery module number and capacity. Regarding similar parameter optimization Wu X. et al. [23] used the parallel chaos optimization algorithm to achieve the minimal drivetrain cost of a PHEV. Also aiming to minimize the cost of the drivetrain, Hegazy O. et al. [24] optimized the size of the fuel cell and ultracapacitor with PSO and GA algorithms. Also using genetic algorithms for the components sizing, Jain M. et al. [25] performed a multi-objective optimization of a FC-PHEV with an electrolyser aiming to reduce the fuel consumption and the weight of the vehicle, and additionally performed a cost analysis. Both FC-HEV and FC-PHEV powertrains are regarded in studies from the author Melo P. et al [26] and Ribau J. et al. [27]; where a transit bus and a taxi vehicle, respectively, were optimized using single and multi-objective metaheuristic optimization, aiming cost and fuel consumption minimization, simulated in official and real driving cycles. In Ribau J. et al. [27] the all-electric range of the PHEV taxi was also maximized. Ribau J. et al. [28] compared heuristic and metaheuristic optimization methods regarding FC-PHEV taxi powertrain cost. Also using an heuristic method Xu L. et al. [29] optimized a fuel cell bus and performed on-road testing, aiming to reduce the cost and improve the performance of the vehicle.

4.1.3. Life cycle analysis

The implementation of alternative technologies in the transport sector aims to increase the efficiency of the vehicle itself but also the vehicle environmental impact. One important tool to evaluate a vehicle utilization impact, including the energy used, is the life cycle analysis (LCA) methodology. Regarding the fuel life cycle (fuel production and utilization in the vehicle), also known as Well-to-Wheel (WTW) analysis, Ferreira A. et al. [30] and Ribau J. et al. [31] studied

alternative hydrogen fuel production pathways, and the energy consumption and CO₂ emissions associated to the fuel production and use in the fuel cell vehicles is evaluated. A detailed WTW analysis for several alternative fuels and powertrains can be found in Concawe [32], and the impact of the penetration of such alternative technologies in Silva C. [33]. More specifically, in China, about 40 alternative fuels were studied regarding the respective energy intensity and Greenhouse gas emissions (GHG) [34]. Regarding WTW analysis and the vehicle's materials life cycle (Cradle-to-Grave, CTG), a FC-HEV taxi vehicle was analyzed by Baptista P. et al. [4]. In Bartolozzi I. et al. [35] life cycle assessment was used to evaluate and compare the environmental impacts of the alternative scenarios for the hydrogen production pathways, and also to analyse the influence of electric vehicles. Also considering WTW and CTG, Silva C. et al. [36], studied the analysed of internal combustion engine powered PHEVs. A detailed WTW and CTG analysis for several vehicle technologies can be found in Kromer M. et al. [37]. A WTW evaluation and a first approach in vehicle optimization using an heuristic method was made by Ribau J. [38] where a HEV and a PHEV taxi were optimized aiming the powertrain downsizing, and simulated in official and real driving cycles.

4.1.4. Proposed approach

This study highlights the significance of the driving conditions and the conflict between the optimization of investment cost, efficiency and LCA impact in powertrain design optimization of FC-HEV and FC-PHEV city buses in analyzing their advantages relatively to conventional diesel buses.

A single-objective (minimization of cost, fuel or LCA CO_{2eq}) and multi-objective genetic algorithms (minimization of the couples cost and fuel, cost and LCA CO_{2eq}, fuel and LCA CO_{2eq}), linked with the vehicle simulation software ADVISOR[7], are used to perform the powertrain components optimization.

The suitability of Europe Transient Driving Cycle for heavy-duty vehicles (ETC), a combined urban and extra-urban driving cycle, for urban Oporto city bus optimization problem is discussed as well as optimized fuel cell buses advantages regarding conventional diesel buses. Potential financial savings are assessed for the alternative vehicle solutions.

The fuel cell buses are based on the chassis of a Mercedes-Benz Citaro bus [11]. A real driving cycle measured in the city of Oporto (*PortoDC*) is used, as well as the reference ETC. Optimal

configurations are discussed and proposed, and compared to a reference conventional transit bus and a direct fuel cell bus.

4.2. Methodology

Two different types of passenger buses are considered as reference vehicles in order to compare the optimization results: a conventional internal combustion engine powered bus (ICEV bus), and a direct fuel cell powered bus (DFCV bus), and its specifications are based on the HYFLEET:CUTE project [11], and in [6] (Table 23). Table 24 shows the performance of the reference vehicles in the real measured and standard driving cycles simulated in ADVISOR platform.

Table 23- Reference bus main characteristics

		ICEV bus	DFCV bus
Diesel engine	Nominal Power (kW @ rpm)	210 @ 2200	--
	Max. Torque (N.m @ rpm)	1120 @ 1200-1800	--
AC Electric motor	Nominal Power (kW @ rpm)	--	200 @ 2100
	Max. Torque (N.m @ rpm)	--	1050 @ 800
Fuel Cell	Nominal Power (kW)	--	250 (30 power dump)
Auxiliaries (W)		9000 mechanical	17000 electrical
Volume (length/height/width) (m)		12.11 / 3.12 / 2.55	12.11 / 3.67 / 2.55
Curb weight (kg)		11460	14200

Table 24- Reference buses LCA and cost data, and performance in ETC and PortoDC driving cycles. Diesel fuel is used in ICEV (0.840 kg/l, 42.8 MJ/kg), and hydrogen (23.36 g/l, 120 kJ/g) is used in DFCV.

	ETC						PortoDC						Performance		Cost (\$ 1000)
	Energy Consumption (MJ/km)			CO ₂ eq emissions (g/km)			Energy Consumption (MJ/km)			CO ₂ eq emissions (g/km)			Max. Speed (km/h)	Time (s) 0-50km/h	
	TTW	WTT	LCA	TTW	WTT	LCA	TTW	WTT	LCA	TTW	WTT	LCA			
ICEV	10.50	1.68	12.32	931.2	149.1	1088.3	26.40	4.22	30.80	2341.3	374.9	2724.2	88.10	10.20	8.500
DFCV	9.20	7.22	17.38	0	639.0	703.8	22.40	17.58	40.90	0	1555.9	1620.6	93.40	16.40	34.805

A FC-HEV and a FC-PHEV, based on the frame of the reference DFCV bus in Table 23, are optimized considering a range of different components of the powertrain. In Table 24 the powertrain cost is associated to the Original Equipment Manufacturer (OEM) cost of the engine, transmission, and exhaust for ICEV [32], and to the fuel cell system and electric motor and controller for the DFCV. The cost range for the DFCV has into consideration one replacement of the fuel cell during the vehicle lifetime ([39], [40]).

In the DFCV vehicle the torque and speed is transmitted to the wheels by a final drive connected to an electric motor, whose power and energy are supplied directly by the fuel cell. Similarly to the

DFCV, the traction of a FC-HEV vehicle is provided by an electric motor; however, besides the fuel cell a battery pack can also supply power to the vehicle (Figure 34) in a *series* configuration.

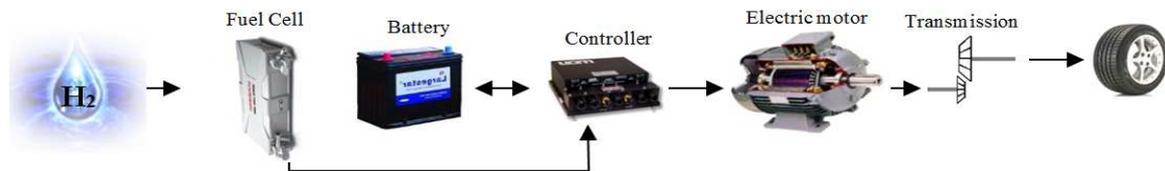


Figure 34- Basic configuration of a fuel cell series hybrid powertrain.

The configuration in *series* is based on the fact that all the traction power to the wheels is provided by one source of mechanical power, in this case an electric motor which is fed by the fuel cell and by the battery. The objective of the battery in a hybrid vehicle is to operate like a buffer between the main power/energy supply (in this case the fuel cell), and the power demand (the electric motor in a *series* configuration). The battery besides delivering power and energy can also store it. If for any reason the fuel cell produces more energy than required by the electric motor, the excess energy can be stored in the battery. Moreover, this function can also be used to control the fuel cell energy flow operation aiming to increase its efficiency, controlling its power rate and its ON/OFF threshold. The battery pack allows in some events for the fuel cell to operate in lower power rates or in high efficiency modes and compensate the power required by the electric motor. Depending on the battery power and energy capacity the battery can in some cases supply enough power to the vehicle allowing the fuel cell to be off for a limited time. However, in a hybrid vehicle the battery cannot be fully depleted and its energy level (state-of-charge, SOC) should be kept above a certain level (charge sustaining level, CS) (Figure 35). Therefore the fuel cell is used to help propulsion and to provide additional energy in order to maintain the battery SOC. Additionally, when the vehicle is decelerating (and braking), the electric motor can immediately operate as a generator and convert the mechanic energy in the wheels into electric energy storing it in the battery.

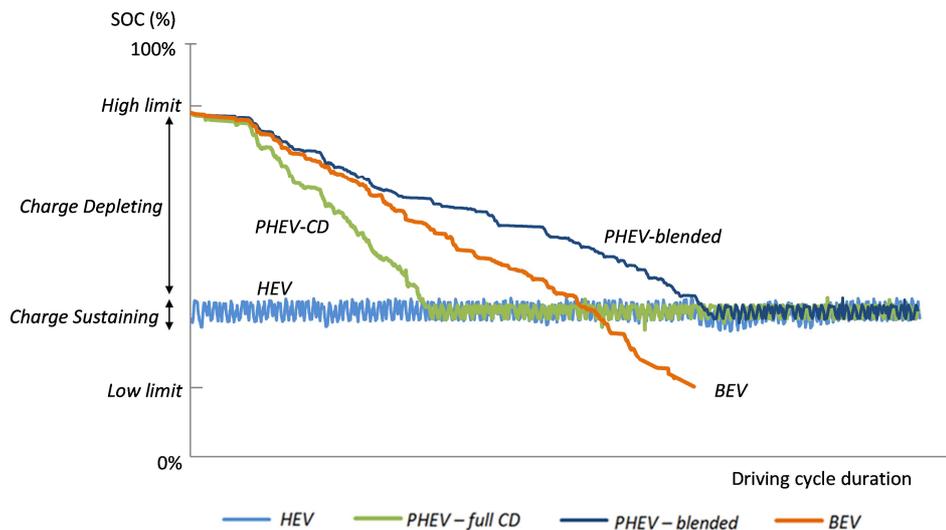


Figure 35- Examples of different battery usage strategies for pure battery electric vehicle (BEV), hybrid (HEV), and plug-in hybrid vehicles (PHEV), highlighting battery's charge depleting (CD) and sustaining (CS) zones. (Source: Own data.)

