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Assessment of hydrogen supply chains based on dynamic bi-objective optimization of costs and greenhouse gases emissions: case study in the context of Balearic Islands

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Highlights:

- A dynamic method for optimization of hydrogen supply chains is illustrated.
- Greenhouse gases emissions and costs of hydrogen chains are assessed.
- Trade-offs between environmental and economic performances are analyzed.
- Study shows the impact of electrolyzer management on the environmental results.
- Future analyses should include more environmental impact categories.
- Comparison with alternative territorial decarbonization options should be engaged.

Abstract:

Balearic Islands are facing challenges related to energy demand and reliance on imported fossil fuels. In this context, hydrogen vector could be part of the technical solutions for increasing the contribution of renewable energies towards various energy demand sectors. This paper explored the use of dynamic simulation and optimization as a mean for assessing the achievable economic and environmental performance of hydrogen pathways under the specific fluctuating boundary conditions of these Islands. A bi-objective dynamic optimization approach based on a Mixed Integer Linear Programming approach has been implemented using PERSEE software to assess the tradeoffs between costs and carbon emissions of hydrogen supply chains. The chosen case study has been built using some of the technical features of the European GreenHysland project located in Balearic Islands. The optimization of the design and operating conditions of hydrogen chains involving two modes of hydrogen transport (trucks and pipeline) has been addressed, for the supply of hydrogen to fuel cell buses and taking into account the possibility of injecting hydrogen into the natural gas network. The economic and environmental optimizations resulted in different electrolyzer's operation strategies. On one hand the economic optimization led to high use rate of the electrolyzer (92%) and high carbon impact of hydrogen due to high carbon content of grid electricity. On the other hand the environmental optimization led to a PV-following strategy with a low use rate of the electrolyzer (50%). It was shown that in current situation, due to the high greenhouse gases intensity of Balearic electrical grid, the conditions for hydrogen to provide a net carbon advantage compared with fossil reference scenario would be to ensure a minimal direct PV share of 40% in the electricity consumed by the electrolyzer, thus resulting in a running time availability lower than 63% and an average use rate lower than 75% of nominal capacity. From a greenhouse gas perspective, it was shown that the best choice would be to encourage direct solar electricity sourcing for the electrolyzer as well as maximizing injection into the natural gas grid. Finally, results showed that the choice of truck or pipeline for hydrogen transport does not have a significant influence on the total emissions compared to the influence of operation strategy. This study confirmed the interest of the dynamic optimization approach combined with epsilon-constraint method for the design of hydrogen projects to comply with future certification requirements for green or low-carbon hydrogen. In future work, the comparison of hydrogen systems with alternative energy supply chains should be extended to other categories of environmental impact through multi-objective optimization methods. Finally, innovative modeling and optimization methods should be developed to evaluate different hydrogen deployment strategies and infrastructure planning in the Balearic Islands' future energy landscape.

Keywords:

GreenHysland; Hydrogen; Supply chains; Optimization; Environmental impacts; Scenarios; PERSEE.

Nomenclature

List of acronyms

BOP	Balance of Plant
CEA	Commissariat à l'énergie atomique et aux énergies alternatives
CO ₂ -eq	Carbon dioxide equivalent
EU	European Union
GHG	Greenhouse gases
GWP	Global warming potential
H ₂	Hydrogen
HVDC	High Voltage Direct Current
LCA	Life Cycle Assessment
LCAC	Levelized Cost of Avoided CO ₂ -eq
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LCOH	Levelized Cost of Hydrogen
MILP	Mixed Integer Linear Programming
NG	Natural gas
NPV	Net Present Value
PEM	Proton Exchange Membrane
PV	Photovoltaic
RED	Renewable Energies Directive
RFNBO	Renewable Fuels of Non Biological Origin
SDG	Sustainable Development Goals
UIB	Universitat de les Illes Balears

1. Introduction

1.1. Background and motivations

1.1.1 Background

As nations across Europe and globally commit to ambitious decarbonization targets for 2030 and aim for net-zero greenhouse gas emissions by 2050, energy systems are progressively shifting from non-sustainable carbonated fossil fuels to low carbon and renewable energy sources [1]. This transition in the energy sector is taking place as part of the sustainable development goals (SDG) defined by United Nations to prepare a desirable, resilient and climate neutral future for the next generations [2]. In this context, islands face an important challenge with regard to energy supply due to their small size and isolated energy systems. They are heavily dependent on fossil fuel imports for electricity generation, transport, and heating. Fossil fuels are not only a major source of greenhouse gases (GHG) emissions, but they are also more expensive than on the mainland which represents a financial burden for the islanders [3]. Moreover the renewable energy potential on island territories can be limited by the strained electrical grids.

This paper deals with the specific context of Balearic Islands, located in the Mediterranean sea close to the East coast of Spain. These islands are characterized by a mass tourism-based economy with millions of visitors each year. As many islands, the energy mix of Balearic Islands relies mainly on fossil fuels import (gas, diesel, coal) as well as electricity import through a sub-marine cable linking the archipelago to the peninsula. Renewable energy production in Balearic Islands remains relatively limited at present. In terms of greenhouse gas emissions, accessible public assessments highlight the significant share of transport (road, air and sea), which accounted for 66% in 2019, while energy production represented 27% of emissions [4]. The future

1 evolution of the Balearic energy system complies with the Spanish national program [5] and the 2019 law,
2 which sets decarbonization targets compared to 1990 (-40% in 2030, -90% in 2050), reduction in primary
3 energy consumption compared with 2005 (-26% in 2030, -40% in 2050) and growth in the share of renewable
4 energies in the archipelago's energy mix (35% in 2030, 100% in 2050, from which 70% produced in the
5 territory) [6].

6 Technical solutions such as hydrogen could play a role in achieving these objectives with respect to the
7 flexibility it could bring to future energy landscape. Complementary to direct electrification, hydrogen and its
8 derivatives could play a role in the decarbonization of hard-to-abate sectors such as steel industry, high-
9 temperature industrial heat, heavy transport (shipping, aviation, heavy road transport), combined heat and
10 power for buildings, among others. Focusing on heavy mobility, hydrogen could also contribute to improve the
11 air quality and reduce noise pollution. Electrolytic hydrogen is also recognized as a mean for facilitating the
12 expansion of intermittent renewable energy penetration resolving curtailment issues in grid-constrained areas
13 [7]. However, the deployment of hydrogen as an energy carrier is still at an early stage [8]. Financial support
14 from public policies is put in place over regional, national and European perimeters to increase the maturity of
15 hydrogen technologies and hydrogen markets. At EU level these deployments are supported through regional
16 projects selected in the frame of dedicated call for proposals concerning all necessary steps in the hydrogen
17 value chain, from production (and often even dedicated renewable electricity production) to subsequent
18 storage and its transport & distribution to various off-takers in mobility, industry or combined heat and power
19 applications.

20 The study presented in this paper has been performed in the frame of the GreenHysland project [9]. This
21 project has been selected by the European Clean Hydrogen Partnership under the 2020 call for proposal
22 related to small scale Hydrogen Valley [10], [11]. This five years project (2021-2025) located on the island of
23 Mallorca aims to deploy a fully functioning hydrogen ecosystem turning the island into the first hydrogen hub
24 in Southern Europe. It can be considered as a territorial demonstration of H₂ technologies and demonstration
25 of synergies between stakeholders from production to transport and use of this energy vector. The project
26 comprises (i) the development of hydrogen production, transport and distribution infrastructure (green
27 hydrogen production plant, hydrogen truck trailers, deployment of a hydrogen pipeline and hydrogen refuelling
28 station), (ii) the demonstration of three types of end-use applications (hydrogen vans and buses, stationary
29 fuel cells and hydrogen injection into the natural gas grid) and (iii) the analysis of the economic, environmental
30 and social impacts of larger scale deployment of hydrogen as an energy carrier, including the development of
31 a multi-criteria analysis methodology and the elaboration of a hydrogen roadmap towards 2050 in the Balearic
32 Islands.

33 This paper refers to the impact analysis work performed within the GreenHysland project, the goal
34 being to contribute to the development of relevant methodologies for the assessment of hydrogen supply
35 chains. The purpose of such methodologies would be to help stakeholders involved in the energy transition of
36 Balearic Islands to clarify the benefits and drawbacks of hydrogen technologies in comparison with other
37 decarbonization options and finally to support decision-making.

38 **1.1.2 Motivations**

39 The decarbonization of end-uses through hydrogen depends on the direct and indirect environmental
40 impacts generated from the primary energy from which hydrogen is produced as well as life cycle impacts of
41 the newly developed technologies over the whole hydrogen supply chains. As an example, water electrolysis
42 is often considered as an environmental-friendly method for hydrogen production. However even though
43 hydrogen produced by electrolysis from low carbon sources tends to minimize environmental impact, the
44 impact is not zero since electricity production involves environmental footprints as well as electrolysis and
45 associated processes such as water treatment or desalination [12]. Hence several initiatives are being
46 undertaken at National, European and International levels in order to support ramping-up of clean hydrogen
47 market and related industry in the next years and decades by setting new rules and certification processes.
48 The new version of the European Renewable Energy Directive commonly referred as RED II (2018) defines
49 the global rules and targets for increasing deployment of renewable energies across European Union.
50 Complementary to this directive, a specific Delegated Act recently published (February 2023) establishes a
51 "Union methodology setting out detailed rules for the production of renewable liquid and gaseous transport
52 fuels of non-biological origin" (RFNBO) [13]. These rules refer to consideration of additionality (new dedicated
53 renewable power plants associated with hydrogen production plant), temporal correlation (from calendar
54 month basis to hourly correlation basis) and geographical correlation (notion of bidding zone). Thus the
55 regulatory framework that is put in place at European level imposes rules for certification of low carbon or
56 green hydrogen and consideration of temporal correlation between renewable production and hydrogen
57 production. A second Delegated Act establishes the minimum threshold for greenhouse gas (GHG) emissions
58 savings of RFNBO fuels at -70% compared to reference process (production of hydrogen from steam methane
59 reforming with a reference emission of 94 gCO_{2-eq}/MJ). Hence, hydrogen stakeholders may be facing a new
60 challenge regarding the optimized size and optimized operation of hydrogen equipment to fulfill the afforded
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mentioned GHG emission requirements while maximizing the profitability of the production plants. Therefore appropriate methods and tools will be needed in order to simulate the economic performances associated to these constraints while taking into account the intermittent characteristics of renewable resources, electricity prices, carbon intensity of grid electricity or intermittency of the hydrogen demand. These methods should help to assess trade-offs between economic viability of hydrogen supply chains and environmental benefits such as avoided carbon emissions. In summary, the first motivation of this study is related to the evolving regulatory context about low carbon hydrogen certification that will imply implementation of appropriate dynamic assessment methods for pre-design studies of hydrogen projects.

The certification of hydrogen relates to the way the gas is produced. However in the future hydrogen transport infrastructure such as truck trailers or pipelines will have to be deployed to convey the gas from production sites to utilization sites. The choice of one or the other mode of transport depends on the volume to be transported. But from an environmental point of view, the question arises about their impact in comparison with the environmental impact of other stages in the supply chain. Therefore the impact of transport has to be taken into account in the analysis. In this study the objective is to go beyond the existing framework by extending the scope of the perimeter and considering impact of infrastructure. Additionally the analysis should consider the impacts related to the manufacturing and use of all components of the hydrogen supply chain (electrolyzers, compressors, storages, pipeline, fossil fuel used for truck trailers, etc.), *i.e.* not restricted to the nature of electricity consumed for hydrogen production. Thus the second motivation of this study is related to the fact that the analysis of environmental benefits of hydrogen should imply considering the impacts of the entire energy supply chain in order to be able to compare these impacts with alternative decarbonization options.

From a stakeholder perspective, ensuring economic viability is a key parameter for hydrogen market uptake. Cost minimization requires favourable electricity price conditions and maximizing the use of assets to ensure amortization of initial investments. However this economic objective may be conflicting with the minimization of environmental impacts depending on the carbon intensity of the electricity consumed. Therefore it appears important to study the influence of the operation of the electrolyzer on costs and impacts and to assess the best dynamic utilization of these equipments over the entire hydrogen supply chain in order to minimize costs and emissions. Such analysis may help in the assessment of the best cost and performances achievable by the hydrogen supply chain while taking into account the variability of sources and possibility of arbitrage regarding downstream demand (hydrogen injection in natural gas grid for instance). From a territorial point of view, another question arises related to the best use of hydrogen for maximizing decarbonisation, and the economic value of the hydrogen produced. Ultimately, the potential benefits of hydrogen should be evaluated considering a wider set of criteria (such as the levelized cost of avoided emissions) and compared with alternative decarbonisation options and measures. Thus the third motivation of the study is related to the fact that optimal sizing and operation of hydrogen supply chains may not be equivalent between cost minimization and environmental impact minimization. Hence appropriate numerical tools could play a role for the analysis of the optimal solutions and related economic and environmental performances, in order to support decision-making in the frame of preliminary opportunity studies of hydrogen projects implementation on a given territory.

In summary, the motivation of this paper is to address the need of appropriate dynamic optimization methods to study the trade-offs between cost and environmental impact minimization of hydrogen supply chains. This method has to tackle simultaneously (i) the dynamic nature of the problem (variable electricity prices, variable GHG emissions from grid electricity, variable PV production, variable amount of hydrogen that can be injected in natural gas grid for a given maximal percentage and depending on natural gas flow rate) and (ii) the consideration of greenhouse gases emissions related to manufacturing and use of all equipments.