The default control strategy for the fuel cell powertrains used in this study is the "thermostat" strategy implemented in ADVISOR [7], where the fuel cell turns on when the SOC reaches the low limit point (low SOC) of the charge sustaining range, and turns off when the SOC reaches the high limit point (high SOC). The fuel cell is used to produce electricity for the propulsion power and for the battery, to maintain the battery state-of-charge. The fuel cell power rate is also dependent on the SOC target. The SOC target used in this study was 40% (CS level), and the high and low SOC limits selected were 45% and 35% respectively (Charge Sustaining range in Figure 35). In this strategy the fuel cell has a limit for the minimum operation power of around 10% its nominal power, allowing the fuel cell when ON to deliver power at a minimum of 50% of efficiency. Note that the battery has also operating limits (Low limit and High limit in Figure 35) which constraints the energy capacity due to physical and safety properties of the battery pack.

A PHEV has the particularity of having two operation modes: CD (charge depleting) and CS. In CS mode the vehicle operates similarly to a HEV as described earlier. In CD mode the use of battery power is the priority and therefore a full electric operation can be used like a pure battery electric vehicle, where only electricity is used (in Figure 35 this option is represented as PHEV- full CD). Nevertheless, some plug-in vehicles have the option to use the fuel converter in the CD mode in order to help the propulsion system in more demanding power events or to slow down the battery depletion, being known as blended mode (represented in Figure 35 as PHEV- blended). Unlike the HEV, the PHEV battery can be recharged by an external source of electricity. This allows the use of

a wide range of the battery capacity in the CD mode. In general, the CS mode is only engaged when a specified battery state-of-charge is achieved (CS level).

In this study a PHEV with full electric CD operation is regarded, and the distance travelled using electric power only is designated as all-electric range (AER). In Figure 35 an example of the PHEV, HEV, and BEV operation modes are shown.

4.2.1. Hybrid vehicle components

In order to perform the vehicle powertrain optimization different components were taken as a possible hypothesis: 4 different proton exchange membrane fuel cell models (FC), 4 electric motors (MC, including controller), and 8 batteries (BAT) were available in this study, and are presented in Table 25-Table 27.

Table 25- FC models. (source: [4], [6], [11], and [41])

	FC_1	FC_2	FC_3	FC_4
Nominal power (kW)	32	50	120	250
System weight (kg)	170	223	706	1470

Table 26 - MC models. (source: [6], [11], and [42]). ^aPermanent Magnet ^bInduction.

	MC_1	MC_2	MC_3	MC_4
Nominal power (kW)	104 ^a	145 ^a	200 ^b	240 ^b
System weight (kg)	102	66	171	200

Table 27- Battery models. (source: [43], and [44]) ^aLithium ion. ^bNickel-metal hydride

	BAT_1	BAT_2	BAT_3	BAT_4	BAT_5	BAT_6	BAT_7	BAT_8
Nominal voltage (V)	3.6 ^a	3.6 ^a	3.6 ^a	3.7 ^a	12 ^b	6 ^b	12 ^b	6 ^b
Low/High limit voltage (V)	2.5/4	2.5/4	2.5/4	2.7/4.2	10.3/14	10.3/14	10.3/14	10.3/14
Energy capacity (Ah)	7	20	30	40	34	68	100	200
weight (kg)	0.37	0.8	1.1	1	9	9	18.6	18.6

Besides the model selection of the fuel cell and the electric motor, the power scale for each component is also an important parameter considered in component sizing. The software ADVISOR has a scaling function that sizes the component regarding its nominal power, as also its weight accordingly to the scaling value Melo P. et al. [26]. A scaling range between 0.5 and 3 is used (a value of 1 represents the original component as in Table 25-Table 27). For example, if a scaling value of 0.5 is selected for a specific component model it means that the component is downsized to 50% of its original capacity; on the other hand, the maximum scaling value of 3 means that the component has its capacity and power sized to 3 times more its original characteristics. Power scaling is not considered for the battery; however the number of battery

modules is a variable parameter in the vehicle design. The battery's SOC charge sustaining level was maintained 40% for both FC-HEV and FC-PHEV.

A OEM cost for each component was estimated and used to attribute a "virtual" cost to the designed vehicle's powertrain. The costs estimated (Eqs. (1) to (4)) were based in several cost analysis studies which assumed large volume production scale ([32], [37], [40], [45], [46], [47], [48] and [49])

From the previous studies the main data for each component were collected: nominal power, energy capacity (battery), mass, and cost. The respective data for each component were plotted in a scatter diagram indexed by the variables of cost and specific power (kW/kg) of the component. For the battery, the same method was performed but for the variables of cost and power/energy capacity rate (kW/kWh). The data was analyzed and the best fitted trend was used in this study.

$$FC^{cost}(\$) = P (159 (P/m_{FC}) + 33) (REP + 1) \quad (1)$$

$$MC^{cost}(\$) = P (20 (P/m_{MC}) + 0.25) \quad (2)$$

$$BAT_{Lithium}^{cost}(\$) = E (368 |\ln(P/E)| + 177) (REP + 1) \quad (3)$$

$$BAT_{NiMh}^{cost}(\$) = 0.8 E (368 |\ln(P/E)| + 177) (REP + 1) \quad (4)$$

Where *Li* and *Nimh* regard to the battery chemistry, Lithium or Nickel-metal hydride, and *P*, *m*, and *E* to power (kW), mass (kg), and energy capacity (kWh) respectively.

It is known that the fuel cell and specially the battery had a limited lifetime that usually is less than the vehicle itself. The lifetime expectancy varies with the component, from which many published values aren't in accordance ([37], [39], [40]). Therefore, in this study one replacement (*REP*) is accounted for the fuel cell and for the battery, attempting to highlight an additional impact of those components in the vehicle powertrain. No influence of the replacement and maintenance of the components were accounted, neither the incremental efficiency degradation. The cost estimations (Eqs. (1) to (4)) although optimistic are in agreement with the large scale production estimations for alternative technologies. In [39] estimations indicates that the cost of fuel cell systems can be expected to decrease by 78%/kW (in short term) and component costs for batteries by 48%/kWh by 2020, due to economies of scale (1 million fuel cell vehicles in the EU by 2020) and incremental improvements in technology and production facilities. Nevertheless, the cost optimizations results should maintain their relation between the different solutions.

4.2.2. Driving cycles

A real driving cycle was used for which data were measured within the city of Oporto (*PortoDC*) metropolitan area, by using a speed sensor, a GPS system equipped with a barometric altimeter and data recovery from the OBD (On-Board Diagnostic) vehicle interface [6]. Additionally, an official driving cycle was also used, the ETC (European Transient Cycle) for heavy duty vehicles [50]. Both cycles are present in Table 28 and Figure 36. The synthetic driving cycle, ETC, is clearly very different than the real driving cycle which will allow to achieve distinct results in different driving conditions. The *PortoDC* is a urban bus route, with more stops and idle time, higher average acceleration but lower speeds, throughout a very shorter distance. The road grade, measured in *PortoDC*, is also an important property. Note that the speeds achieved in ETC are representative of extra-urban events.

Table 28- Driving cycle characteristics.

Driving cycle	Time (s)	Distance (km)	Average speed (km/h)	Max. speed (km/h)	Average acceleration (m/s^2)	Max. acceleration (m/s^2)	# stops	Idle time (s)
<i>PortoDC</i>	2138	7.67	12.91	54.0	0.52	2.5	29	621
ETC	1799	29.48	58.97	91.1	0.20	3.83	4	75

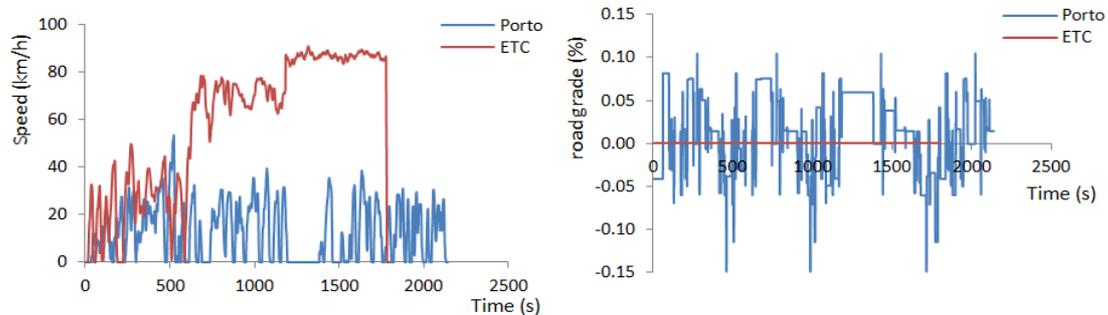


Figure 36- Speed (left) and road grade (right) profile of the official driving cycle ETC (red) and real driving cycle *PortoDC* (blue).

4.2.3. Life Cycle Analysis

A LCA methodology implies analyzing a product's flows during all its lifetime, since it is produced, to its utilization and its end-of-life, including its recycling process. Regarding the vehicle life cycle analysis, it can be divided in the fuel life cycle and the vehicle materials life cycle, i.e., three major stages: fuel production, distribution and storage, Well-to-Tank (WTT), fuel use in the vehicle, Tank-to-Wheel (TTW), and materials production, vehicle assembling, maintenance, dismantling and

recycling, CTG. The majority of the research works focuses on the WTW part of the vehicle life cycle, on energy use and GHG or CO₂ equivalent emissions ([51] and [52]). In this study the powertrain component sizing is the goal, so we consider important to cover also the materials CTG impact. The fuel consumption is a good indicator of the efficiency of the vehicle and the life cycle CO_{2eq} an indicator of the environmental impact of the vehicle itself and its use. The boundaries of the LCA can be found in Figure 37. Components sizing has potential impact on bus hydrogen consumption due to weight implications and on CTG impact.