1.2. Literature review

Despite the various benefits resulting from renewable energy and hydrogen production, there are still new issues to overcome, such as system losses caused by inadequate operation, sizing or selection of location of systems [14]. By including optimization techniques, the design and operation of energy systems can be addressed, resulting in more efficient and cost-effective scenarios [15]. Numerous optimization techniques have been implemented in this area, and one of the most widely used is mixed integer linear programming (MILP) [16]. The main advantage of a MILP Solver method is the accuracy of the solution. If the problem is well defined (objective function, boundary conditions, constraints), the solution found with the use of MILP Solver is the global optimal solution of the problem. The other advantage is that the optimal dispatch is found without the need to adjust the operating strategy of the units [17]. In addition, energy system optimization inherently involves multiple and conflicting objectives. For instance, the most efficient energy processes are not necessarily the most economical ones, or a system with low GHG emissions can suppose high investment costs. Therefore, energy system optimization is more realistic and reliable if different evaluation aspects, such as cost, technical and environmental concerns, are explicitly taken into account. This can be accomplished by

1 giving them an explicit role as objective functions, rather than aggregating them into a single economic
2 indicator objective function [18]. Thus, the problem of optimizing energy systems can be addressed with a
3 multi-objective approach, where the solution vector is not determined by a single technical solution, but by a
4 set of optima. The optimal solution points form what is commonly referred to as a non-dominated set or Pareto
5 optimum. For each of the Pareto arrangements, improving one objective without worsening another is not
6 possible. For the calculation of the Pareto front, the epsilon-constraint method is widely used, especially for
7 cases where there are two objectives. This is due to the fact that it provides high reliability of the results within
8 brief computational time [19]. Optimization techniques are used in various simulation software packages to
9 plan energy systems. These pieces of software have been developed not only to evaluate the technical and
10 economic potential of energy systems, but also to simplify the design and operation process of systems that
11 include renewable sources maximizing, at the same time, their profitability [20]. However even though the use
12 of software programs seeks to maximize the use of renewable energies and thus, minimize the environmental
13 impact, most of them do not include environmental impact as a decision variable. Moreover when
14 environmental information is considered the impact related to equipment manufacturing is often excluded from
15 the analysis perimeter. A recent review [21] related to multi-objective optimization including environmental
16 criteria for hydrogen systems highlights that the environmental indicator most frequently used is GHG
17 emissions. Furthermore, the authors of this review show that most of the conducted studies are bi-objective,
18 and that one of the most used methodologies for this type of optimization is the epsilon-constraint. Although
19 there are some studies in this field with other methodologies such as evolutionary algorithms or inclusion of
20 machine learning [23], the epsilon-constraint methodology is currently still widely used [24].

21 This short literature review shows that the optimization of energy systems involves a wide field of numerical
22 approaches and tools. In terms of optimization methods, MILP formalism is largely used to obtain optimal
23 sizing and operation strategies of energy systems. There are increasing research in the field of optimal
24 operation of hydrogen energy systems however there are still few developments that take into consideration
25 simultaneously the dynamic conditions, the operation of the entire hydrogen supply chains and the embedded
26 environmental impact of all components involved.

27 **1.3. Objectives, paper organization and limitations**

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30 The analysis of the literature shows that optimization with simultaneous consideration of costs, all GHG
31 emissions (direct and indirect) of each component and dynamic behavior of hydrogen supply chains, is not
32 frequently addressed. Thus, based on previous motivations and literature review, the objective of the method
33 proposed in this paper is to go beyond state-of-the-art approaches by coupling simultaneously a dynamic
34 optimization using MILP modeling approach using linear technical and economic models as well as
35 incorporating cradle-to-gate environmental models in the optimizer covering all components involved in the
36 hydrogen supply chain. In this paper, this method is illustrated on a case study inspired by some of the
37 characteristics of the GreenHysland project.

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39 In alignment with Sustainable Development Goals (SDGs) such as Goal 7 (Affordable and Clean Energy)
40 and Goal 13 (Climate Action), this study focuses on optimizing hydrogen supply chains to mitigate greenhouse
41 gas emissions while ensuring economic viability. The objectives for this study were set as follows:

- 42 • Objective 1: To model hydrogen supply chain scenarios and to identify which optimal operation and design
43 are obtained when minimizing GHG emissions compared to minimizing costs (What would be the optimal
44 operating strategy for an electrolyzer from the point of view of decarbonization, given the nature of the
45 electrical energy consumed and the uses of hydrogen?);
- 46 • Objective 2: Analysing trade-offs and relationship between economic viability and environmental
47 sustainability using common indicators (such as levelized cost of hydrogen, levelized cost of avoided
48 emissions, specific emissions per kilogram of hydrogen);
- 49 • Objective 3: Highlighting how the choice of hydrogen transport mode influences economic and
50 environmental results;
- 51 • Objective 4: To provide insights about the most influencing components regarding cost and GHG emissions
52 breakdown of these hydrogen chains (comparing the share of hydrogen infrastructure with the share of
53 energy supply).

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56 It is worth noting that the support of decision-making for the implementation of hydrogen infrastructure
57 over a given territory involves multiple aspects such as technical, social, environmental, regulatory, economic,
58 or political considerations. This paper do not pretend to cover the whole spectrum of decision-making criteria
59 involved in this process. Moreover other aspects are excluded from the analysis:

- 60 • This study does not aim at establishing a multi-year investment planning for hydrogen infrastructure.
 - 61 • There are no consideration in terms of business model.
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- The goal is not to provide a full Life Cycle Assessment (LCA), despite the fact that general LCA principles are used
- The study presented in this paper has to be considered as an illustration of a method only.

The next section 2 provides the description of the method (case study definition, bi-objective optimization model formulation, scenario presentation). The results are presented and discussed in section 3. Finally conclusions and perspectives are provided in section 4.

1.4. Disclaimer

The study presented in this article contributes to the development of appropriate methodologies for impact analysis activities planned within GreenHysland project. The authors do not pretend to provide here an evaluation of economic or environmental performance of this EU project in itself. The case study detailed in this paper consists in a theoretical evaluation of an energy system inspired by some of the technical characteristics of the GreenHysland project. This theoretical evaluation aims at illustrating a bi-objective optimization methodology based on dynamic simulation. This study does not refer to potential hydrogen upscaling scenarios within the Balearic Islands. This paper constitutes a first step towards the development of multi-criteria analysis methodology for the assessment of hydrogen deployment scenarios.

2. Methods

2.1. System description

The architecture of the considered hydrogen system (Figure 1) is based on some of the characteristics of the GreenHysland project. The specifications of each element are provided below.

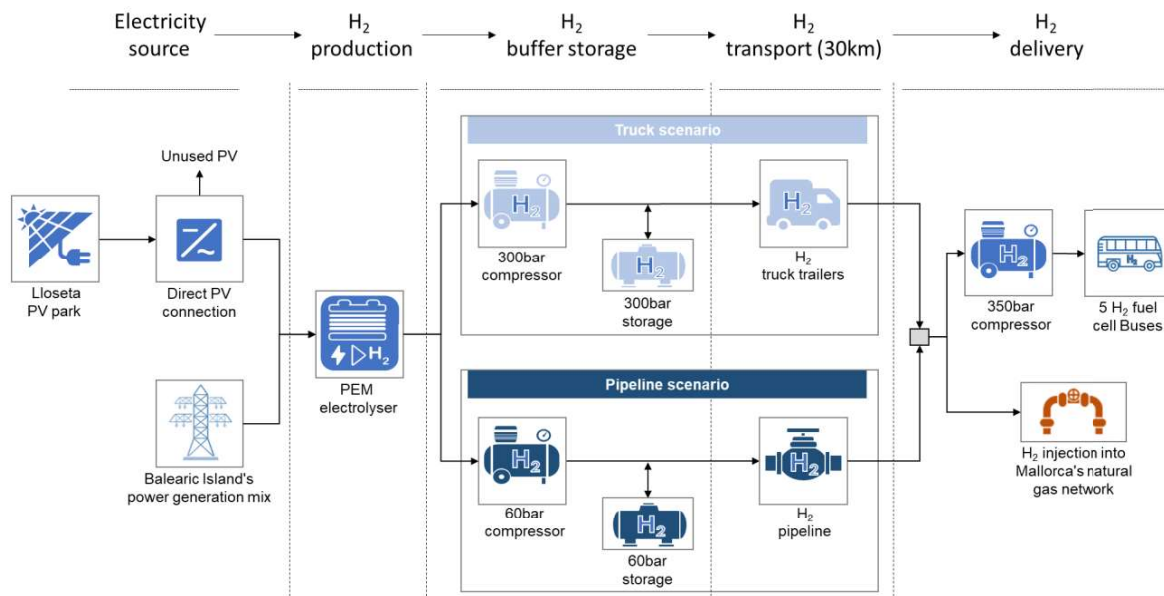


Figure 1: Illustration of the considered hydrogen supply chains and applications. (Note: electrical consumption of compressors is not represented in this graph).

- Electricity sources:

The system comprises a PV plant located in Lloseta with a peak power of 8.56 MW_p [9]. The electrolyzer and compressors are also connected to the electrical grid of Balearic Islands.

- Hydrogen production:

Hydrogen is produced using a centralized 7.5 MW Proton Exchange Membrane (PEM) electrolyzer placed in the municipality of Lloseta, at the same site as the PV plant. The electrolysis plant comprises three pressurized “HyLYZER® - 500” units connected to the PV park and to the islands’ electricity power grid. It produces hydrogen at 30 bar at a maximal flow rate of 135 kgH₂/h.

- Hydrogen compression, storage and transport:

Once produced, hydrogen is compressed, stored and transported to Palma de Mallorca over a distance of 30 km.

- In the Truck transport scenario, hydrogen produced by the electrolyzer is compressed from 30 bar to 300 bar in order to fill the truck trailers. This pressure level corresponds to the operating pressure selected in GreenHysland project for truck trailers [9]. A hydrogen buffer storage capacity is considered at the electrolysis plant location. This buffer storage consists in on-site additional trailer capacity, therefore the same maximum hydrogen pressure of 300 bar is considered. Hydrogen is then transported at 300 bar towards the hydrogen end-use applications.
- In the Pipeline scenario, hydrogen is compressed from 30 bar to 60 bar. The 60 bar hydrogen pressure assumption for the hydrogen pipeline has been chosen based on potential operating pressures mentioned in the European Hydrogen Backbone study [25] where a range of 50 bar to 80 bar is mentioned for distribution and transportation pipelines respectively. A hydrogen buffer storage capacity is also considered at the electrolysis plant location. This buffer storage is supposed to be designed for a maximum operating pressure of 60 bar. Hydrogen is then transported at 60 bar towards the hydrogen end-use applications.

- Hydrogen applications:

Hydrogen is delivered to a hydrogen buses refueling station. In this study the technical model of the refueling infrastructure is simplified considering only a single compressor for direct delivery of hydrogen at 350 bar (no high pressure buffer storage at refueling station). Hydrogen is used as a fuel for a fleet of five fuel cell buses. The refueling station is placed in Palma de Mallorca. Each bus has five 350 bar hydrogen tanks of 312 litres each (1,560 litres in total). It is assumed that this volume is equivalent to a usable capacity of 37.5 kg of hydrogen. It is supposed that all buses are refueled once a day; hence ~70 tons of hydrogen are needed in a complete year corresponding to an average flow rate demand of 8 kgH₂/h. For simplification, this value as been considered as a constant and mandatory demand at each hour of the year, assuming that the buses are refuelled sequentially. In parallel the hydrogen produced in Lloseta can be injected into the Mallorca's natural gas grid. The injection point is also placed in Palma de Mallorca. The injection of hydrogen into the NG grid is supposed to be a flexible injection with a maximal allowable hydrogen flow rate of 4%_{vol} (target for GreenHysland project).

2.2. Optimization approach

2.2.1 Overview

The technical and economic study presented in this paper is carried out with PERSEE software developed at CEA by members of LSET laboratory in Grenoble, France. PERSEE is a tool for optimizing the sizing and management of multivector energy systems, based on MILP formulation [24]. The software allows the modeling and multi-objective optimization of energy systems, such as industrial processes or energy production facilities. Two approaches can be implemented. If the size or production capacity of an existing facility is already known, optimization is performed to optimally operate the system over several years of operation. Conversely, if the facility size or production capacity is an unknown variable, it is optimized in order to determine the system optimal size. Whatever the case, from all the information entered by the user, PERSEE creates a system of equations containing the objective function and all the constraints of the problem. Subsequently, this system of equations is solved using a commercial solver, such as Cplex. PERSEE software gives various optimization options to the user: (i) Economic optimization through the minimization of the Total Cost function (or maximization of the Net Present Value, NPV), expressed in €; (ii) Environmental optimization through the minimization of one environmental impact, among a set of available impact categories (for instance: minimization of the cumulated GHG emissions over the entire industrial project lifetime, expressed in kgCO_{2-eq}). In order to build the front of optimal solutions, the epsilon-constraint method is currently implemented in PERSEE but interface with specific multi-objective optimization algorithms is also possible. Once the environmental, technical and economic constraints are set, the optimization is spread over a period of one year, with a specific time step, for example, one hour. Then PERSEE has to meet the imposed constraints minimizing the Total Cost and/or minimizing the considered environmental impact.