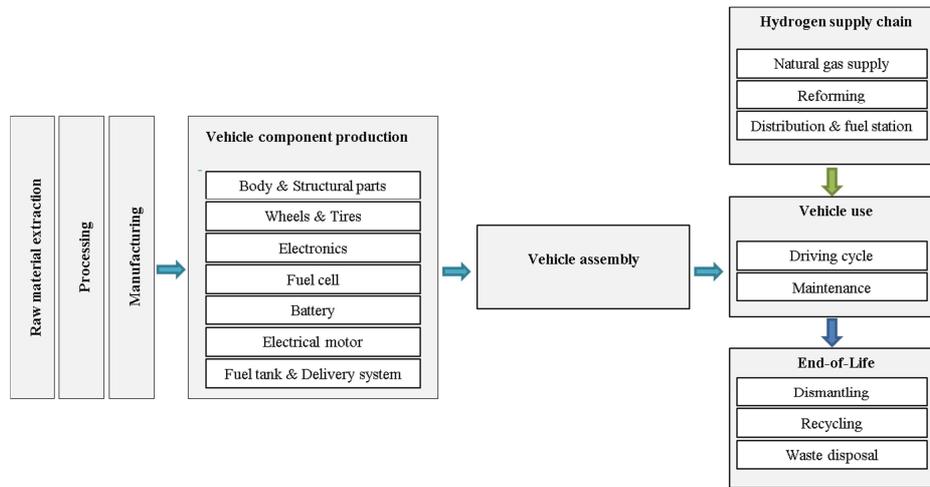


Figure 37- Life cycle stages simplified flow chart applied to a bus lifetime. Functional unit: MJ or grams of CO_{2eq} per lifetime km, if energy or emissions is regarded. (Source: Own data.)

Eq. (5) resumes the life cycle calculations for the energy use and CO_{2eq} emissions in fuel WTW and material CTG stages.

$$\begin{cases} LCA \text{ energy use } \left(\frac{MJ}{km} \right) = \left\{ WTT \left(\frac{MJ_{exp}}{MJ_{final}} \right) * TTW \left(\frac{MJ}{km} \right) + TTW \left(\frac{MJ}{km} \right) \right\}^{WTW \text{ stage}} + CTG \left(\frac{MJ}{lifetime \text{ km}} \right) \\ LCA \text{ CO}_{2eq} \left(\frac{g \text{ CO}_{2eq}}{km} \right) = \left\{ WTT \left(\frac{g \text{ CO}_{2eq}}{MJ_{final}} \right) * TTW \left(\frac{MJ}{km} \right) + TTW \left(\frac{g \text{ CO}_{2eq}}{km} \right) \right\}^{WTW \text{ stage}} + CTG \left(\frac{g \text{ CO}_{2eq}}{lifetime \text{ km}} \right) \end{cases} \quad (5)$$

4.2.4. Tank-to-Wheel

The TTW stage corresponds to the energy utilization during the vehicle operation namely to the fuel/electricity directly consumed by the vehicle and the emissions from the vehicle's tailpipe. In the ICEV bus only diesel fuel is regarded as energy source, and in the DFCV and FC-HEV buses the

hydrogen fuel is the only energy source. In the plug-in option, the FC-PHEV bus, the energy source is hydrogen fuel and electricity from the grid (external source).

The daily travelled distance for the bus was estimated from STCP [53] and CUTE [11] having an average value of 132.6 km per day (*lifetime km*). In the FC-PHEV bus, it was assumed that one battery charge is made per day, meaning that of the 132.6 km, there is a distance, AER, in which the vehicle is using only electric power.

In the TTW stage a clear comparison between the vehicle technologies is done, namely their efficiency in energy conversion and driving performance. In order to evaluate the vehicles in the TTW stage, a vehicle simulation software is used, ADVISOR [7]. This software, developed by NREL, uses a combined backward-forward approach that enables the software to model advanced batteries and powertrain components while maintaining a relatively fast simulation speed. It has been demonstrated in the research community as a reliable tool for studying energy consumption and vehicle performance and for testing energy-related control schemes ([5] and [7]).

4.2.5. Simulation tool validation

As a mean to validate the simulation model for this work, a simulation of the DFCV bus (Table 1) over the *PortoDC* real driving cycle was compared to the published results in Gonçalves G. et al. [6], since both the vehicle and the driving cycle were based on the CUTE project [11]. Using the same vehicle mass to perform the validation (16000 kg), a relative error of 0.32% was achieved between the simulation model used in this study (1562.93 g of hydrogen consumed) and the results measured in Gonçalves G. et al. [6] for the same vehicle and driving cycle (1567.95 g of hydrogen consumed).

Drive cycle specifications and vehicle specifications (Table 15 and Table 16) represent the main inputs in this software. In this study the simulations are performed in two different driving cycles, the real measured driving cycle, *PortoDC*, and the official European driving cycle for heavy duty vehicles, ETC.

4.2.6. Fuel cycle (Well-to-Tank and Well-to-Wheel)

The WTT stage in the life cycle refers to the extraction and production, distribution, and storage of the fuel or energy itself, and is used to account the energy consumption and CO_{2eq} emissions associated in those processes.

The total energy of the WTT pathways (MJ) does not include the energy content of the produced fuel (or energy), so WTT only regards the energy used (consumed) to provide the fuel to the vehicle tank.

The energy sources evaluated in the WTT stage for this study, are: diesel for the ICEV bus, hydrogen for the fuel cell buses (DFCV, FC-HEV, FC-PHEV), and electricity only for the FC-PHEV.

The diesel WTT factor is estimated by CONCAWE [32] and per 1 MJ of diesel produced 0.16 MJ is expended in the WTT stage and 14.2 g/MJ of CO_{2eq} emitted (0.16 MJ_{exp}/MJ_{final diesel} and 14.2 gCO_{2eq}/MJ_{final diesel} respectively).

The electricity production in Portugal depends on the Portuguese primary energy mix share for electricity generation. The primary energy sources mix used in the Portuguese electricity production in year 2012 is present in Table 29.

Table 29- Average Portuguese electricity generation share by energy source in 2012 [54]

Fossil			Renewable					Importations (Spain)
Cogeneration	Natural Gas	Coal	Solar	Small Hydro	Biomass & Waste	Hydro	Wind	
11%	11%	24%	1%	1%	5%	11%	20%	16%

The electricity generation regards the power plants used to convert the primary energy and the importations share. The resulting WTT factor for the electricity, regarding primary energy losses and CO_{2eq} emissions per 1 MJ of electricity produced is 2.206 MJ/MJ_{elec} and 110.22 gCO_{2eq}/MJ_{elec} respectively by using the physical content method for nuclear and renewables ([54], [55] and [56]). Disregarding the 1 MJ energy content in the electricity produced, the WTT factor becomes: 1.206 MJ_{exp}/MJ_{final elec} and 110.22 gCO_{2eq}/ MJ_{final elec} respectively, is used in Eq. (5). The electricity used in this study was considered to be generated by the average yearly generation mix, and no influence of the marginal or daily variation of the mix was accounted.

The hydrogen fuel considered in this study was produced via steam reforming of natural gas. It was assumed that the natural gas is received in Portugal such as the method used nowadays: around 58% is transported to Portugal in liquid state via ship from west Africa (Nigeria), around 40% is transported via pipeline from north Africa (Algeria), and 2% via pipeline from Europe [57] The natural gas is used in centralized steam reforming, and the produced hydrogen is compressed and distributed by truck to fuel stations. Table 30 shows the natural gas WTT factor (expended energy per 1 MJ of natural gas produced) associated to its production and importation to Portugal.

Table 30- Portugal natural gas estimated WTT factor. [32] and [57]

Origin / share (%)	Algeria 40%		Nigeria 58%		EU 2%	
Processes	MJ/MJ _{NG}	gCO _{2eq} /MJ _{NG}	MJ/MJ _{NG}	gCO _{2eq} /MJ _{NG}	MJ/MJ _{NG}	gCO _{2eq} /MJ _{NG}
• Extraction and Processing	0.03	3.3	0.03	3.5	0.02	3.3
• Pipeline	0.02	1.9	--	--	0.02	1.9
• Liquefaction	--	--	0.09	5.8	--	--
• Transport (shipping)	--	--	0.09	5.6	--	--
• Receipt	--	--	0.03	1.8	--	--
Weighted Total (100%)	MJ/MJ _{NG} 0.210			gCO _{2eq} /MJ _{NG} 16.08		

In Table 9 the estimations for the hydrogen WTT factor regarding energy and CO₂ and considering the natural gas importation is shown.

Table 31. Portugal hydrogen estimated WTT factor.

	MJ/MJ _{H2}	gCO _{2eq} /MJ _{H2}
NG importation (LHV _{hydrogen} / LHV _{NG} → 2.44 MJ _{hydrogen} /MJ _{NG})	0.511	39.260
Reforming*		
• Central Reforming	0.210	23.230
• Gaseous Hydrogen distribution & compression	0.060	6.960
Total (MJ _{exp} /MJ _{final H2})	0.785	69.458

*The reforming stage is performed in Portugal. Then, the CONCAWE [32] estimations were adapted and the required electricity energy used in reforming and transport accounted the calculated Portuguese electricity factor of 1.206 MJ/MJ_{elec} and 110.22 gCO_{2eq}/MJ_{elec}.

For each MJ used in the vehicle (TTW stage), the WTT factor for each energy source (diesel, hydrogen, or electricity) must be accounted in order to estimate the fuel life cycle, (WTW,) as described in Eq. (5). Note that in Eq. (5) the WTW stage must account both hydrogen and electricity used in the FC-PHEV.

4.2.7. Vehicle materials cycle (Cradle-to-Grave)

The CTG stage regards the energy consumption and CO_{2eq} emissions of the materials used in the production of the vehicle, assembly and recycling processes of the vehicle life cycle. However, in this study only the CO_{2eq} emissions will be considered in the optimization objectives.

In order to account the impact of the vehicle fabrication during its lifetime the total expected travelled distance of the vehicle during its life must be considered.

A Portuguese study [58] points to an average of 1046667 km per bus lifetime (km_{life}), which includes data from real bus manufacturers and operators in Portugal (STCP, MAN, AVIC,

Barraqueiro...). The life cycle results in this study are regarded to the vehicle lifetime expectancy, and therefore are defined as per *lifetime km* (accounting 1046667 km) (Eq. (6)). In this study, only the main powertrain components, fuel cell, electric motor, controller, and battery, are considered in the CTG analysis since the main frame of the vehicle is maintained the same for the different vehicle options studied. The CO_{2eq} emissions associated to the CTG stage for each component are described by Eqs. (6) and (7), and added in Eq. (5) for the total vehicle's lifetime, and are function of the components weight (*m*, in kilograms). The energy consumption calculations are similar. Note that alike to the cost estimation one replacement of the fuel cell and battery is accounted (*REP*). The CTG CO_{2eq} emissions factor for each component (gCO_{2eq}/kg_{component}) was estimated from the GREET [59] and CONCAWE [32] database, with the respective values of: 22669.58 gCO_{2eq}/kg_{FC}, 10093.56 gCO_{2eq}/kg_{MC}, 13438.45 gCO_{2eq}/kg_{BAT Lithium}, 11719.48 gCO_{2eq}/kg_{BAT NiMh}.

$$\left\{ \begin{array}{l} CTG_{CO_{2eq}}^{FC}(g) = \left(\frac{gCO_{2eq}}{kg_{FC}} \right) m_{MC} (REP + 1) \\ CTG_{CO_{2eq}}^{MC}(g) = \left(\frac{gCO_{2eq}}{kg_{MC}} \right) m_{MC} \\ CTG_{CO_{2eq}}^{BAT_{Lithium}}(g) = \left(\frac{gCO_{2eq}}{kg_{BAT_{Lithium}}} \right) m_{BAT_{Lithium}} (REP + 1) \\ CTG_{CO_{2eq}}^{BAT_{NiMh}}(g) = \left(\frac{gCO_{2eq}}{kg_{BAT_{NiMh}}} \right) m_{BAT_{NiMh}} (REP + 1) \end{array} \right. \quad (6)$$

$$CTG_{CO_{2eq}}(g) = CTG_{CO_{2eq}}^{FC} + CTG_{CO_{2eq}}^{MC} + CTG_{CO_{2eq}}^{BAT_{Lithium}} + CTG_{CO_{2eq}}^{BAT_{NiMh}} \quad (7)$$

4.2.8. Lifetime Operation costs

In order to evaluate the potential financial savings between the investment cost of the powertrain and the fuel savings, a lifetime analysis must be made for each vehicle. The powertrain investment cost is accounted as referred above. The operational costs account only the fuel and electricity consumption, and its associated cost to the user. In this study, Portuguese average costs were assumed for diesel (1.375 €/liter or 0.0512 \$/MJ_{diesel} [60]) and for electricity (0.0589 \$/MJ_{elec.} or 0.15 Euro cents/kWh [56]). For hydrogen a range of cost possibilities 0.0416 \$/MJ_{hydrogen} to 0.1666 \$/MJ_{hydrogen} were assumed [61]. Note that the energy costs are far from being stationary.

One way to evaluate the lifetime cost savings derived from the cost investment in the powertrain and the fuel costs related to the vehicle lifetime, is to compare the results with the reference vehicle, ICEV. The financial balance (*P*) is defined by a simple balance between the costs of the fuel

cell vehicles and the reference ICEV (Eq. (8)). Therefore, negative values imply that is worthwhile to invest in such optimized powertrains.

$$P\left(\frac{\$}{km}\right) = \left\{ \frac{J}{(lifetime\ km)} + \left(\left(\frac{\$}{MJ} \right)_{H_2\ fuel} TTW(MJ/km)_{H_2} + \left(\frac{\$}{MJ} \right)_{elec.} TTW(MJ/km)_{elec.} \right) \right\}_{FC\ veh} - \left\{ \frac{J}{(lifetime\ km)} + \left(\frac{\$}{MJ} \right)_{diesel} \left(\frac{MJ}{km} \right)_{diesel} \right\}_{ICEV} \quad (8)$$

where *FC veh* refers to the optimized fuel cell vehicles and to the DFCV, *ICEV* to the reference ICEV vehicle, *J* is the powertrain cost (*J(x)*), *lifetime km* is the traveled distance considering the life time expected in kilometers, $(\$/MJ)_{fuel}$ is the cost (in dollars, \$) of the fuel (hydrogen or diesel) or electricity per MJ, *TTW(MJ/km)* is the fuel or electricity consumption of the vehicle in TTW stage. Only the FC-PHEVs have electricity consumption. The electricity consumed during the FC-PHEV life time is calculated by accounting the vehicle electric consumption (in CD mode) during the daily AER.

4.3. PHEV and HEV optimization

The objective is to optimize the powertrain of a FC-HEV and FC-PHEV bus aiming to reduce the vehicle cost, reduce the fuel consumption, and reduce the CO_{2eq} emissions regarding its life cycle. Single-objective and multi-objective genetic algorithms are used to optimize the fuel cell vehicles. In Single objective optimization each objective independent minimization is regarded. In this study multi-objective optimization aims to minimize two simultaneous objectives: cost & LCA CO_{2eq} emissions, and LCA CO_{2eq} emissions & Fuel consumption.

The optimized vehicles must be capable to perform a certain driving cycle and comply with specific performance constraints: minimum top speed of 80 km/h and a maximum acceleration time from 0-50 km/h of 12 s. Only for the FC-PHEV bus a minimum AER of 33 km constraint must be accounted (around ¼ of the daily distance).

The object of optimization is the main powertrain components sizing (fuel cell, electric motor, and battery). In order to perform the powertrain sizing, a range of potential electric motors, fuel cells, and batteries, are available for the optimization. Additionally the power scaling of the MC and FC, and the number of modules of the battery, are also design variables of the optimization Table 32.

The reference DFCV, although not having a battery has its fuel cell and electric motor available in the optimization variables.

4.3.1. Cost Minimization

Assuming that the vehicle chassis, transmission, and auxiliary systems are maintained for the different vehicle designs (FC-HEV and FC-PHEV), the objective function ($f_{cost}(x)$), aiming cost minimization, focuses on direct comparison between the different component choices, and in this case can be expressed as the sum of the estimated costs of the components (see Eqs. (1) to (4) and Eq. (9)):

$$\text{Min } f_{cost}(x) \rightarrow \text{Min } \{C_{FC}(x) + C_{MC}(x) + C_{BAT}(x)\} \quad (9)$$

where x is the cost currency in dollars (\$), $f_{cost}(x)$ is the objective function of cost minimization, C_{FC} is the cost of 2 fuel cell systems (since one replacement is assumed during the vehicle expectancy), C_{MC} is the cost of the motor and controller, and C_{BAT} regards to the cost of 2 battery packs (accounting one for replacement during vehicle life).

4.3.2. Fuel Consumption Minimization

Alike to cost objective, the fuel consumption optimization focuses on direct comparisons between the different vehicle designs, aiming to minimize the hydrogen fuel consumption. The fuel consumption for the PHEV-FCs is calculated in charge sustaining mode when the vehicle uses the fuel cell alike to FC-HEV, thereby not influenced by the use of the electric energy in pure electric mode. The electric consumption is not accounted in this type of optimization. The fuel consumption (TTW fuel consumption) objective function ($f_{fuel}(x)$) is the sum of the fuel consumption rate (g/s) throughout the driving cycle (with the duration of t seconds), and is a direct result from the simulation software (Eq. (10)).

$$\text{Min } f_{fuel}(x) \rightarrow \text{Min } \{\sum \text{fuel grams } (t)\} \quad (10)$$

4.3.3. Life Cycle CO_{2eq} Minimization

The vehicles are also optimized aiming to reduce their life cycle impact in terms of greenhouse gas emissions. LCA accounts with the energy (fuel or electricity) utilization in the vehicle, the energy production, and vehicle fabrication impact. The minimization of LCA impact is described by the Eq. (11).

$$\text{Min } f_{LCA\ CO_{2eq}}(x) \rightarrow \text{Min } \{CTG_{CO_{2eq}}(x) + WTW_{CO_{2eq}}(x)\} \quad (11)$$

where $f_{LCA\ CO_{2eq}}(x)$ is the objective function regarding CO_{2eq} emissions minimization relatively to the LCA impact, x is the quantity of CO_{2eq} emissions per kilometer of the vehicle lifetime (gCO_{2eq}/km), CTG and WTW are the LCA stages regarding respectively to the vehicle materials and to the energy production and use in the vehicle (see Eq. (5)).

4.3.4. Multi-objective Minimization

Using multi-optimization methods allows optimizing two or more objectives simultaneously. Multi-objective optimization problems can sometimes be formulated as a single weighted objective function, assigning a weight coefficient to each “sub-objective”, and therefore transforming the multi-objective into a single-objective problem. However, sometimes the determination of the weights is difficult since the importance share of each sub-objective can be complex to define, and metaheuristic methods become appropriate. In this method, a multi-objective genetic algorithm is implemented and the objective evaluation process is performed similarly to the single-objective genetic algorithm. In this study only two objectives are optimized simultaneously.

The couples of objectives to be minimized are *Cost & LCA CO_{2eq} emissions* (Eq. (12)), *LCA CO_{2eq} emissions & Fuel consumption* (Eq. (13)), and *Cost & Fuel consumption* (Eq. (14)).

$$\text{Min } G(x) \rightarrow \text{Min } (f_{cost}(x), f_{LCA\ CO_{2eq}}(x)) \quad (12)$$

$$\text{Min } H(x) \rightarrow \text{Min } (f_{LCA\ CO_{2eq}}(x), f_{fuel}(x)) \quad (13)$$

$$\text{Min } L(x) \rightarrow \text{Min } (f_{cost}(x), f_{fuel}(x)) \quad (14)$$

where $f_{cost}(x)$ regards to the cost of components objective, as in Eq. (9), and $f_{fuel}(x)$ is the fuel consumption, as in Eq. (10), and $f_{LCA\ CO_{2eq}}(x)$ regards to LCA CO_{2eq} emissions objective as in Eq. (11).

4.3.5. Single-objective optimization algorithm – GA

A genetic algorithm, GA, was used to perform the optimization. A GA is a metaheuristic method which is an iterative process that uses an algorithm to guide simple heuristics in the search of global optima of a problem, combining different kinds of search space exploration, and using preliminary solutions in order to improve the search process to find near-optimal solutions. The GA is a method that seem particularly suited to the considered optimization problem. It fits to a vast objective function formats, and it is a very robust algorithm to solve nonlinear, nonconvex, discrete, and analytically complex problems, alike to the vehicle optimization problem in this study [62]. Other advantages in this method are that it is a derivative free method and its great search efficiency in large domains. The case study accounts for different models of components and its sizing (using a mathematical scaling function, provided by ADVISOR) that assembles a solution, providing a perfectly adapted structure to the implementation of the GA chromosome (Figure 38). The selection of the components and the scaling factor are both generated by the GA, and they represent a vehicle which is evaluated by ADVISOR.