The Figure 2 below presents an overview of the steps involved in the present study. The first step consists in the choice and modelling of dynamic data and equipment data. The second step relates to the optimization process itself and the third step consists in the analysis of optimization results. These steps are detailed in the next parts of the paper. Dynamic data are provided in section 2.2.2, environmental approach is described in section 2.2.3, followed by economic approach in section 2.2.4 and the formulation of the bi-objective optimization problem in section 2.2.5. A summary of the technical, economic and environmental data used to perform this study is presented in Appendix A.

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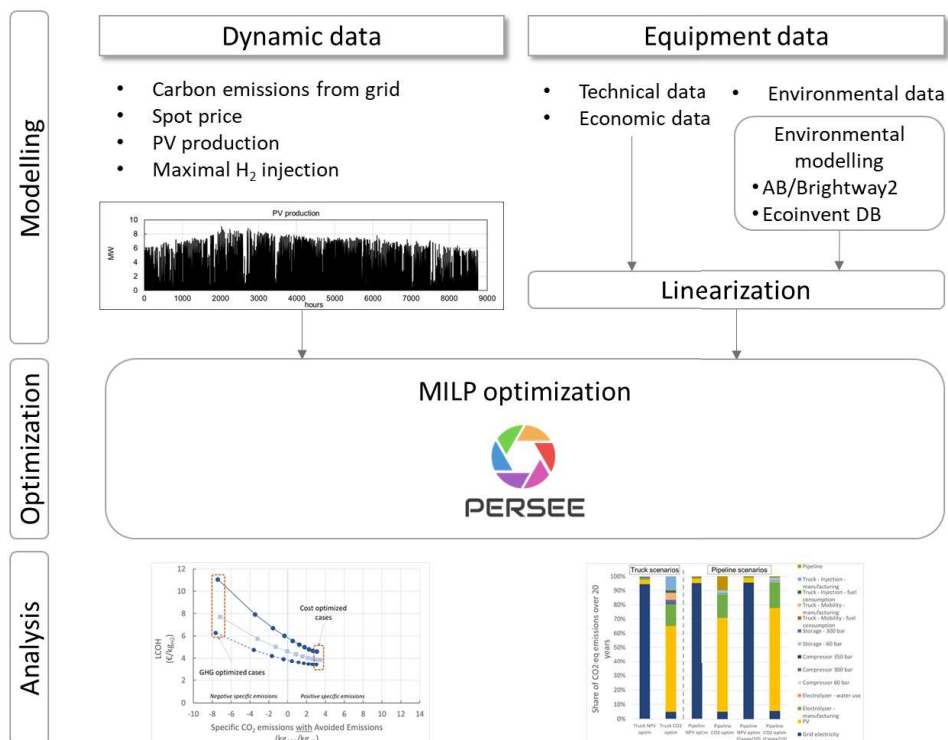


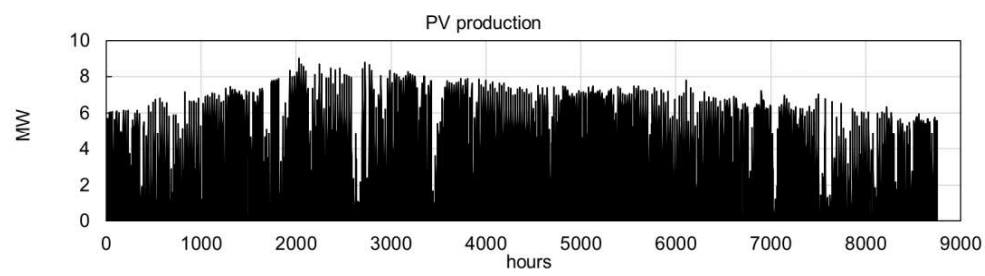
Figure 2: Overview of the optimization process.

2.2.2 Dynamic data

2.2.2.1 Overview

The dynamic optimization approach presented in this paper has been performed based on a set of variable temporal data over a period of 1 year and a time step of 1 hour (Figure 3):

- PV production has been determined using PVGIS platform for Lloseta location [28];
- Grid electricity hourly data (power generation mix, spot price, emissions) in 2019 have been obtained courtesy from the Engineering Department of Universitat de les Illes Balears (UIB) [26]. Even though data series from 2020 and 2021 were also available, they were not considered in the present study given that both 2020 and 2021 were atypical years due to the COVID-19 pandemic. Additional calculations have also been performed in order to take into account emissions related to import of electricity from Spanish mainland through High Voltage connexion, as detailed in the next section.
- Maximal allowable hydrogen injection profile (4%vol) has been obtained based on natural gas (NG) consumption, which has been approximated from the electrical production of NG-based power plants as these plants are the main NG consumers in Balearic Islands.
- As mentioned in section 2.1, hydrogen demand for the mobility application was fixed at a constant mass flow of 8 kgH₂/h all over the simulated year.



(a)

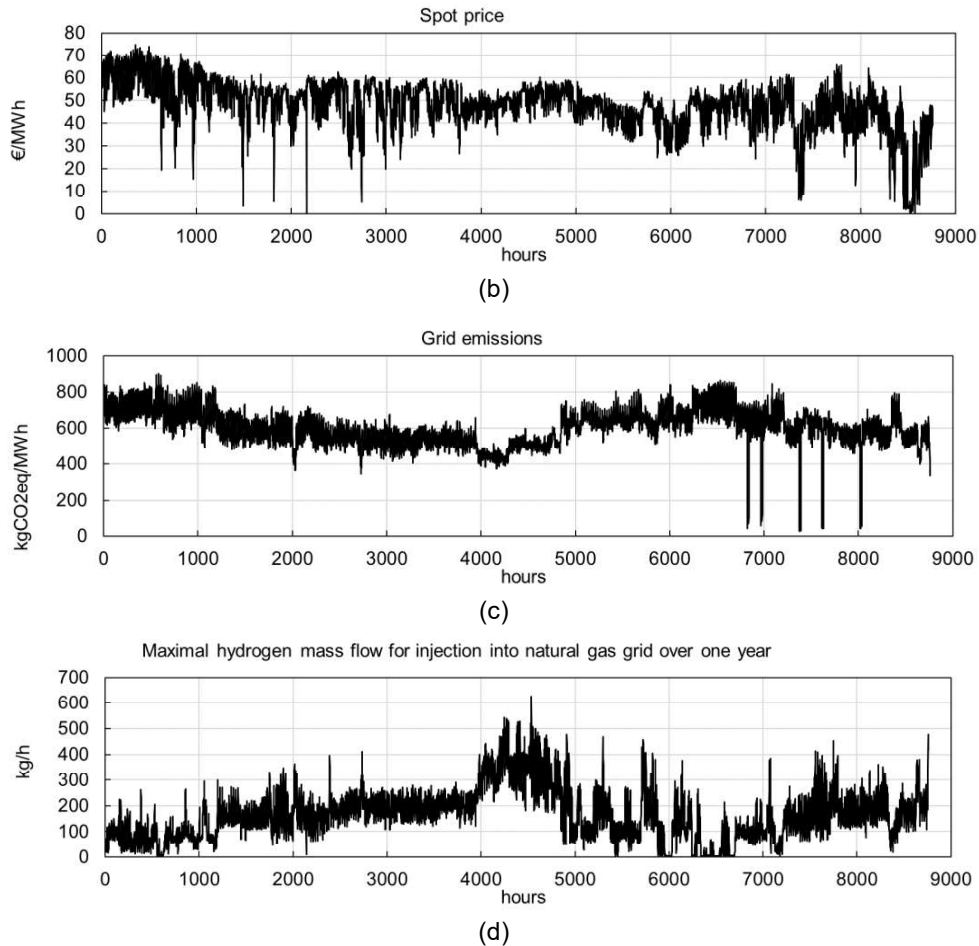


Figure 3: Overview of the temporal data used in this study: (a) PV production, (b) Grid electricity price, (c) Grid emissions and (d) Maximal hydrogen mass flow rate for injection into natural gas grid.

2.2.2.2 Focus on GHG emissions of Balearic electrical grid

Since the objective of the study was to optimize dynamically the hydrogen production including the environmental impact, hourly data of GHG emissions of the Balearic Islands' electricity grid have been calculated. In order to know the GHG emissions of the electricity consumed in the Balearic Islands, emissions from energy imports have been taken into account. For this purpose, ENTSOE emission data of power generation in Spain mainland [27] were used and added to the GHG temporal data provided by the Industrial Engineering Department of the University of the Balearic Islands [26]. Emission factor for PV production was also considered based on [29]. Thus the temporal evolution of the 2019 GHG emission factor of the Balearic electrical grid was obtained (Figure 4) with a corresponding yearly averaged emission factor of 590 kgCO₂-eq/MWh. In addition, a reduction of carbon intensity of the electrical grid over the years has been considered based on the scenario proposed by the Ministry for Ecological Transition and the Demographic Challenge of the Balearic Islands [5] and assuming an emission factor below 160 kgCO₂-eq/MWh for year 2039 as the optimization is performed over a 20 years duration (from 2019 to 2039). Thus, a reduction coefficient was implemented in PERSEE in order to take into account this decrease in grid GHG emissions over the supposed 20 years lifetime of the hydrogen supply chain considered in this study.

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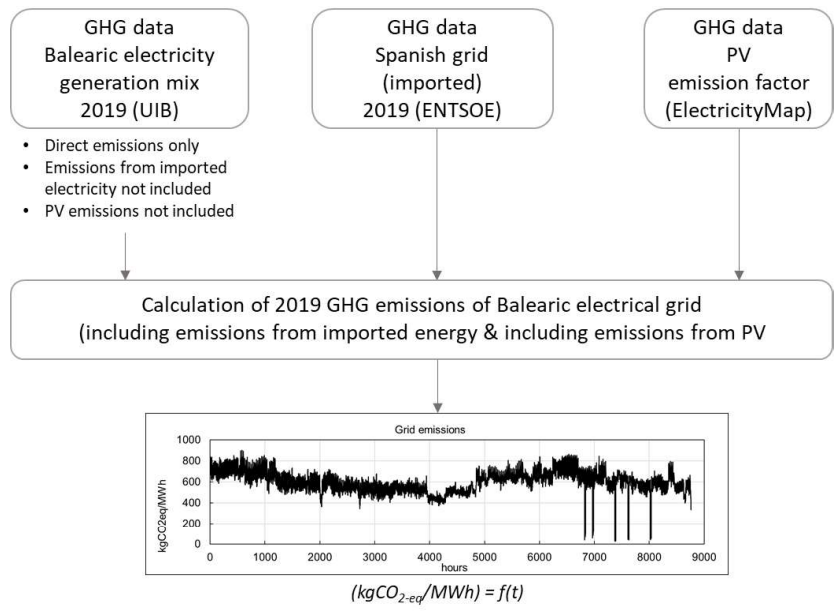


Figure 4: Process for elaborating temporal GHG emission factor ($kgCO_{2-eq}/MWh$) of Balearic electrical grid, including emissions from imported energy.

2.2.3 Environmental approach and data

2.2.3.1 Overview

In this study, the goal is not to conduct a full and formal Life Cycle Assessment (LCA) study as recommended by ISO standards [22] as no formal critical review is foreseen. The objective is to illustrate the coupling between optimization process and environmental impact analysis. However, in the next paragraphs the environmental approach implemented in this study is highlighted following some of the typical steps of the LCA methodology.

- **Goal:**

The goal of this study is (i) to quantify the greenhouse gases emissions over the entire hydrogen supply chain and (ii) to compare truck and pipeline scenarios. The aim is to take into consideration impacts related to grid electricity consumption as well as embedded emissions related to equipment life cycle and avoided emissions related to substitution of fossil fuels by hydrogen for two applications (mandatory energy delivery to five hydrogen buses and a flexible injection in natural gas grid).

- **Scope:**

A cradle-to-gate perimeter was chosen, meaning that the cradle-to-gate impacts of each equipment involved in the supply chain were considered. End-of-life of equipment is out of the scope of this study. The perimeter of the environmental analysis is provided in Figure 5. In addition to electricity consumption, the use phase of the components was considered through consumption of treated water for the electrolyzer as well as consumption of diesel fuel for the truck trailers.