A GA is a stochastic global search and optimization method, and its creation was inspired in natural biological evolution based on Darwin's theory of survival of the fittest, which applies the principle of survival of the fittest preliminary solutions to produce successively better approximations to a solution ([63] and [64]). The developed GA used in this study was based on a real-coded Genetic and Evolutionary Algorithm Toolbox (GAtbx) for MATLAB software [63] and [65].

The chromosome structure and the genes range were adapted to the optimization problem, including the communication between the GA and the ADVISOR to perform the evaluation of each candidate solution. The communication between the GA and ADVISOR is performed entirely by using MATLAB files, from which a special file included in ADVISOR package, *adv_no_gui.m*, allows to run simulations automatically without needing the use of the graphical user interface. This file is therefore responsible to read the chromosome information, attach the remaining input data and start the simulations.

Since the optimization constraints are mandatory for this study, a penalty condition was implemented which applies a high enough penalty to the fitness value of each solution that misses to comply with the specified constraints. Those penalized solutions are therefore excluded from the main solution population due to the elitist properties of this algorithm.

Other improvement implemented in the developed GA was the generation of an initial population in complete agreement with the constraints, which consequently can accelerate the convergence of the algorithm, since it will already start with a set of not penalized candidate solutions.

Additionally, a method of incest prevention was employed. The incest in GAs is usually responsible for the premature convergence of the algorithm in local optima solutions [66]. In the applied method, if two equal parent individuals (sharing the same genetic material) are chosen to breed (crossover), automatically the two expected offsprings are randomly generated, and therefore preventing the simple duplication of their parents genotype and at the same time inducing diversity to the solutions. A simple resume of the used algorithm is followed.

The genetic algorithm works by building a random population of individuals which is a set of possible solutions to the optimization problem. The individuals are represented by the GA's chromosome (Figure 38). The GA chromosome structure is composed by the individuals that contain information, genes, representing the respective components and all the design variables to be optimized (see Table 32). Each possible gene combination forms an individual which can be seen as a candidate solution regarding to a designed FC-HEV or FC-PHEV bus.

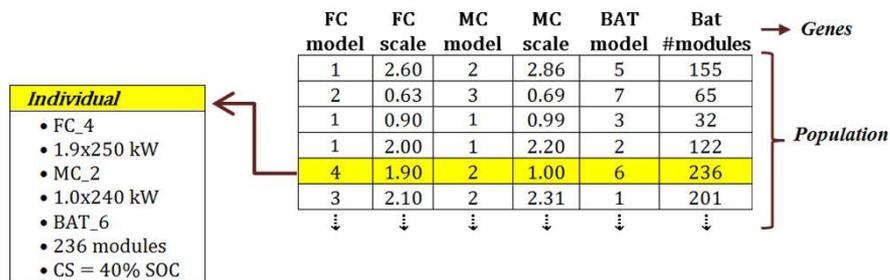


Figure 38- Chromosome structure for GA.

Table 32- Range of available genes used to assembly a vehicle.

FC model	FC power scale	MC model	MC power scale	BAT model	BAT modules
FC_1 to FC_4	0.5 - 3	MC_1 to MC_4	0.5 - 3	BAT_1 to BAT_8	50 - 250

The available genes, the constraints to be achieved, the size of population, and the maximum number of generations, are the initialization parameters of the GA in this study. A maximum of 500 generations and 50 individuals of population size were used. A resume of the used GA is represented in Fig. 6.

After the initial population is generated randomly, a first evaluation of each individual is performed (Fig. 6). In the evaluation process the ADVISOR software is used to simulate the vehicle (individual) in the desired driving cycles, and afterwards the cost and LCA calculations are

performed. ADVISOR besides checking the feasibility of each individual, it also outputs valuable information on the vehicle performance: energy consumption, maximum speed, maximum acceleration, and battery behavior. These output data for each designed vehicle are evaluated regarding the constraints requirements. The cost and LCA calculations also use the output data from ADVISOR.

A ranking profile is assigned to each individual of the population, where better fitness is assigned to individuals with lower cost, lower fuel consumption, or lower CO_{2eq} emissions depending on the case study. Accordingly to the individual's fitness, a selection process is performed in order to properly choose the individuals for breeding and generate a new population of offspring. The selection uses stochastic universal sampling method (default routine).

Accordingly to a specified generation gap of 0.8, the size of the offspring population is 80% of the initial population. The breeding (crossover) routine uses an intermediate recombination operator, with 0.8 of crossover probability. In geometric terms, intermediate recombination is capable of producing new variables within a slightly larger hypercube than that defined by the parents but constrained by a scaling factor chosen uniformly at random over some interval typically [-0.25, 1.25][64]. From each pair of best ranked individuals in the population two individual child individuals are formed. Next a mutation process occurs (mutation rate of 1/(variables per individual)), changing a gene value, and adding diversity to a generated population. At this point the offspring population is completed.

After the offspring population is evaluated the offspring individuals are reinserted into original population maintaining the best fitted individuals, by replacing the least fitted. The totality of the offspring population is reinserted in the parent population, and only 20% of the best fitted parents are maintained.

The termination criterion of the GA is the maximum number of generations (Figure 39), which for this study is 500 generations. The convergence of the algorithm is analyzed when the final solutions are achieved. If a convergence tendency or if the final solutions are not satisfactory according to the computational time and the quality of solutions the optimization process is repeated.

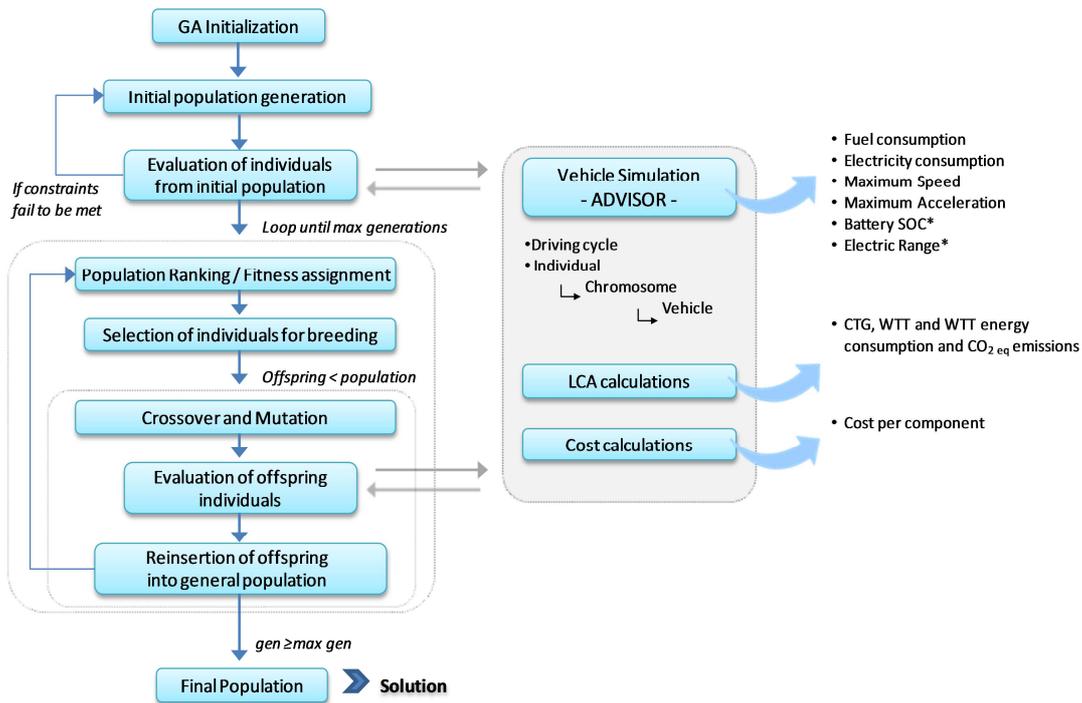


Figure 39- Scheme of the GA including its integration with ADVISOR platform, LCA calculations and cost calculations. *refer to indirect results

4.3.6. Multi-objective optimization algorithm – NSGA-II

A Non-dominated Sorting Genetic Algorithm (NSGA-II) developed by [67] and [68], was used to develop the multi-objective optimization in this study.

In multi-objective problems it is often not possible to have a single solution which simultaneously optimizes all objectives, especially if they are in conflict. Generally, in this kind of formulation improving in one objective may deteriorate another. A balance between the optimization objectives represented by trade-off solutions is achieved when a solution cannot improve any objective without degrading other objectives. These solutions are called non-dominated solutions. The set of these solutions is a *non-dominated set* or a Pareto-optimal set, for which the corresponding objective vectors are referred to as the Pareto-front [27], [68]. The Non-dominated Sorting Genetic Algorithm (NSGA) proposed in [27] was one of the first such evolutionary algorithms.

The NSGAII developed for this study was based on the Global Optimization Toolbox for MATLAB software [69], and in order to evaluate a solution's objective value, a simulation tool, ADVISOR, and a cost and LCA model were used similarly to the GA.

The main core of the NSGA-II is a genetic algorithm; therefore there are many similarities in the optimization process between the NSGA-II and the GA. Alike to the GA, in the NSGA-II a population of individuals (candidate solutions) is sorted accordingly to its ranking, and the ranking attribution is performed by comparing the solutions with each other regarding its non-domination level [67]. A simple non-domination concept is described as follows. Consider a population of individuals, or candidate solutions, $X=[x_1 \ x_2 \ \dots x_n]$, and a certain number of objectives, k . A decision vector x_1 dominates a decision vector x_2 , if and only if: x_1 is not worse than x_2 in all objectives, i.e. $f_k(x_1) \leq f_k(x_2), \forall k$; and x_1 is strictly better than x_2 in at least one objective, i.e.: $\exists k: f_k(x_1) < f_k(x_2)$. A solution x_n is a non-dominated solution if there isn't any other solution that dominates x_n , in the terms defined above. A set of non-dominated solutions in each run/generation of the algorithm makes a Pareto set. In this study a maximum of 75% of the population (34 individuals of a total of 50) is selected to form the Pareto sets, during 500 generations (similarly to the GA). Besides the maximum number of generations other important stopping criteria was adopted for NSGA-II: the algorithm stops if the weighted average relative change in the best fitness function value over 150 generations is less than or equal to 0.003. The optimization variables regarding the vehicle are represented by the same chromosome structure as in GA, presented in Figure 39 and Table 32, in which a range of components for the powertrain design are available for selection, including its sizing. The evaluation of the optimization objectives, minimization of cost & LCA CO_{2eq} emissions and minimization of cost & fuel consumption, is performed.