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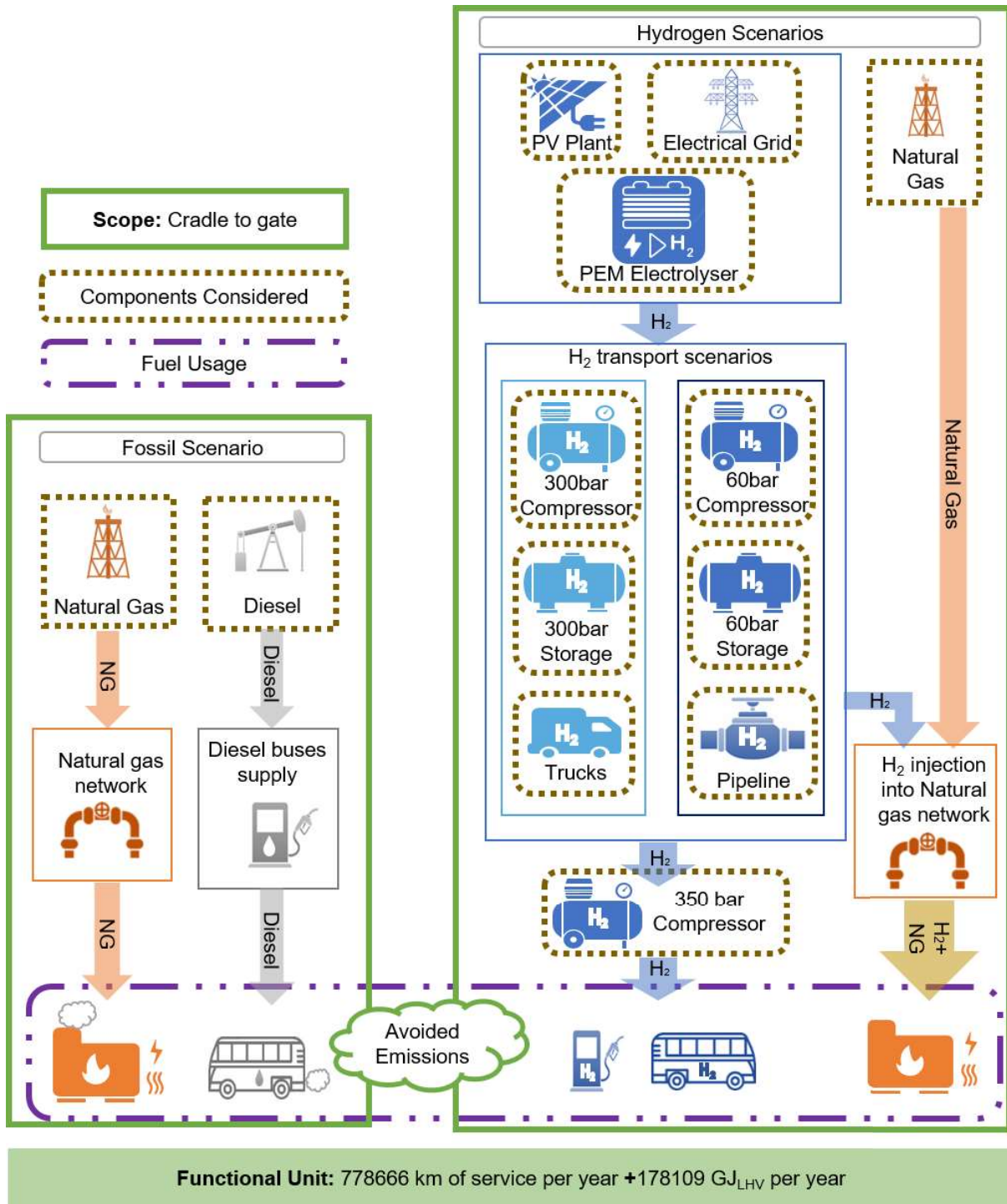


Figure 5: Perimeter of the environmental analysis for the case study.

• **Functional unit:**

In order to be able to compare the scenarios between them and to compute properly the avoided emissions when comparing with fossil fuel scenario, it is necessary to define a functional unit related to the equivalent service provided. Therefore the functional unit considered in this study is representing the two end-uses of the hydrogen delivered and is formulated as follows: "a fixed yearly distance of 778 666 km of service for urban buses AND a maximum of 178 109 GJ of thermal energy content injected into the natural gas network".

- "a fixed yearly distance of 778 666 km of service for urban buses" : this distance corresponds to a consumption of 9 kgH₂/100km and assuming a constant hydrogen demand of the 5 buses fleet over the entire year (8760 hours at 8 kgH₂/h);

- “a maximum of 178 109 GJ of thermal energy content injected into the natural gas network”: this value comes from the assumption of a maximal hydrogen injection of 4%_{vol} in the natural gas network, based on the estimated yearly natural gas consumption in Balearic Islands. With such definition, the amount of hydrogen injected is a degree of freedom for the optimization.

- **Alternatives:**

The alternatives compared for this functional unit are Hydrogen supply and Fossil supply. The avoided emissions are then calculated considering the same service provided by diesel buses (yearly distance of 778 666 km) and same thermal energy provided by natural gas (flexible part of the optimization) with a quantity depending on the amount of hydrogen injected, with a maximum of 178 109 GJ per year.

- **Methods:**

Despite the fact that different LCA software have been developed over the past two decades, the research community has always developed its own software implementations that could be adapted and extended to build advanced, non-standard LCA models. As a way of example, Brightway version 2 has been developed since 2012 as an open source Python-based LCA framework, and has been widely used throughout the research community [33]. This software has been chosen for this study due to its flexibility for building parametrized environmental impact models. In order to obtain the results of the direct and indirect emissions of the different components of the system, it is necessary to define the boundaries and the impact categories. In this case, only the end-of-life stage of the components is not considered (Figure 5). The environmental impact category selected for the Life Cycle Impact Assessment (LCIA) is the Global warming potential (GWP) of the EV3.0 method. Ecoinvent 3.8 database ([34],[35]) is used for the selection of the activities for the diverse components. It is important to highlight that when selecting the Ecoinvent activities, a geographic prioritization is established. For this study, priority was given to Spain data in the database. When no Spain reference was available, European data (RER) was selected and, if the latter was not available, "global" (GLO) and "rest of the world" (RoW) data was chosen.

- **Link with optimization:**

Environmental information has to be included in the linear optimization problem considering the life cycle impacts of all components of the energy system. Therefore the emissions for most of the elements of the system have been linearized in relation with system sizes with the aim of achieving an accurate modelling within the framework of the MILP formalism. An overview of the data sources and environmental modelling is presented in Table 1 while the linear relations are provided in Appendix A - Table A.2.

Table 1

Data sources and Environmental modelling chosen for each type of equipment

Component	Modelled with AB/Brightway + linearization	Direct use of existing environmental data	Comments
PV plant	No	Yes	Based on [29]
Electrolyzer	Yes	No	Modelled with [33] and data from [34], [35], [36], [37]
Compressors	Yes	No	Modelled with [33] and data from [34], [35], [36], [38]
Hydrogen buffer storages	Yes	No	Modelled with [33] and data from [34], [35], [39] & internal data for steel tanks
Truck trailers	Yes	No	Modelled with [33] and data from [34], [35], [39]
Pipeline	No	Yes (Ecoinvent)	Using NG pipeline data from [34], [35]
NG emissions	No	Yes (Ecoinvent)	Modelled with [33] and data from [34], [35]
Diesel bus emissions	No	Yes (Ecoinvent)	Modelled with [33] and data from [34], [35]

2.2.3.2 Modelling and linearization of equipment's embedded emissions

- **PEM Electrolyzer**

The PEM electrolyzer inventories used in the present work are updated from [37]. GHG emissions for the production phase of the PEM system have been calculated for 10 system capacities using Activity Browser software, since some components of the Balance of Plant (BoP) of PEM systems do not increase in a linear way. For this purpose, reference [36] was used. The information obtained has been adjusted so that it can be added to the MILP optimization problem. Therefore, a linear adjustment is made for the system, giving as a result the linear function shown in Appendix A Table A.2.

- **Compressors**

1 In order to obtain the GHG emissions values of compressors, the study published by Ghandehariun and
2 Kumar [38] was used. Since the assumptions between the literature and the studied system are different,
3 particularly the system capacity, the exponential rule has been applied for the calculation of energy and
4 material inputs applying the extrapolation equation suggested in [36]. The value of the GHG emissions has
5 been calculated for different compressor capacities and a linear regression was made resulting in the linear
6 function expressed in Appendix A Table A.2.

- 7 • *Hydrogen Storages*

8 The linear functions for calculating indirect product emissions related to the manufacturing of type I tank for
9 60 bar storage and type II tank for 300 bar storage are given in Appendix A Table A.2, referring to hydrogen
10 storage capacity expressed in kgH₂. Numerical coefficients were based on internal data and inventory from
11 [39] as well as data from Ecoinvent database ([34],[35]) from which dedicated linear relations were built.

- 12 • *Truck trailers*

13 The environmental impact of truck trailers was considered only through the trailer part of the truck (hydrogen
14 storage vessels and trailer materials). The same hydrogen storage technology was considered for 300 bar
15 storage of the truck trailer as for 300 bar buffer storage (type II tanks mounted on trailer) therefore the equation
16 for estimating the GHG emissions from truck trailers is equivalent to the one obtained for 300 bar hydrogen
17 storage (Appendix A Table A.2).

- 18 • *Hydrogen pipeline*

19 Emissions related to the life cycle of hydrogen pipeline has been derived from natural gas pipeline data
20 from Ecoinvent database ([34],[35]).

21 **2.2.4 Economic approach and data**

22 2.2.4.1 Hydrogen price

23 Hydrogen price depends on many factors. It is influenced not only by production and distribution costs, but
24 also by the selected end-use application [44]. The specific requirements and conditions of each hydrogen end-
25 use application (e.g. energy carrier, fuel, feedstock for industry) determine some crucial aspects, such as
26 hydrogen level of purification or storage conditions. In addition, taxes also play a critical role in establishing
27 hydrogen prices. For instance in the field of mobility, green hydrogen might only be subject to Value Added
28 Taxes (VAT), as no environmental taxes may apply during the initial steps of introduction into the transport
29 sector [45].

30 Various studies analyze the future on hydrogen prices. The International Energy Agency (IEA) declares
31 that the drop in the renewable energy costs can make the cost of green hydrogen decreasing to a range of
32 1.3-4.5 USD/kgH₂ by 2030 [46]. When considering the mobility sector, McKinsey & Company establish a
33 hydrogen 2030 breakeven cost between 4.4 and 4.6 USD/kgH₂, without any cost of carbon emissions [47].
34 The Fuel Cells and Hydrogen Joint Undertaking (FCH JU) has determined the goal to reach a hydrogen price
35 between 4.5 and 7 €/kgH₂ by the year 2025 [45]. Additionally, authors in [45] assumed a final selling price for
36 hydrogen equal to 4 €/kgH₂. According to them, this value covered green hydrogen production costs, and it
37 provided some profit.

38 Therefore, in the present study, the hydrogen selling price for the mobility application has been also set to
39 4 €/kgH₂. When considering hydrogen selling price for the natural gas grid injection, the same value (4 €/kgH₂)
40 was adopted. This price value would correspond to a situation where hydrogen is being significantly
41 incentivized as its magnitude differs from the price calculated on a heat content basis from current natural gas
42 price. The main reason of this choice lies in maintaining for both applications the same conditions in terms of
43 hydrogen selling prices. In forthcoming publications, additional research could be conducted to explore
44 breakeven costs for green hydrogen across different applications and conducting sensitivity studies on the
45 hydrogen price and analyzing the impact of these assumptions on the optimization results and shape of Pareto
46 fronts.

47 2.2.4.2 Project lifetime and discount rate

48 A project lifetime of 20 years was considered. Data series were based only on information of the year 2019.
49 For this reason, each time series was replicated over the years in order to guarantee the optimization over the
50 20-years period. The Net Present Value optimization was performed considering a discount rate of 7%.

51 **2.2.5 Formulation of the bi-objective optimization problem**

52 2.2.5.1 Optimization objectives

53 The aim of this study is to compare hydrogen supply scenarios and analyse trade-off and relationship
54 between costs and cumulated emissions. In this study the system is optimized through the computation of two
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main indicators which are the Total Cost TC and the Cumulated Emissions E , over the entire industrial project lifetime Y .

The Total Cost function (eq. 1) expressed in Euro (€) is calculated considering both Capital expenditures and Operational expenditures, including revenues from hydrogen delivery.

$$TC = \sum_{el=1}^N \left[CA_{el} * S_{el} + \sum_{i=1}^Y \frac{OP_{el} + \sum_{t=1}^{8760} BC_b * F_t^b - \sum_{t=1}^{8760} SP_s * F_t^s}{(1+k)^i} \right] \quad (\text{eq. 1})$$

el	Element of the system (-)
N	Number of elements of the system (-)
CA_{el}	Specific capital expenditures of each element el (€/size_unit)
S_{el}	Size of element el (size_unit)
OP_{el}	Operational expenditures (annual basis) of each element el (€/year)
BC_b	Buying cost of energy b consumed by each element el (€/flux_unit)
SP_s	Selling price of energy s sold by each element el (€/flux_unit)
F_t^b	Flow of bought energy b at time t
F_t^s	Flow of sold energy s at time t
k	Discount rate (%)
Y	Project lifetime (years)
t	time step (hour)

In this study, the Cumulated Emissions function (eq. 2) refers specifically to GHG emissions, expressed in mass of CO₂ equivalent (kgCO_{2-eq}). The considered environmental analysis perimeter has been described in part 2.2.3. It comprises both direct and indirect emissions of the hydrogen supply chains. Direct emissions are related to diesel combustion in truck trailers. Indirect emissions are related to grid electricity consumption and manufacturing of each element (also referred as “CAPEX-related emissions”). In this paper avoided emissions refer to the amount of emissions that would have been emitted with conventional fossil fuel-based solution (substitution of diesel in buses by hydrogen and substitution of natural gas in the grid by hydrogen). The manufacturing of diesel buses, hydrogen buses, gas generators are out of scope (Figure 5).

$$E = \sum_{i=1}^Y \left[\sum_{t=1}^{8760} DE_t + \sum_{t=1}^{8760} IEG_t + \sum_{el=1}^N IPE_{el} - \sum_{t=1}^{8760} AE_t \right] \quad (\text{eq. 2})$$

DE_t	Direct emissions from combustion of diesel in truck trailers (kgCO _{2-eq} /h)
IEG_t	Indirect emissions from grid electricity consumption (kgCO _{2-eq} /h)
IPE_{el}	Indirect product manufacturing emissions of element el (kgCO _{2-eq})
AE_t	Avoided emissions compared to reference fossil scenario (kgCO _{2-eq} /h)

Based on this definition, the solutions characterized by negative values of E will correspond to situations where greenhouse gases emissions generated throughout the hydrogen supply chain are lower than the fossil fuel scenario. Therefore these solutions will be considered as more “sustainable” from the greenhouse gases emissions perspective. Of course these “negative” emissions do not refer to carbon removal from the atmosphere.

2.2.5.2 Problem formulation

• 2.2.5.2.1 Formulation

The minimization of Total Cost function can be written as follows:

$$TC_{\min} = \min : TC \quad (\text{eq. 3})$$

Leading to a set of both *sizing* and *operation* optimal variables:

$$\left\{ \begin{array}{l} \varphi \\ T \end{array} \right\} \xrightarrow{TC_{\min}} \left\{ \begin{array}{l} S^{TC_{\min}} \\ O_T^{TC_{\min}} \end{array} \right\} \quad (\text{eq. 4})$$

φ System to be optimized

T	Optimization horizon (hours)
$S^{TC_{min}}$	Sizing variables: set of optimized equipment sizes
$O_T^{TC_{min}}$	Operation variables: matrix of optimized energy and mass flows over the optimization period T

The minimization of Cumulated Emissions function can be written as follows:

$$E_{min} = \min : E \quad (\text{eq. 5})$$

Leading to another set of both *sizing* and *operation* optimal variables:

$$\left\{ \begin{array}{l} \varphi \\ T \end{array} \right\} \xrightarrow{E_{min}} \left\{ \begin{array}{l} S^{E_{min}} \\ O_T^{E_{min}} \end{array} \right. \quad (\text{eq. 6})$$

$S^{E_{min}}$	Sizing variables: set of optimized equipment sizes
$O_T^{E_{min}}$	Operation variables: matrix of optimized energy and mass flows over the optimization period T

Regarding the sizing variables S , the only variables considered were 60 bar and 300 bar hydrogen storage capacities in order to see if the optimizer finds an interest in investing in these equipment as it brings possibility of desynchronization of production and demand. The main upstream operation variables are related to the PV and grid power consumed at time t . The optimization is performed in PERSEE taking into account a set of technical constraints formulated for each element as well as general constraints to ensure the equilibrium of energy and mass balance in the system. In this study, the bus demand can be considered as a constraint while hydrogen mass flow injected in NG network stands for a downstream optimization variable with an upper bound set at 4%_{vol} of NG flow rate at each time t . The following (eq. 7) expresses the constraints related to the minimal delivery of hydrogen demand for buses and maximal hydrogen injection into the natural gas grid.

$$\dot{m}_{H2Bus}(t) \leq \dot{m}_{H2delivered}(t) \leq \dot{m}_{H2Bus}(t) + \dot{m}_{H2InjectMAX}(t) \quad (\text{eq. 7})$$

$\dot{m}_{H2Bus}(t)$	Hydrogen demand for buses at time t
$\dot{m}_{H2delivered}(t)$	Total hydrogen mass flow rate delivered (buses and injection) at time t
$\dot{m}_{H2InjectMAX}(t)$	Maximal allowable hydrogen mass flow rate into the natural gas grid at time t

- 2.2.5.2.2 Formulation of the epsilon-constraint approach

A bi-objective optimization has been performed to evaluate the solution space at the interplay of the two conflicting objectives (Total Cost minimization and Cumulated Emissions minimization). In order to build the Pareto front, two mono-objective optimizations are performed (eq. 8 and eq. 9): (i) in the first one, Total Cost is minimized without applying any Cumulated Emission constraint; (ii) in the second one, Cumulated Emissions are minimized:

- Minimization of Total Cost generates one extreme point of the Pareto front:

$$\left\{ \begin{array}{l} \varphi \\ T \end{array} \right\} \xrightarrow{TC_{min}} \left\{ \begin{array}{l} S^{TC_{min}} \\ O_T^{TC_{min}} \end{array} \right. ; (TC_{min}; E_{TC_{min}}) \quad (\text{eq. 8})$$

- Minimization of Cumulated Emissions generates the other extreme point of the Pareto front:

$$\left\{ \begin{array}{l} \varphi \\ T \end{array} \right\} \xrightarrow{E_{min}} \left\{ \begin{array}{l} S^{E_{min}} \\ O_T^{E_{min}} \end{array} \right. ; (TC_{E_{min}}; E_{min}) \quad (\text{eq. 9})$$

- Then 10 intermediate scenarios were defined with equidistant Cumulated Emissions constraint between E_{min} and $E_{TC_{min}}$:

$$E_i \in [E_{\min}; E_{TC_{\min}}] \quad (\text{eq. 10})$$

$$E_i = E_{\min} + \left(\frac{E_{TC_{\min}} - E_{\min}}{10} \right) * i$$

- The optimal points of the Pareto front are then obtained by minimizing the Total Cost function for each intermediate Cumulated Emissions constraint:

$$\min : TC \quad (\text{eq. 11})$$

s. t.

$$E \leq E_i$$

- Then the coordinates of the points of the Pareto front were obtained:

$$\left\{ \begin{array}{l} \varphi \\ T \end{array} \right\}_{E_i} \Rightarrow \left\{ \begin{array}{l} S^{E_i} \\ O_{E_i} \end{array} \right\}; (TC_{E_i}; E_i) \quad (\text{eq. 12})$$

2.2.5.3 Indicators

It has been chosen to focus on specific indicators that are commonly used for analysis of economic and environmental performance of hydrogen systems:

- Levelized cost of hydrogen
- Specific emissions
- Levelized cost of avoided CO_{2-eq}.

2.2.5.3.1 Levelized cost of hydrogen

In particular, the Levelized Cost of Hydrogen (LCOH) expressed in €/kgH₂ is defined as the ratio between the Total Cost (without revenues) and the levelized hydrogen production over the project lifetime:

$$LCOH = \frac{\sum_{e1=1}^N [CA_{e1} * S_{e1} + \sum_{i=1}^Y \frac{OP_{e1} + \sum_{t=1}^{8760} BC_b * F_t^b}{(1+k)^i}]}{\sum_{i=1}^Y \frac{M_{H_2}}{(1+k)^i}} \quad (\text{eq. 13})$$

with

M_{H_2} Annual mass of hydrogen delivered to the final applications (kgH₂/year)

2.2.5.2 Specific emissions

Similarly, in this paper the indicator “specific emissions” was used, expressed in kgCO_{2-eq}/kgH₂ as the ratio between the cumulated emissions and the cumulated hydrogen production over the project lifetime. The specific emissions indicate the amount of greenhouse gases emitted per unit of hydrogen produced (expressed as kgCO_{2-eq}/kgH₂). This environmental impact is quantified for various scenarios in order to determine their sustainability. As for cumulated emissions, solutions characterized by negative values of specific emissions indicate a net reduction in emissions compared to reference fossil solutions, even if they come with higher costs.

$$e_{GHG} = \frac{E}{\sum_{i=1}^Y M_{H_2}} \quad (\text{eq. 14})$$

2.2.5.2.3 Levelized cost of avoided CO_{2-eq}

Finally it has been chosen to focus on the Levelized Cost of Avoided CO_{2-eq} (LCAC) expressed in €/tCO_{2-eq_avoided} which can be calculated when the results from optimization lead to negative Cumulated Emissions, meaning that the avoided emissions compared to reference fossil case become higher than the emissions from the hydrogen case:

$$LCAC = \frac{\sum_{e=1}^N [CA_{e1} * S_{e1} + \sum_{i=1}^Y \frac{OP_{e1} + \sum_{t=1}^{8760} BC_b * F_t^b}{(1+k)^t}]}{|E|} \quad (\text{eq. 15})$$

With $E < 0$

2.3. Scenarios

In the present three hydrogen supply scenarios were considered performed:

- [Truck scenario]: Truck trailers are supposed to be used to transport hydrogen from Lloseta photovoltaic plant to Palma de Mallorca, where the applications of mobility and injection into the natural gas grid are placed. In this case, it is assumed that all hydrogen produced by the PEM electrolyzer is transported by trucks. Here, 2 trucks are used to supply hydrogen to the refuelling station, whereas other 4 are involved in potential hydrogen injection into the natural gas grid. These numbers of trucks have been pre-determined based on electrolyzer maximal flowrate, hydrogen demand and unitary truck capacity ensuring, therefore, permanent availability of transport capacity at production site.
- [Pipeline scenario 1]: A pipeline specifically designed to convey 135 kgH₂/h flow rate is used for the transport of hydrogen from Lloseta to Palma.
- [Pipeline scenario 2]: In this scenario, the pipeline capacity is supposed to be oversized by a factor of 10 in order to cover an increase in the hydrogen production capacity of the production plant, compared to the initial value (135 kgH₂/h). Therefore, the capital cost and embedded GHG emissions of the pipeline are adjusted to the scale of the case study, being divided by a factor 10.

3. Results & Discussion

3.1. Pareto Front

3.1.1 Overview

Figure 6 provides the Pareto front obtained for each hydrogen transport scenario. The graph shows the Net Present Value (Y axis) as a function of the cumulated emissions (X axis) over the 20 years project time. The NPV is equal to the opposite of the Total Cost. This indicator is chosen here for facilitating interpretation of graph with positive values of Y axis showing profitable solutions. The objective of getting a front for each scenario is to obtain an overview of the costs and emissions ranges for each option showing the impact of hydrogen transport mode and corresponding assumptions on emissions and cost results. The Pareto front represents the best economic performances that can be achieved for a given amount of cumulated greenhouse gases emissions. Moreover, it allows getting all points to confirm the trend of each indicator for each scenario, and highlighting relationship and trade-offs between cost optimization and environmental impact optimization. The scenarios have been separated to highlight the distinct outcomes under different sets of assumptions. By presenting each transport scenario individually, a transparent comparison of the optimal costs and greenhouse gas emissions is provided. The graph can be interpreted considering four zones:

- ⇒ Green zone : profitable and sustainable : this zone corresponds to positive values of the NPV and negative values of the cumulated emissions which represent the fact that emissions from the hydrogen chain are lower than those of the reference fossil scenario.
- ⇒ Orange zone: profitable but not sustainable : this zone corresponds to positive values of the NPV and positive values of the cumulated emissions which represent the fact that emissions from the hydrogen chain are higher than those of the reference fossil scenario.
- ⇒ Blue zone: non profitable but sustainable : this zone corresponds to negative values of the NPV (non-profitable) and negative values of the cumulated emissions which represent the fact that emissions from the hydrogen chain are lower than those of the reference fossil scenario.
- ⇒ Red zone: non profitable and not sustainable : this zone corresponds to negative values of the NPV (non-profitable) and positive values of the cumulated emissions which represent the fact that emissions from the hydrogen chain are higher than those of the reference fossil scenario.

Figure 7 provides the yearly hydrogen delivery obtained in the case of the Truck NPV optimization case and Truck GHG optimization case, highlighting the difference in hydrogen production between both optimizations.

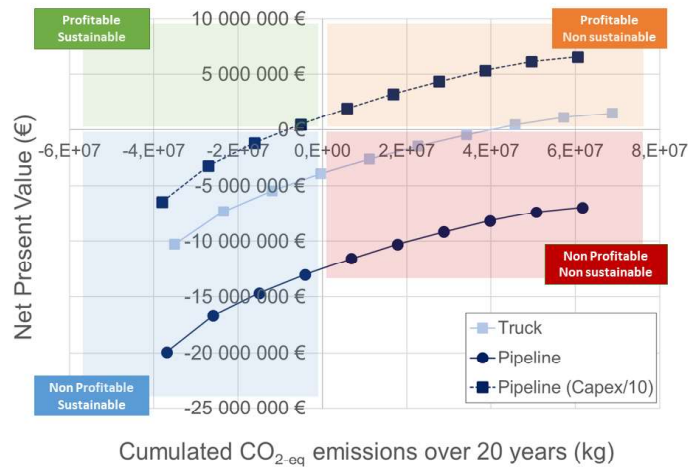


Figure 6: Pareto Front obtained for each of the three scenarios

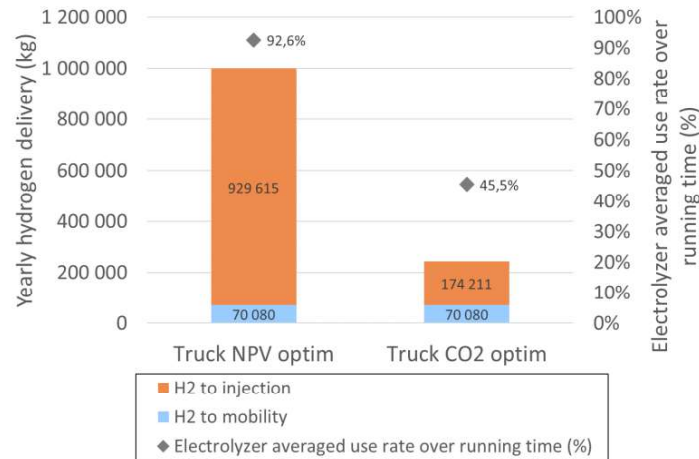


Figure 7: Yearly hydrogen quantity delivered to hydrogen buses and injected into the natural gas network in the case of the Truck scenario, for the two optimal solutions obtained when minimizing costs ("NPV optim") and minimizing GHG emissions ("CO₂ optim")

3.1.2 Net Present Value

The negative values of net present value (NPV) in the analysis are crucial indicators of the economic viability of hydrogen supply chain scenarios. They show that focusing only on environmental optimization, without considering economic factors, can lead to unprofitable systems. The significant economic differences between scenarios emphasize the importance of CAPEX assumptions. The pipeline scenario becomes the most profitable when CAPEX costs are lower. This suggests the need for careful evaluation of investment expenses to determine the economic feasibility of hydrogen supply chain options. Negative values of NPV come from under utilization of assets and much less hydrogen sold (as shown in Figure 7) leading to less amortization of investments. These negative values indicate that within the specified parameters, the analyzed systems lack economic profitability when focusing solely on environmental optimization. Moreover, the notable economic divergences among scenarios underscore the sensitivity of outcomes to assumptions, with the pipeline scenario emerging as the most profitable under reduced CAPEX costs assumptions. This highlights the necessity of carefully evaluating investment and operational expenses in appraising the economic feasibility of hydrogen supply chain options.