4.4. Results and Discussion

The optimization results for the hybrid bus, FC-HEV, and for the plug-in hybrid version, FC-PHEV, are presented in Table 33, for single-objective optimization, and in Figure 40 and Table 34 for multi-objective optimization.

In Table 33 and Table 34 the optimization results are described for both ETC and *PortoDC* driving cycles, and include the powertrain main characteristics, the optimization achievements regarding the objectives (included in energy consumption, CO_{2eq} emissions, and cost results), and the financial savings relatively to the conventional vehicle (P_{best} and P_{max} if considering the lowest or highest hydrogen price respectively). Note that the FC-HEV, unlike the FC-PHEV, does not have AER (and TTW_{elec}) since it doesn't have the possibility to use electricity from the electrical outlet.

Figure 40 shows the NSGA-II (multi-objective) solutions. In some cases the constraints were alleviated in order to achieve a greater number of solutions when possible: minimum top speed of 60 km/h, maximum acceleration time from 0-50 km/h of 20 s, and only for the FC-PHEV a minimum AER of 20 km. This only produces additional results in some cases (as seen in Figure 40). The optimal non-dominated solutions from NSGA-II contain a wide variety of powertrain components for each vehicle configuration and driving cycle. Each line of Table 34 regards to the minimum or maximum values of the genotype and phenotype of each Pareto set result.

Table 33- Results from FC-HEV and FC-PHEV single-objective optimization, in ETC and *PortoDC* driving cycles. ¹Lithium battery, the remaining batteries are Nickel based. *Same vehicle was achieved for *Min Fuel* and *Min LCA CO_{2 eq}*.

Vehicle -- Driving cycle	Objective	FC (kW)	MC (kW)	BAT		Vehicle mass (kg)	AER (km)	Energy Consumption (MJ/km)				CO ₂ emissions (g/km)			Cost (\$1000)	<i>P_{best}</i> (\$/km)	<i>P_{max}</i> (\$/km)
				(kW)	(kWh)			TTW _{fuel}	TTW _{elec}	WTT	LCA	TTW	WTT	LCA			
FC-HEV	Min <i>Cost</i>	166	189	115 ¹	3.0	13288	--	8.81	--	6.92	16.38	0	611	655	33.7	-0.137	0.964
--	Min <i>Fuel</i> *	88	281	699	226.8	16349	--	7.32	--	5.74	14.78	0	400	610	231.7	-0.010	0.905
ETC	Min <i>LCA CO_{2 eq}</i>	88	281	699	226.8	16349	--	7.32	--	5.74	14.78	0	400	610	231.7	-0.010	0.905
FC-PHEV	Min <i>Cost</i>	114	257	981	77.9	14710	33	8.41	5.09	6.48	15.18	0	578	646	158.2	-0.048	0.741
--	Min <i>Fuel</i>	80	298	922	299.1	17416	122	6.84	5.31	6.32	13.88	0	576	701	299.4	0.060	0.125
ETC	Min <i>LCA CO_{2 eq}</i>	112	259	1102	87.5	14907	37	8.30	5.09	6.41	15.00	0	572	645	175.0	-0.036	0.710
FC-HEV	Min <i>Cost</i>	82	201	168 ¹	8.9	12715	--	18.92	--	14.85	34.05	0	1314	1332	39.4	-0.511	2.654
--	Min <i>Fuel</i> *	25	256	944	306.5	17137	--	11.20	--	8.79	21.93	0	777	889	299.2	-0.585	1.616
<i>PortoDC</i>	Min <i>LCA CO_{2 eq}</i>	25	256	944	306.5	17137	--	11.20	--	8.79	21.93	0	777	889	299.2	-0.585	1.616
FC-PHEV	Min <i>Cost</i>	42	209	427	138.5	14590	33	13.84	10.48	11.31	25.40	0	1009	1073	161.9	-0.595	1.503
--	Min <i>Fuel</i>	25	256	944	306.5	17137	60	11.20	10.97	10.81	23.84	0	974	1085	299.2	-0.503	1.061
<i>PortoDC</i>	Min <i>LCA CO_{2 eq}</i>	20	252	918	297.9	16986	51	11.43	10.71	10.48	23.25	0	942	1035	247.7	-0.555	1.036

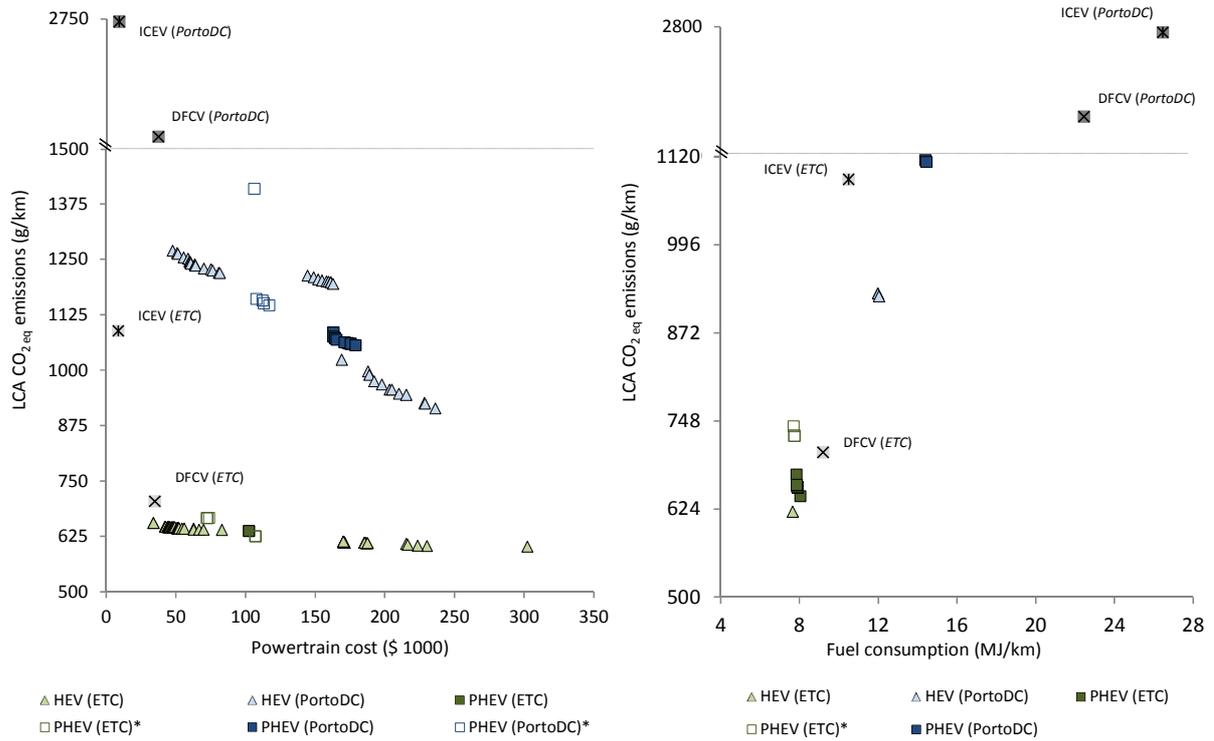


Figure 40- Pareto solutions from FC-HEV and FC-PHEV multi-objective optimization, in ETC and *PortoDC* driving cycles, and comparison to the reference vehicles. *alleviated constraints

From the optimization results it can be seen that it is difficult to highlight one vehicle or technology as the best for each driving cycle. As expected, each desired objective (minimization of cost, fuel consumption, or LCA emissions) results in its optimal powertrain. Nevertheless for the FC-HEV the minimization of fuel consumption and LCA emissions are dependent, and lead to the same results (Table 33). Since the FC-HEV only uses hydrogen, the fuel consumption and LCA CO_{2eq} emissions are highly correlated (since the fuel cycle is predominant in the LCA impact, Fig. 8). On the other hand, in FC-PHEV, fuel and electricity are consumed in the vehicle, and therefore the fuel consumed in the vehicle has not the same proportionally in the LCA as in the FC-HEV. In addition to the electricity use the battery also influences the LCA impact (Figure 41 and Figure 42). Unlike single-objective, the multi-objective genetic algorithm was used to find trade-off solutions between two objectives (Figure 40 and Table 34). Note that powertrain cost and energy consumption can be concurrent objectives, and therefore the decreasing energy consumption influences a raise in the cost of the vehicle (the same can be concluded regarding the powertrain cost and LCA emissions). The use of single-objective and multi-objective methods allows us to analyse and discuss a wider range of possible and optimal powertrain technologies for the fuel cell bus. The multi-objective optimization may not provide absolute results as the single-objective; nevertheless, the trade-off results between several objectives may also be important for decision makers.

The multi-objective optimization of *Cost & LCA CO_{2eq} emissions* for the FC-HEV is able to highlight a wide range of possible vehicle compositions by achieving a great amount of Pareto solutions, unlike the objective *LCA CO_{2eq} emissions & Fuel consumption* (Figure 40). Similarly to the single-objective optimization the dependency of the LCA CO_{2eq} emissions and the fuel consumption could guide the optimization algorithm towards similar FC-HEV compositions. Although the electricity consumed in the FC-PHEV influences the LCA and the vehicle powertrain selection, the fuel consumption still remains as the major responsible for the TTW stage.

Table 34- Pareto solutions range (minimum and maximum values) from FC-HEV and FC-PHEV multi-objective optimization, in ETC and *PortoDC* driving cycles.

Vehicle -- Driving cycle	Objective	FC (kW)	MC (kW)	BAT		Vehicle mass (kg)	AER (km)	Energy Consumption (MJ/km)				CO ₂ emissions (g/km)			Cost (\$1000)	<i>P_{best}</i> (\$/km)	<i>P_{max}</i> (\$/km)	
				(kW)	(kWh)			TTW _{fuel}	TTW _{elec}	WTT	LCA	TTW	WTT	LCA				
FC-HEV -- ETC	Min <i>Cost</i> & Min <i>LCA CO₂ eq</i>	80	182	113	3.0	13180	--	7.31	--	5.74	14.60	0	507	603	33.9	0.059	0.980	
		163	284	925	300	17228	--	8.80	--	6.91	16.40	0	611	654	302.6	-0.138	0.900	
FC-PHEV -- ETC		110	297	268	87	14359	35	8.25	5.30	6.47	15.69	0	576	636	102.6	-0.103	0.654	
FC-HEV -- <i>PortoDC</i>		27	209	206	14	12893	--	11.86	--	9.31	22.72	0	824	913	47.7	-0.500	1.690	
		74	287	1065	239	16150	--	17.91	--	14.06	32.35	0	1244	1269	236.3	-0.620	0.870	
FC-PHEV -- <i>PortoDC</i>		34	211	498	161	14949	33	13.26	10.47	11.04	25.49	0	986	1056	163.2	-0.588	0.723	
		39	224	551	179	15208	37	14.01	10.53	11.42	26.53	0	1020	1084	179.1	-0.596	0.601	
FC-HEV -- ETC		Min <i>TTW fuel</i> & Min <i>LCA CO₂ eq</i>	95	288	186	4.8	13488	--	7.66	--	6.02	15.10	0	532	619	187	-0.038	0.920
FC-PHEV -- ETC			88	234	427	138	15104	57	7.85	5.17	6.23	15.61	0	563	641	150.4	-0.004	0.310
			107	390	751	244	1649	100	8.05	5.26	6.30	15.87	0	571	672	252.7	-0.012	0.284
FC-HEV -- <i>PortoDC</i>	28		234	714	231	16016	--	11.99	--	9.41	23.01	0	833	923	228	-0.598	0.901	
	29		258	785	255	16349	--	12.05	--	9.46	23.04	0	837	927	250	-0.616	0.890	
FC-PHEV -- <i>PortoDC</i>	41		392	513	175	15184	34	14.40	10.58	11.71	27.30	0	1044	1116	180.5	-0.497	0.836	
	41		395	540	166	15312	36	14.46	10.56	11.72	27.33	0	1045	1113	172.5	-0.505	0.815	
FC-HEV -- ETC	Min <i>Cost</i> & Min <i>TTW fuel</i>		80	182	113	3.0	13180	--	7.31	--	5.74	14.60	0	507	602	33.9	0.059	0.980
			163	284	925	300	17228	--	8.80	--	6.91	16.40	0	611	654	302.6	-0.138	0.900
FC-PHEV -- ETC			91	175	521	78	14653	33	7.42	5.08	6.13	15.19	0	553	638	156.6	-0.013	0.41
		116	243	1092	221	16178	91	8.43	5.26	6.50	16.04	0	580	658	223.6	-0.055	0.277	
FC-HEV -- <i>PortoDC</i>		27	209	206	14	12893	--	11.86	--	9.31	22.72	0	824	913	47.7	-0.500	1.690	
		74	287	1065	239	16150	--	17.91	--	14.06	32.35	0	1244	1269	236.3	-0.620	0.870	
FC-PHEV -- <i>PortoDC</i>		25	214	514	167	15023	34	11.53	10.48	11.07	25.60	0	989	1059	167.6	-0.564	0.666	
		36	240	771	250	16267	50	13.64	10.74	11.40	26.40	0	1017	1083	245.5	-0.596	0.328	

The optimized FC-HEV powertrain, with a smaller battery than the FC-PHEV (Figure 43), achieved the minimum cost for ETC and *PortoDC*, with less 67% and less 76% of the cost respectively. Although the fuel cell hybrid technology clearly allows great improvements in the powertrain, the cost minimized FC-HEV costs 3 times more than a conventional ICEV.

The optimized FC-PHEV powertrain achieved the minimum fuel consumption at the expense of a larger battery, allowing a maximum of 6% less fuel consumption than the FC-HEV. Compared to the reference ICEV, the FC-PHEV achieved less 35% and less 58% fuel consumption in ETC and

PortoDC respectively, and 26% and 50% compared to the DFCV. Although the FC-HEV can also achieve similar fuel consumption values with a larger battery it has not the advantage of using CD mode if needed (more efficient).

Concerning to the LCA emissions the FC-HEV bus achieves up to 16% less CO_{2 eq} emissions than the FC-PHEV. Although the FC-PHEV can use a more efficient operation mode when using electricity only (CD mode), the larger battery and the electricity generation at the WTT stage increase the overall LCA impact (Figure 41 and Figure 42). In comparison to the reference ICEV, the optimized FC-HEV achieved 45% less and 67% less LCA CO_{2 eq} emissions in ETC and *PortoDC* respectively; and 14% less and 45% less LCA emissions when compared to the DFCV.

Although analysing the single-objective and the multi-objective results as a whole set of optimal solutions can highlight optimized powertrains for each objective or couple of objectives, sometimes knowing the financial advantages is sufficient or the priority. The potential financial advantages in acquiring a fuel cell bus relatively to a conventional ICEV bus were estimated for each solution (P_{best} and P_{max}). Negative values represent that there exists a gain and that in that specific conditions the use of the fuel cell vehicle is worth it when compared to the ICEV. There is a major influence of the energy costs. Only if the lower prices of hydrogen are assumed a financial compensation could be potentially achieved. The optimized FC-HEV powertrain has the highest potential gains for ETC and *PortoDC*, with gains of 0.138 \$/km and 0.620 \$/km respectively. This result was achieved in multi-objective optimization by minimizing the cost and the fuel consumption. This indicates that the multi-objective optimization is clearly an advantage when combining those two objectives. Although achieving smaller financial savings, the FC-PHEV has a financial benefit of 0.103 \$/km and 0.596 \$/km for ETC and *PortoDC* respectively.

In order to better understand the dissemblance between the solutions regarding each objective, the LCA solutions and powertrain cost are further analysed in Figure 41 to Figure 43 for the best solutions achieved.

In order to lower the cost of the FC-HEV powertrain, two main tendencies can be observed: a shift between the power supply from the battery to the fuel cell component, and the selection of a lighter and smaller battery (like the Lithium based batteries relatively to Nickel), allowing the vehicle to weigh less. Note that the battery in the FC-HEV since it doesn't use electricity is always smaller than in the FC-PHEV if the cost is the objective. These selections can be verified in Figure 43, where the optimized vehicles for minimum cost are composed with more powerful fuel cells, but with smaller electric motors and batteries. In cost optimization the battery represents 27%

and 57% of the powertrain total cost for ETC and *PortoDC*, however in the fuel and emissions optimization the battery represents 91% and 96% in average for ETC and *PortoDC* respectively; followed by the fuel cell and the motor and controller (see Figure 43).

A battery is capable to “absorb” some of the fuel cell losses and to better control the energy flow in the powertrain, resulting in larger batteries aiming to achieve better fuel efficiencies. This effect, may present sudden increases in cost even for a little reduction in fuel consumption. A lower power fuel cell can be the best choice in terms of fuel economy, if the combined battery and fuel cell power is enough for the peak power demands, since the use of battery power is usually more efficient than using a fuel converter. Since the fuel utilization and production stages (TTW and WTT) are responsible for the major share in the life cycle of the vehicle (Figure 41), the objectives of fuel consumption in TTW and the CO₂_{eq} emissions in LCA minimization are in agreement for the FC-HEV. The fuel stage (TTW plus WTT) accounts with a share of more than 90% of the total LCA CO₂_{eq} emissions. On the other hand, the majority of life cycle CO₂_{eq} emissions for the FC-PHEV are not only associated to the fuel consumption, but also to the electricity consumption (Figure 41).

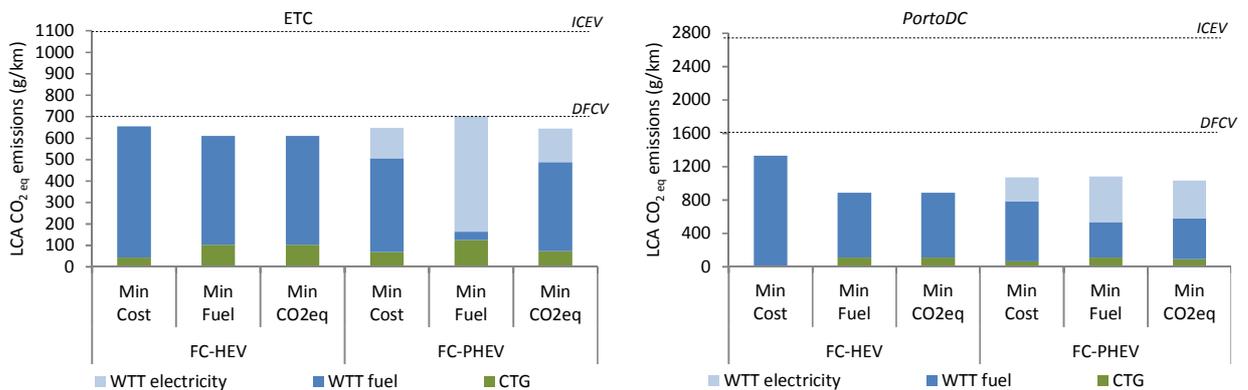


Figure 41- Best solutions achieved for minimum LCA CO₂_{eq} emissions (in grams per lifetime kilometer) regarding FC-HEV and FC-PHEV optimization (different minimization objectives), in ETC (left) and *PortoDC* (right) driving cycles. (Reference vehicles in dashed line)

The use of electricity is usually an advantage in terms of efficiency in the vehicle during the AER, however it has a higher impact in the LCA, since in WTT stage the electricity is responsible for higher energy consumption and emissions than hydrogen production. Consequently, the fuel consumption minimization in the FC-PHEV leads to different vehicle powertrain compositions than in LCA emissions minimization, unlike the FC-HEV. This is a very important fact to consider in

optimizing LCA CO₂ eq emissions in the FC-PHEV. Concerning the electricity supply, the time of the day choose to charge the vehicle battery is important since it is related to different powerplants, which will lead to different emission factors and energy losses in the electricity supply. However, the use of the electricity from the grid in this study did not account electricity generation mix daily variations neither the marginal mix influence. It is clear from Figure 41 that the CTG stage, although important, has less impact in life cycle than the energy used in the vehicle.