3.1.3 Cumulated emissions

Due to the consideration of avoided emissions compared to reference fossil solutions, it is possible to interpret some information by considering two zones in this graph:

- "Positive" emissions:

- In this zone, emissions from hydrogen chain are higher than reference situation despite accounting for avoided emissions. This zone corresponds to high electrolyzer use rate using carbonated grid electricity and leading to lower total cost (resp. higher Net Present Value).
- “Negative” emissions:
 - Cumulated emissions are negative meaning that there is a larger amount of avoided emissions compared to direct and indirect emissions from the hydrogen chain. This zone corresponds to solutions where PV electricity is prioritized, injecting PV based hydrogen into natural gas grid instead of using carbon intensive grid electricity, which in turns leads to reduced electrolyzer use rate and higher total cost (resp. lower Net Present Value).

These fronts show that the cumulated GHG emissions could become negative mainly due to the GHG emission savings from substitution of natural gas by PV-based hydrogen injection in the natural gas grid.

3.1.4 Interpretation

The Pareto fronts obtained for each transport scenario show similar range of GHG emissions (even if pipeline is slightly better than truck scenario). However NPV results show significant differences between scenarios revealing the important influence of the cost of hydrogen transport modes on the overall profitability of the hydrogen supply chain. Despite lower CAPEX, the truck scenario is less economically interesting compared to low CAPEX pipeline scenario, due to higher OPEX coming from fuel consumption. Pipeline scenario leads to the lowest NPV due to high CAPEX and under utilization compared to hydrogen flow rate capacity. Low CAPEX pipeline scenario leads to highest NPV result. The significant difference between cumulated GHG emissions obtained for environmental optimization compared to economic optimization shows the strong influence of hydrogen chain operation strategy on the environmental performance given the specific conditions of the case study (local PV farm and highly carbonated electrical grid).

3.2. Levelized Cost of Hydrogen (LCOH) and specific emissions

3.2.1 Overview

Complementary to the original Pareto front, the Figure 8 shows the relationship between the Levelized cost of hydrogen (€/kgH₂) and the Specific greenhouse gases emissions (kgCO_{2-eq}/kgH₂), comparing the results obtained with consideration of avoided emissions and those obtained without consideration of avoided emissions. For each scenario, the reported LCOH values determine the minimum H₂ averaged sell price from which the overall supply chain is profitable.

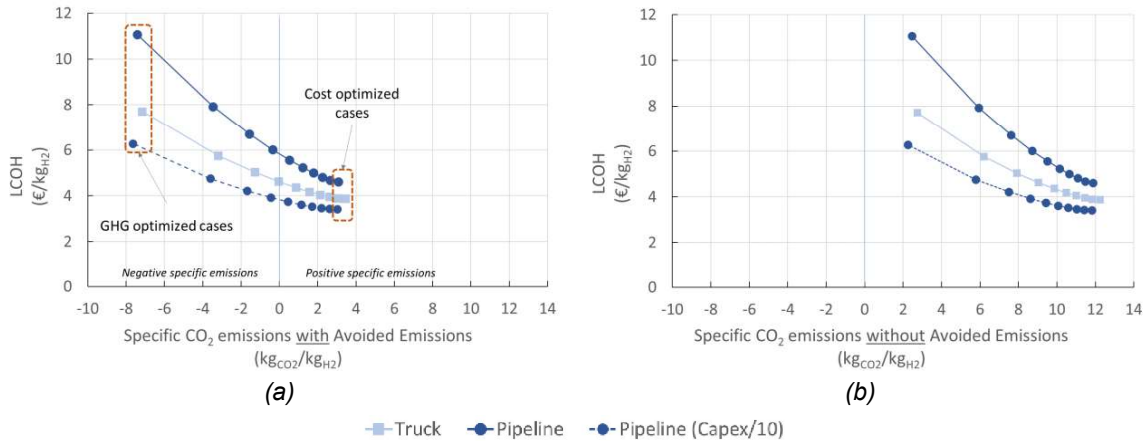


Figure 8 : Levelized Cost of Hydrogen compared with Specific CO_{2-eq} emissions. Optimization results converted into $LCOH = f(e_{GHG})$ - (a) with Avoided Emissions, (b) without Avoided Emissions.

3.2.2 LCOH

The following observations can be made based on results presented in Figure 8. Results for “GHG optimized cases” are located on the left side of each graph. For these cases the LCOH ranges from 6 to 11 €/kgH₂.

- Original pipeline scenario reaches the highest LCOH at approximately ~11 €/kgH₂.
- For Tube trailer scenario, the LCOH is around ~8 €/kgH₂.
- Pipeline with reduced CAPEX scenario exhibits the lowest LCOH value, approximately 6 €/kgH₂.

Results for “Cost optimized cases” correspond to the right side of each graph. For these cases, the LCOH narrows to 3.5 to 5 €/kgH₂.

- Original pipeline scenario leads to highest LCOH at approximately ~4.6 €/kgH₂.
- For Tube trailer scenario, the LCOH is around ~3.9 €/kgH₂.
- Pipeline with reduced CAPEX scenario exhibits the lowest LCOH value, approximately 3.4 €/kgH₂.

Thus a greater difference can be observed between hydrogen transport scenarios for GHG optimized cases, compared to cost optimized cases. This comes from the fact that the quantity of hydrogen produced is significantly lower for GHG optimized cases compared to cost optimized cases, as shown in Figure 7.

3.2.3 Specific emissions

The specific emissions give hint of which group of solutions generates a reduction in current emissions. This implies that the solutions with positive specific emission values lead to higher overall emissions. Therefore, the solutions considered as more sustainable would be the ones that present negative values of specific emissions despite higher cost. Thus, prioritizing solutions with negative specific emissions values aligns with sustainability objectives, as they contribute to mitigating climate change and reducing overall environmental impact. Under the set of assumptions considered in this study, the specific emissions without considering avoided emissions range between 2 and 12 kgCO_{2-eq}/kgH₂ for all scenarios, whereas it ranges between -8 and 4 kgCO_{2-eq}/kgH₂ when avoided emissions are considered. Such analysis could be used to estimate the subsidies needed per kilogram of hydrogen as a function of the targeted GHG content (kgCO_{2-eq}/kgH₂) and depending on price threshold that is acceptable for end-uses of hydrogen.

3.2.4 Use rate of electrolyzer and share of electricity sources

Figure 9 below shows the share of photovoltaic energy in the total energy consumed by the electrolyzer, and the evolution of the electrolyzer's running time availability (proportion of the time where hydrogen production is not zero), as a function of specific GHG emissions (with avoided emissions taken into account) in the specific case of truck scenario.

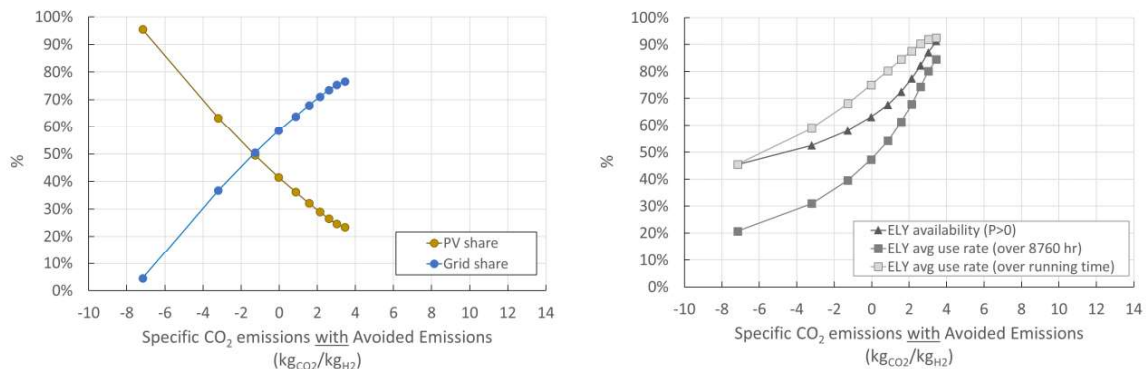


Figure 9 : Share of electricity sources and Electrolyzer use rate for Truck scenario.

This graph shows that the lowest specific emissions are achieved when the electrolyzer uses local photovoltaic generation as its main source of electricity. The electrolyzer's utilization rate is then less than 50%, resulting in higher hydrogen costs. On the other hand, the highest specific emissions are obtained for low PV share (but still 20%) and higher use of electrical grid, leading to higher use rate of the electrolyzer and lower LCOH values.

These results show that for cost optimized case (respectively highest specific emissions, on the right side of each graph), the electrolyzer averaged use rate over running time reaches 92% with a time availability of 90% (power>0). The availability does not reach 100% even for cost optimization case, which comes from the limitations regarding the maximal hydrogen flow rate that can be injected in low NG demand periods. Indeed the production capacity of the electrolyzer is 135 kgH₂/h, with 8 kgH₂/h dedicated to bus demand, and resulting in 127 kgH₂/h capacity available for injection into NG grid. However the instantaneous maximal hydrogen mass flow that can be accepted in the gas network is sometimes inferior to this value and even reaches 0 at some moments of the year as shown in Figure 3-d. Thus in some of these periods the optimizer prefers to limit the use of the electrolyzer and to use the buffer storages to provide hydrogen to the mandatory demand for buses (8 kgH₂/h) while also avoiding highest grid price hours.

In the set of solutions where emissions are exclusively optimized, the generation behavior of the electrolyzer follows the trend of the PV production, as it avoids the use of the grid. However, the hours of use of the electrolyzer are considerably reduced, generating an economically oversized system.

Thanks to these graphs, the conditions for switching from Positive to Negative specific emissions can be determined, and thus providing an assessment of decarbonization potential depending on LCOH level. For instance in the case of Truck scenario:

- PV share should be higher than 40% (maximizing the use of direct PV);
- Grid use should be lower than 60%;
- Electrolyzer running time availability should be lower than 63%;
- Electrolyzer use rate average over running time should be lower than 75% of nominal capacity;
- The LCOH might be higher than 4.5 €/kgH₂ (Figure 8) meaning that this should be the minimal price of hydrogen to ensure the financial equilibrium while reducing emissions compared to reference fossil-based applications.

The conditions for achieving the lowest specific emissions require maximizing use of direct PV, and minimizing grid utilization. The consequences of such situation would be:

- An electrolyzer running time availability (power > 0) of about 45% of the time (meaning that the system would be kept without any production more than 55% of the time);
- An average electrolyzer use rate over running time of ~45% of nominal power, due to the shape of the daily solar production;
- An LCOH as high as 8 €/kg.

3.3. Levelized Cost of Avoided CO₂-eq (LCAC)

The Figure 10 shows the Levelized Cost of Avoided CO₂-eq expressed in €/tCO₂-eq_{avoided}, as a function of the annualized GHG emission reduction (incl. avoided emissions). The following observations can be made:

- The lowest LCAC is obtained for the highest CO₂-eq emissions reduction. The energy system considered in this study could reach a reduction of ~1.800-1.900 tCO₂-eq /year for a LCAC in the range ~466-845 €/tCO₂-eq_{avoided}.
- Such result would mean that if all costs are supported by the collectivity, once the hydrogen system is installed, the best operation in terms of cost and decarbonization efficiency would be a PV following operation strategy as shown in Figure 9.
- The values of LCAC obtained for the minimal points (~466-845 €/tCO₂-eq_{avoided}) could be used as a basis for comparison with alternative decarbonization strategies for the considered end-use applications.
- These optimal values of LCAC (~466-845 €/tCO₂-eq_{avoided}) correspond to the highest LCOH (~6-11 €/kgH₂). In that case if all costs of the hydrogen chain were supported by private stakeholders, then the economic viability for hydrogen chain stakeholders would be reached only if hydrogen price paid by end-users is in the same range as the LCOH (~6-11 €/kgH₂) which is higher than the hydrogen price assumptions that was considered in this study (4 €/kgH₂ for both applications).

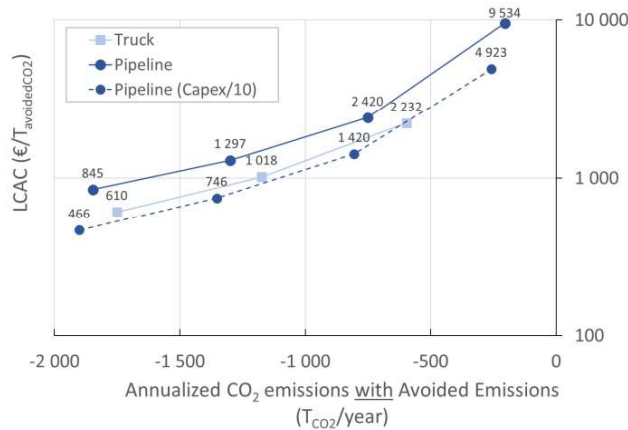


Figure 10 : Levelized Cost of Avoided CO₂-eq (€/tCO₂-eq_{avoided}).

From the point of view of decarbonization cost, it is then preferable to make the electrolyzer working in a synchronous way with PV plant. There will be less hydrogen injected in the Natural gas grid but this would be more efficient from decarbonization perspective due to less use of highly carbonated electricity from grid. The lowest LCAC are achieved for highest PV share which will lead to intermittent use of the electrolyzer with a low capacity factor and high production costs. In such situation, the flexible operation of the electrolyzer must be guaranteed from a technical stand-point by the equipment manufacturer. One perspective could be to envisage hybridization with alternative low carbon electricity routes in order to increase the use rate of the

electrolyzer. Additionally these preliminary results do not take into account the change in optimal use of electrolyzer correlated with changes in the electrical mix. Indeed additional electricity import from Spain will occur as a new submarine cable will be put in service [48]. In this situation, the profile of carbon content of grid electricity consumed by the electrolyzer may evolve and taking advantage of the higher share of renewables in Spanish mix (mainly due to wind and hydro power) which will increase the use rate of electrolyzer. However such situation require detailed analysis considering also the updated hourly cost of such low carbon electricity. Such analysis of levelized cost of avoided CO_{2-eq} should be conducted in comparison with other decarbonization alternatives at territorial level in future studies.

3.4. Cost and emissions structure

3.4.1 Overview

In the present section, the cost and emissions breakdown analysis of the projects is performed. Figure 11 depicts the components relative contribution to the levelized cost, while Figure 12 shows their relative contribution to the emissions. These results show the impact of electrical grid. From an economical point of view the optimizer find interesting using the grid to produce more hydrogen and at lowest cost, but this electricity consumption represents the main contribution to emissions.

3.4.2 Structure of costs

The Figure 11 shows the structure of costs of optimized solutions obtained for NPV and GHG optimization cases and for each transport scenario. These figures do not include the revenues from hydrogen sales but only capital and operational expenditures of the hydrogen supply chains.

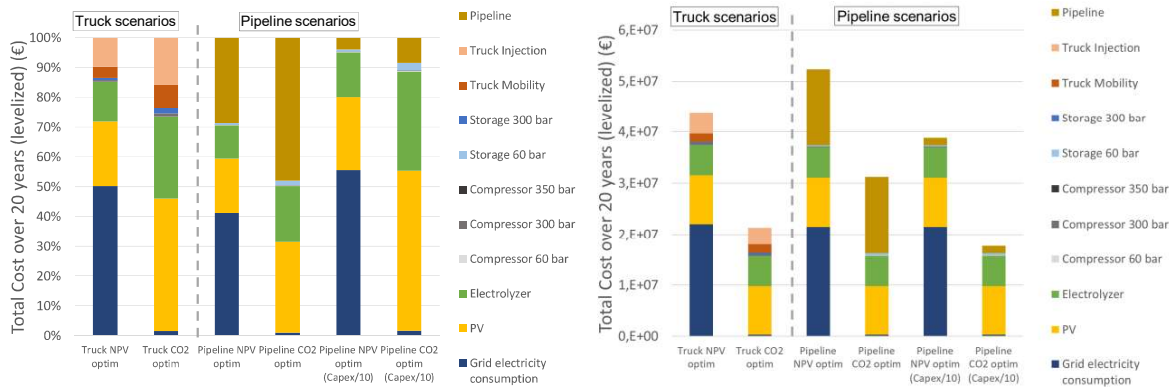


Figure 11 : Structure of costs (a) relative and (b) absolute

These results show the role of electrical grid in NPV and GHG optimization cases:

- Considering that the size of the components such as the photovoltaic farm, the electrolyzer, the compressors and the gas transport medium are fixed, the variations of the cost breakdown between the solutions are mainly due to the use of the electrical grid.
- For NPV optimization cases, the optimizer takes advantage of the already invested PV plant and considers economically interesting to use grid electricity for additional hydrogen production as the averaged electricity spot price (around 50 €/MWh) makes hydrogen selling price of 4 €/kgH₂ economically profitable. Thus the cost of grid electricity represents about 50% of the total costs.
- For GHG optimization cases, the cost of electricity from electrical grid is almost zero as the optimizer intends to limit the use of highly carbonated grid electricity.

The share of PV production is also highlighted by these figures:

- For NPV optimization cases, PV plant investment represents about 20% of the total levelized cost over the 20 years lifetime
- For GHG optimization cases, the share of the PV plant range between 30% and 55% of the total cost. This is a consequence from the lower electricity consumption for these cases, exacerbating the share of all types of equipments in the total cost.

The results show also the contribution of the components of the hydrogen chain (electrolysis/compression/storage/transport) to the total cost, given the set of considered economic assumptions:

- For NPV optimization cases, the cost of hydrogen equipment represents between 20% and 40% of the total costs

- For GHG optimization cases, this contribution ranges between 45% and 70% of the total cost.
- The results show the significant influence of pipeline CAPEX assumption on the total cost over 20 years ranging from 5% (low CAPEX case) to 30% (high CAPEX case) of total cost for NPV optimized cases.
- Hydrogen transport by trucks stands for about 15% of total costs (including CAPEX and fuel consumption) for NPV optimized cases, which corresponds to similar order of magnitude as the cost of electrolysis process under the considered set of assumptions.

3.4.3 Structure of emissions

The Figure 12 provides the structure of emissions over the 20 years project lifetime. These figures do not include the avoided emissions related to hydrogen substitution to fossil reference but only emissions of the hydrogen supply chains itself.

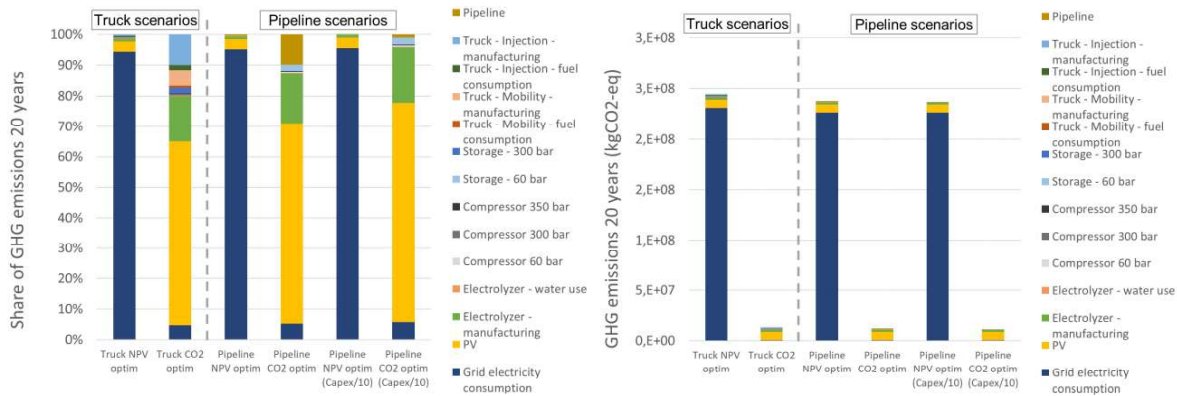


Figure 12 : Structure of emissions (a) relative and (b) absolute

For NPV optimized cases, a limited share of emissions is observed from the hydrogen supply chain with grid electricity being the major carbon emissions contributor (around 95%) even though an emission reduction factor was assigned to the energy extracted from the grid (taking into account future evolution of the electricity mix). For the GHG optimization cases it can be seen that the photovoltaic farm is responsible for most of the emissions. In these optimization cases, the use of the grid is minimized in order to reduce overall GHG emissions. Also, the emissions related to hydrogen production (including grid electricity consumption) are above 80% of the cumulated emissions, with hydrogen transport representing less than 20%. In addition the choice of the hydrogen transport mode (truck or pipeline) does not influence significantly the absolute values of cumulated greenhouse gases emissions over the project lifetime. Finally, under the set of assumptions considered in this study, truck transport seems to generate slightly more emissions than pipeline scenario. However this observation should be further confirmed with detailed life cycle inventories for both hydrogen transport modes.

4. Conclusions and perspectives

4.1 Conclusions

In this paper a bi-objective dynamic optimization approach has been implemented for evaluating the economic performance and GHG emissions of a PV based hydrogen energy chain. A theoretical case study was considered relying on some of the characteristics of the GreenHysland EU project deployed in the island of Mallorca (Spain). The ability to assess the environmental and economic performance of hydrogen chains while taking into account the intermittent nature of the boundary conditions (solar production, prices and emissions linked to the use of the electricity grid, hydrogen demand) has been demonstrated. Several fronts of non-dominated solutions were obtained using the epsilon-constraint method allowing to link economic viability with environmental sustainability and highlighting trade-offs between both objectives. This study leads to the following conclusions:

- The Pareto fronts show that the cumulated GHG emissions could become negative mainly due to the GHG emission savings from substitution of natural gas by PV-based hydrogen injected into the natural gas grid. This means that in current conditions, due to the high GHG intensity of Balearic electrical grid, the solution for reducing emissions with hydrogen might be to encourage direct solar electricity sourcing for the electrolyzer as well as maximizing injection into the natural gas grid.
- The study shows that since the electrical grid of Balearic Islands remains highly carbon intensive, hydrogen cannot be simultaneously produced at low cost and contribute at the same time to reduction of GHG emissions. The results also show that under the given economic assumptions, the economic

viability of environmentally optimal solutions is not guaranteed and may depend on the level of financial public support for hydrogen supply chain.

- Two hydrogen transport modes were compared. The economic results showed the strong influence of cost assumptions on the ranking between pipeline and truck trailer options. However, the choice of one or the other transport mode does not influence significantly the order of magnitude of cumulated GHG emissions over the hydrogen supply chain lifetime.
- It was shown that the total cost minimization does not lead to the same operation strategy compared to the environmental impact minimization. When maximizing the Net Present Value, the grid electricity consumption takes the greatest share of the cost and GHG emissions for all scenarios, as the optimizer tends to maximize the utilization rate of the electrolyzer and the sales of hydrogen. When the cumulated GHG emissions are being minimized, the optimizer prefers using direct production from the local PV plant, which in turn reduces the utilization rate of the electrolyzer and increases the production cost.
- The structures of costs and emissions of optimal GHG solutions were also analyzed. In terms of emissions, the photovoltaic production involves the biggest contribution. However, the share of embedded emissions from “other than Solar” elements (electrolyzer, pipeline, compressors, storages, truck trailers) is not negligible, representing between 25% and 35% of the emissions breakdown. The cost associated with photovoltaic power production represents the highest proportion in the cost structure (except in high CAPEX pipeline scenario where pipeline becomes the highest cost factor).
- In terms of method, this study emphasizes the potential interest of dynamic bi-objective optimization approach to support impact assessment in pre-design phases of hydrogen projects. This approach could bring insights about economic and environmental performance while complying with future assessment methodologies defined at European level (RED II and related Delegated Acts) as well as green or low carbon hydrogen certification processes. By year 2030 the evolution of EU regulation towards mandatory hourly temporal correlation between renewable production and hydrogen production may increase the need of such dynamic multi-objective optimization approaches thus providing support to investment decision-making and daily operation of hydrogen plants.

4.2 Perspectives

The case study investigated in this paper showed that a large number of assumptions have to be defined to be able to reach complete economic and environmental assessment of hydrogen supply chains. Thus several aspects should be investigated in order to increase the robustness of such analysis and several research areas can be identified for improving the accuracy of future studies in this field. The method presented in this paper could be improved through several actions as described below.

At first, sensitivity studies regarding all economic and environmental parameters should be conducted. For economic evaluation, a particular focus should be made on sensitivity about cost assumptions as well as hydrogen selling prices. The cost assumptions should be detailed and consolidated, being for investment part (including studies, installation, EPC costs...) or operational part (including replacement) for all components. In this study an optimistic hydrogen price of 4 €/kgH₂ for injection in NG grid has been considered. Such assumption should be further analysed in relation with differences between H₂ production cost and NG market price. For instance [47] mentions a breakeven production cost of 0.3 to 0.8 €/kgH₂ without carbon tax and 1.2 to 1.5 €/kgH₂ with a 100 €/tCO₂ tax. Also, new financial instruments are being put in place such as the European Hydrogen Bank to support renewable hydrogen production. The influence of these instruments as well as subsidies on a “per kg” basis should be investigated and analysed in the frame of total costs of the hydrogen supply chain, in order to refine the assessment of the economic viability for hydrogen stakeholders involved. In addition, sensitivity studies should be conducted regarding linear environmental models that have been built for each component of the hydrogen chains. A particular focus should be made on the collection of relevant inventory data for truck trailers and hydrogen pipelines, as well as appropriate assumptions regarding lifetime, prospective impacts and replacement costs of these components over the entire considered project lifetime.