Only with respect to the CTG stage (Figure 42) of vehicle components production, clearly the battery is responsible for the largest share (only with exception of the FC-HEV in cost minimization). Consequently in cost minimization optimization, where the components are downsized, both CTG and LCA impact are lower than in other objectives.

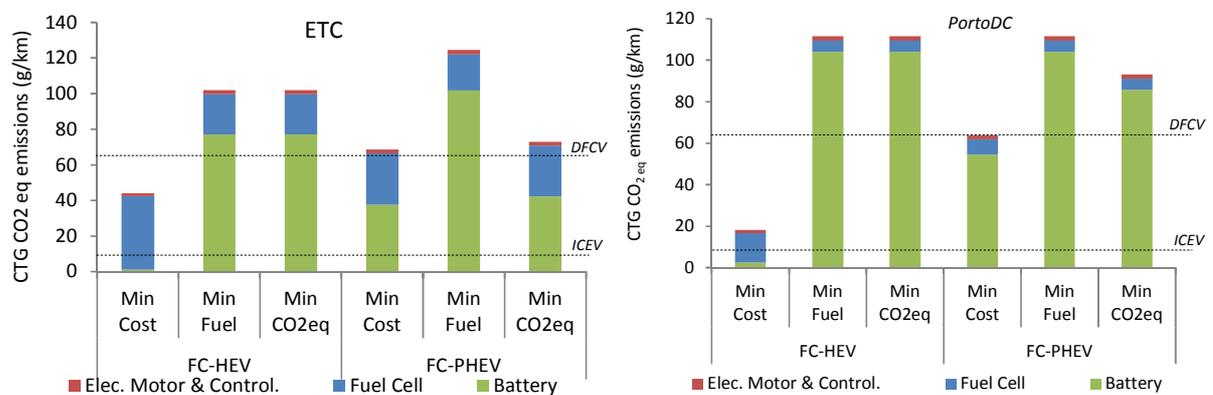


Figure 42- CTG CO₂ eq emissions (in grams per lifetime kilometer) regarding best solutions achieved for minimum LCA emissions regarding FC-HEV and FC-PHEV optimization (different minimization objectives), in ETC (left) and PortoDC (right) driving cycles. (Reference vehicles in dashed line)

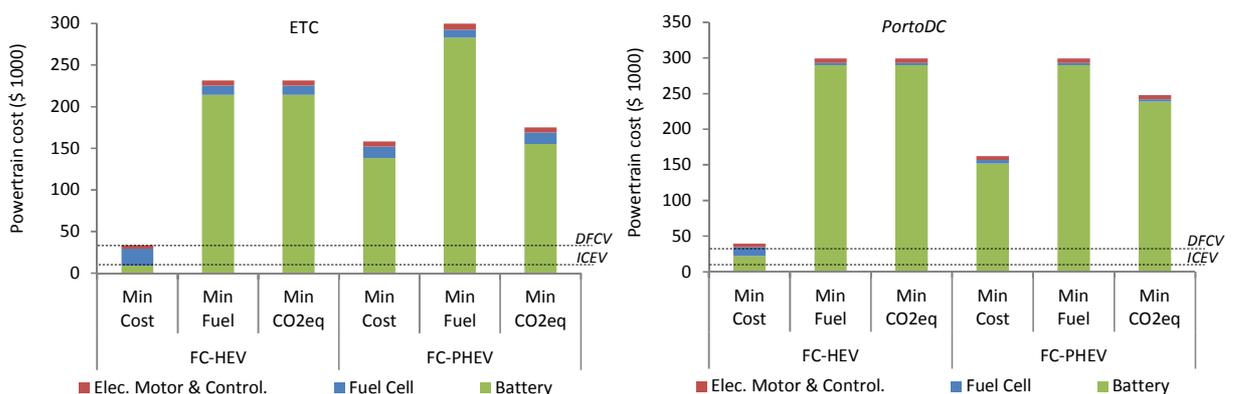


Figure 43- Best solutions achieved for minimum powertrain cost (in thousands of dollars) regarding FC-HEV and FC-PHEV optimization (different minimization objectives), in ETC (left) and PortoDC (right) driving cycles. (Reference vehicles in dashed line)

To observe the suitability of the ETC synthetic standard cycle in design optimization problems, the best solutions achieved (minimum cost, minimum fuel consumption and minimum LCA emissions) for the FC-HEV and FC-PHEV in the ETC were selected and the respective vehicles were simulated in *PortoDC*. The results are shown in Figure 44 and compared with the original optimization results for ETC and *PortoDC*. It can be seen that ETC, usually a driving cycle used in research studies for buses, may not be indicated to estimate the performance of a designed bus in a real driving schedule like the *PortoDC*. The synthetic driving characteristics represented by ETC, aren't appropriated for the reality represented by the *PortoDC*, a bus route within the metropolitan area of the city of Oporto.

When comparing the driving cycles clearly the *PortoDC*, an urban cycle, is on average a more energy demanding driving cycle. ETC, a combined urban and extra-urban driving cycle, has higher average speed, higher maximum acceleration and maximum speed (Table 28), and consequently it has a few peaks of higher power demand. However, *PortoDC* driving cycle has higher average acceleration and torque, since it has variable road grade and also a higher number of stops. Although high demand characteristics exist in ETC, they are scarce, and therefore it maintains the ETC as the driving cycle responsible for less energy consumption in average, however it can influence the optimization process due to its higher power events. The optimization algorithm enforces the choice of components capable to deliver such power.

From the results in Table 34, it can be seen that the ETC, besides being responsible for lower energy consumption, is also responsible to have lower potential for the energy consumption improvement or the LCA impact reduction, than *PortoDC*. Moreover, the ETC also allows fewer saving potential as seen in Table 34. It can be seen that ETC, achieves 30-67% more energy consumption in the *PortoDC*; which represent a lifetime financial balance loss of 0.5-3.5 \$/km (range depending on the hydrogen price).

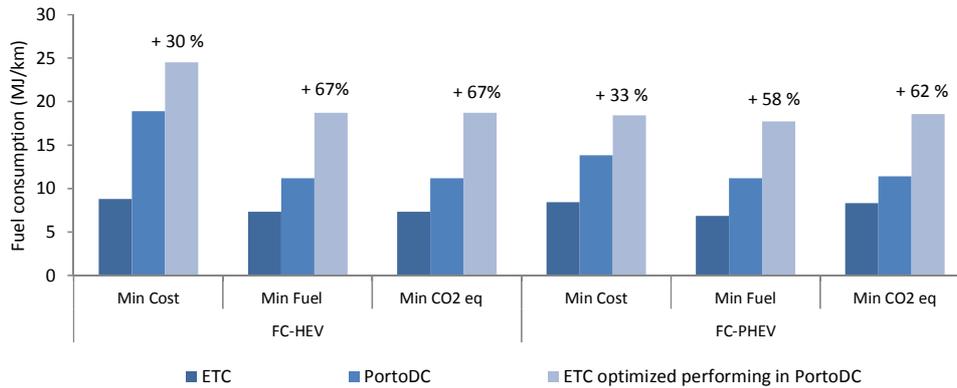


Figure 44- Comparison between fuel consumption of buses optimized for ETC (ETC) regarding cost and fuel minimization, the buses optimized for *PortoDC* (*PortoDC*), and the buses optimized for ETC but simulated in *Porto* driving cycle.

4.5. Conclusions

This study analyzed the significance of the driving conditions and the conflict between the optimization of investment cost, efficiency and LCA impact in powertrain design optimization of FC-HEV and FC-PHEV city buses. The single-objective results showed that lower fuel consumption and LCA CO_{2eq} impact can be achieved at the expense of higher powertrain cost, but depending on the hydrogen price, it can be financially compensatory throughout the bus life time.

The multi-objective optimization results show the conflict between the cost and fuel consumption (and life cycle impact) of the fuel cell vehicle. Further, it presented a wider range of possible optimal solutions for the powertrain technology. The optimization of LCA CO_{2eq} emissions and cost are conflicting because higher capacity batteries allow lower fuel consumption, but increase the cost. Cost and energy consumption can also be concurrent objectives; therefore the decreasing energy consumption requirement resulted in a higher cost of the vehicle.

The cost of the powertrain is mainly composed by the battery, the fuel cell and, the motor and controller. The fuel life cycle (use and production) is responsible for the larger share of the life cycle impact of the vehicle. Consequently, the optimization of fuel and life cycle emissions are coupled for hybrids but not for plug-in hybrid configurations, due to the impact of electricity consumption.

The European synthetic standard cycle ETC is not suitable for pre-dimensioning purposes in real driving conditions, such as the urban *PortoDC* driving cycle. The extra-urban part imposes oversized designs for the fuel cell relatively to the requirements of the *PortoDC*.

Fuel cell buses can reduce the energy consumption by 58%, emit 67% less LCA CO_{2eq} than the conventional diesel buses, and depending on the hydrogen price have the potential to achieve a financial saving of 0.620 \$/km. The FC-PHEV configuration shows more potential for achieving higher operation efficiencies, but the FC-HEV shows to have lower life cycle impact, lower cost in general, and highest financial savings potential.

4.6. Acronyms

AER – All-Electric Range

BAT - Battery

BEV – Battery Electric Vehicle

CAFE - Corporate Average Fuel Economy regulations in the United States of America

CD – Charge Depleting

CO_{2eq} – CO₂ equivalent emissions

CS – Charge Sustaining

CTG – Cradle-to-Grave

DFCV – Direct Fuel Cell Vehicle

FC – Fuel Cell

FC-HEV – Fuel Cell Hybrid Electric Vehicle

FC-PHEV - Fuel Cell Plug-In Hybrid Electric Vehicle

GA – Genetic Algorithm

GPS – Global Positioning System

HEV - Hybrid Electric Vehicle

ICEV – Internal Combustion Engine Vehicle

LCA – Life Cycle Analysis

MC – Motor and Controller

NSGA – Non-dominated Sorting Genetic Algorithm

OBD - On-Board Diagnostic vehicle interface

OEM - Original Equipment Manufacturer

PHEV - Plug-In Hybrid Electric Vehicle

REP – Relative to a component’s replacement number

SOC – Battery State-of-Charge

TTW – Tank-to-Wheel

WTT – Well-to-Tank

WTW – Well-to-Wheel

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