Secondly, the environmental analysis should be extended to other impact categories beyond GHG emissions. The linearization approach implemented in this paper for GHG emissions should be extended to the elaboration of linear models for other impact categories such as land use, local pollution, water use, critical resources depletion, import of fossil fuels, among others. From an optimization perspective, it would be worth studying the influence of the choice of a specific environmental optimization criterion on the sizing and operation of hydrogen supply chains. Once such models will be available, the bi-objective dynamic optimization presented in this paper should be extended towards multi-objective dynamic optimization techniques in order to find the best trade-offs between all these objectives.

Thirdly, the optimization approach should be extended to other optimization variables. In particular the size of all components of the hydrogen supply chain should be considered as optimization variables, such as the size of local PV plant, electrolyzers, compressors, buffer storages and hydrogen transport capacities. The

1 design pressure ranges for stationary buffer storages and gas transport systems (pipeline and truck trailers)
2 should be further validated with the relevant stakeholders in order to increase the credibility of the assessed
3 scenarios. In addition the dynamic method proposed in this paper should be linked to other optimization
4 approaches that have been developed in the literature dealing with multi-agent optimization in order to take
5 into consideration the conflicting interests of the public and private stakeholders involved in the hydrogen
6 ecosystem. Moreover, optimization techniques related to prospective territorial infrastructure investment
7 planning should be implemented as an alternative to the static infrastructure investment approach considered
8 in the present study.

9 Fourthly, the future works should take into account the future evolution of the energy context in Balearic
10 Islands. In this study the dynamic inputs were only based on year 2019 dynamic data and the reduction of
11 carbon intensity of electrical grid has been averaged for calculating the overall 20-year emissions, without
12 simulating the dynamic behaviour of carbon intensity for these future low carbon electricity mix. The cumulated
13 emissions calculated over 20 year project duration were considered with a yearly global reduction factor of
14 electrical grid carbon intensity, without considering any influence of this global evolution on the optimal
15 behaviour of the hydrogen supply chain over the project lifetime. It could be interesting to assess the optimal
16 behaviour of the hydrogen supply chain when considering such future dynamic profiles. Therefore one
17 perspective could be to integrate prospective carbon timeseries related to future evolutions of the electrical
18 grid. As an example, it could be worth considering the evolution of energy mix regarding the launch of the new
19 submarine cable foreseen before year 2030 [48] which will change the carbon content of electrical grid. Indeed
20 the study from Red Electrica de Espana for 2030 mentions the operation of a new submarine cable between
21 Spanish mainland and Balearic Islands, as well as the end of the use of natural gas for electrical production
22 (no more CCGT plant) and a very significant increase of electricity import from the mainland. In this context, if
23 the mix becomes much less carbon intensive, the environmental optimization could lead to more use of grid
24 electricity for low carbon hydrogen production, but on the other hand, if natural gas import is reduced close to
25 zero in 2050, this may influence the possibility of injecting hydrogen into the existing NG network (under current
26 limitation of 4%_{voi}). Moreover, in terms of hydrogen applications, there was no consideration of any evolution
27 of the hydrogen demand over the project lifetime. The forthcoming studies should include assumptions about
28 such evolution and considering hydrogen use in other carbon intensive applications such as maritime, airport
29 and other sectors. Modelling and optimization of hydrogen supply chains should be performed taking into
30 account such evolution of the hydrogen demand.

31 Finally the assessment of hydrogen scenarios and the comparison with other decarbonization options
32 should be carried out taking into a broader set of considerations such as economic aspects, environmental
33 impacts, regulations, safety, technology readiness level, political support or social impacts in order to reach
34 comprehensive analysis of prospective energy scenarios for Balearic Islands. Beyond technical solutions, the
35 question of energy sufficiency and demand-side management in the context of a tourism-based economy
36 should be further investigated to support the sustainable development of the islands.

37 **CRedit authorship contribution statement**

38 Florent Montignac: Conceptualization – Methodology – Writing – Review & Editing

39 Diego Larrahondo Chavez: Conceptualization – Methodology – Writing – Review & Editing

40 Maria-Candelaria Arpajou: Conceptualization – Methodology – Writing – Review & Editing

41 Alain Ruby: Software

42 **Declaration of Competing Interest**

43 The authors declare that they have no known competing financial interests or personal relationships that
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53 **Appendix A**

Table A.2
Technical, economic and environmental assumptions considered.

Component	Parameters	Units	Data	References
Lloseta PV park	Installed peak power	MWp	8.56	[9]
	Solar production	MW/MWp	PV production time series. Lloseta location	[28]
	Lifetime	years	20	Assumption
	CAPEX	€/kWp	1,000	Assumption
	OPEX	€/kWp	1% of investments costs	Assumption
	Embedded emissions	kgCO _{2-eq} /MWh	26	[29]
Balearic Islands power mix	Power production	MW	Hourly power time series.	[26]
	Extraction price	€/MWh	Hourly energy spot price time series.	[26]
	Grid emissions	kgCO _{2-eq} /MWh	Hourly CO _{2-eq} emissions time series.	[26], [27], [29]
Mainland Spain power mix	Electricity price	€/MWh	Hourly energy spot price time series	[27]
	Electricity emissions	kgCO _{2-eq} /MWh	Hourly CO _{2-eq} emissions time series	[27]
PV connection	Efficiency	%	84.2	[30]
PEM Electrolyzer	Nominal power	MW	7.5 ¹	[9]
	H ₂ mass flow rate	kgH ₂ /h	135 ²	[31]
	Efficiency	%	61.7	[31]
	Outlet H ₂ pressure	bar	30	[31]
	Lifetime	years	20	Assumption
	CAPEX	€/MW	500,000	[32]
	OPEX	€/MW	1.8% of investments costs	[32]
	Deionized water consumption	L _{water} /kgH ₂	10	Assumption
	Emissions for water use	kgCO _{2-eq} /kgH ₂	0.0044	[34], [35]
	Embedded emissions	kgCO _{2-eq} /MW	261351*P _{electrolyzer} + 45156	Modelled with [33] and data from [34], [35], [36], [37]
300 bar compressor	Inlet H ₂ pressure	bar	30	Assumption
	Outlet H ₂ pressure	bar	300	Assumption
	H ₂ mass flow rate	kgH ₂ /h	135 ³	Assumption
	Embedded emissions	kgCO _{2-eq} /MW	258027*P _{compressor} + 24217	Modelled with [33] and data from [34], [35], [36], [38]
	Lifetime	years	20	Assumption
	CAPEX	€/MW	700,000	[32]
	OPEX	€/MW	7% of investments costs	[32]
60 bar compressor	Inlet H ₂ pressure	bar	30	Assumption
	Outlet H ₂ pressure	bar	60	Assumption
	H ₂ mass flow rate	kgH ₂ /h	135 ⁴	Assumption
	Embedded emissions	kgCO _{2-eq} /MW	258027*P _{compressor} + 24217	Modelled with [33] and data from [34], [35], [36], [38]
	Lifetime	years	20	Assumption
	CAPEX	€/MW	700,000	[32]
	OPEX	€/MW	7% of investments costs	[32]
300 bar storage tank	Storage capacity	kgH ₂	Optimized	-
	Storage pressure	bar	300	Assumption
	Embedded emissions	kgCO _{2-eq} /kgH ₂	359 (type II H ₂ storage tank)	Same as 300 bar truck trailer
	Lifetime	years	20	Assumption
	CAPEX	€/kgH ₂	550	[32]
	OPEX	€/kgH ₂	0% of investments costs	Assumption
60 bar storage tank	Storage capacity	kgH ₂	Optimized	-
	Storage pressure	bar	60	Assumption
	Embedded emissions	kgCO _{2-eq} /kgH ₂	310 (type I H ₂ storage tank)	Modelled with [33] and data from [34], [35] & internal data for steel tanks
	Lifetime	years	20	Assumption
	CAPEX	€/kgH ₂	550	[32]
	OPEX	€/kgH ₂	0% of investments costs	Assumption

¹ Three 2.5 PEM electrolyzers.

² Hydrogen production for single 2.5MW electrolyzer is 1080 kgH₂/day (45 kgH₂/h). Considering three 2.5 MW electrolyzers, this gives 135 kgH₂/h.

³ Compressor maximal flow rate based on cumulated electrolyzer production.

	Distance	km	30 ⁴	-	
	Fuel consumption	l/100km	30	[41]	
1	Fuel cost	€/l	2	Assumption	
2	Max speed	km/h	60	Assumption	
3	Storage pressure	bar	300	Assumption	
4	Total capacity per trailer	kgH ₂	462	Assumption	
5	Usable capacity per trailer	kgH ₂	370 ⁵	Assumption	
6	Truck trailers	Emissions per km	0.395 ⁶	Modelled with [33] and data from [34], [33][35], [42]	
7		Embedded emissions per truck trailer	kgCO _{2-eq} /kgH ₂	359 ⁷	
8		Lifetime	years	10	
9		CAPEX	€/kgH ₂	550 ^{8,9}	
10		OPEX (other than fuel)	%CAPEX/year	5%	
11				Assumption [32]	
12				Assumption	
13					
14	H ₂ pipeline	H ₂ max mass flow rate	kgH ₂ /h	135 (Scenario 1); 1,350 (Scenario 2)	
15		Efficiency	%	100 ¹⁰	
16		Embedded emissions	kgCO _{2-eq} /km	80,000	
17					Assumption
18					Using NG pipeline data from [34], [35]
19					Assumption
20					[43]
21				Assumption	
22	350 bar compressor	Inlet H ₂ pressure	bar	60	
23		Outlet H ₂ pressure	bar	350	
24		H ₂ mass flow rate	kgH ₂ /h	8	
25		Embedded emissions	kgCO _{2-eq} /MW	258027*P _{compressor} + 24217	
26					Assumption
27				Modelled with [33] and data from [34], [35], [36], [38]	
28				Assumption	
29				[32]	
30				[32]	
31	H ₂ demand for buses	H ₂ fixed flow rate	kgH ₂ /h	8	
32		Avoided emissions	kgCO _{2-eq} /km	1.22 ¹¹	
33					Assumption
34				Modelled with [33] and data from [34], [35], [49]	
35				Assumption	
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⁴ Distance between Lloseta and Palma de Mallorca.

⁵ Assuming a discharge equilibrium pressure of 60 bar, hence usable capacity of 300 bar trailer assumed at 80% of total capacity.

⁶ Calculation: $[\text{truck consumption}] \cdot [\text{fuel density}] \cdot [\text{emission factor}] = 0.3 \frac{\text{L}_{\text{diesel}}}{\text{km}} * 0.85 \frac{\text{kg}_{\text{diesel}}}{\text{L}_{\text{diesel}}} * 1.55 \frac{\text{kg}_{\text{CO}_2\text{-eq}}}{\text{kg}_{\text{diesel}}} = 0.395 \frac{\text{kg}_{\text{CO}_2\text{-eq}}}{\text{km}}$

⁷ Expressed in kgCO_{2-eq} per kg of truck total H₂ capacity.

⁸ Expressed in € per kg of H₂ storage capacity.

⁹ The value of the investments costs of a 300 bar H₂ storage tank is used for estimating the investments costs of 300 bar H₂ tube trailers.

¹⁰ No head losses are considered for the pipeline.

¹¹ GHG emissions of a diesel bus.

¹² Considering emission factor of natural gas and lower heating value of hydrogen.

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Assessment of hydrogen supply chains based on dynamic bi-objective optimization of costs and greenhouse gases emissions: case study in the context of Balearic Islands

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Highlights:

- A dynamic method for optimization of hydrogen supply chains is illustrated.
- Greenhouse gases emissions and costs of hydrogen chains are assessed.
- Trade-offs between environmental and economic performances are analyzed.
- Study shows the impact of electrolyzer management on the environmental results.
- Future analyses should include more environmental impact categories.
- Comparison with alternative territorial decarbonization options should be engaged.

Cover letter

Grenoble, 29/12/2023

Manuscript title:

Assessment of hydrogen supply chains based on dynamic bi-objective optimization of costs and greenhouse gases emissions: case study in the context of Balearic Islands

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Manuscript significance:

This manuscript presents an original method for computing costs and emissions of hydrogen supply chains using a bi-objective optimization approach based on dynamic simulation. The approach includes life cycle emissions related to all components of the supply chains, including primary energy production, hydrogen generation, compression, transport and storage, as well as avoided emissions related to substitution of fossil-based end-uses of final energy. This approach could be implemented in pre-design phases of future hydrogen projects for refined assessments of projected costs and emissions. This study has been conducted in the frame of GREEN HYSLAND EU project.

Submission history:

- Study has been firstly communicated during ECOS 2023 conference.
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- This is the last version of the paper, submitted on 30/06/2024.

Statement:

The manuscript is not being submitted to any other journal.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: