

Multi-criteria optimization of hydrogen energy supply chains considering economic and environmental impacts: theoretical case study in the context of Balearic Islands

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Abstract:

Hydrogen production through water electrolysis can play a role in the decarbonisation of energy systems when powered by electricity obtained from low carbon energy sources. The decision of deploying hydrogen technologies at a large scale in the future implies to get a comprehensive overview of the benefits and drawbacks on a variety of impacts compared to other alternative energy supply scenarios. The aim of this study was to perform a dynamic techno-economic and environmental impact assessment of renewable-based hydrogen supply chains relying on some of the characteristics of the GreenHysland EU deployment project in Mallorca (Spain). In this paper the optimization of the design and operation conditions of two hydrogen transport modes (trucks and pipeline) has been addressed for the supply of hydrogen to fuel cell buses and considering the possibility of injecting hydrogen into the natural gas grid. These hydrogen chains were assessed using PERSEE dynamic optimization tool developed at CEA relying on a Mixed Integer Linear Programming approach. A front of optimal solutions has been obtained considering both economic (Net Present Value) and environmental (cumulated equivalent carbon dioxide emissions) optimization criteria. Finally this study emphasizes the potential interest of such dynamic optimization approach to support impact assessment in pre-design phases of hydrogen projects complying with current and future greenhouse gases savings assessment methodologies defined at European level (e.g. RED II and related Delegated Acts) and corresponding green or low carbon hydrogen certification processes. This initial work opens the way to several perspectives for improvement in order to increase the robustness of these energy chain comparisons including sensitivity studies and the consideration of a broader set of environmental impact categories. These improvements are being reviewed by the research team and will help achieve a more complete analysis of the impacts of potential large-scale hydrogen deployment scenarios in the future energy mix of the Balearic Islands.

Keywords:

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

1. Introduction

1.1. Context: the GreenHysland EU project

The study presented in this paper has been performed in the frame of the GreenHysland EU project. This five years project (2021-2025) aims to deploy a fully functioning hydrogen (H₂) ecosystem on the island of Mallorca (Spain), turning the island into the first H₂ hub in Southern Europe [1]. The project comprises:

- The development of hydrogen production, transport and distribution infrastructure (green hydrogen production plant, hydrogen truck trailers, deployment of a hydrogen pipeline and hydrogen refuelling station)

- The demonstration of three types of end-use applications (hydrogen vans and buses, stationary fuel cells and hydrogen injection into the natural gas grid).

In addition to the technical aspects, the project also addresses the analysis of the economic, environmental and social impacts of the potential larger scale deployment of hydrogen as an energy carrier in the Balearic Islands. Part of these studies relies on dynamic simulation and optimization of current and future energy chains. Therefore, in the present paper, a methodology for a first analysis of hydrogen supply scenarios in the Balearic Islands is addressed considering economic and environmental evaluation criteria.

1.2. Topic of the paper

1.2.1. 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 the 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 project. This theoretical evaluation aims at illustrating a multi-criteria optimization methodology based on dynamic simulation. This study does not refer to potential hydrogen upscaling scenarios within the Balearic Islands

1.2.2. General objectives

The main goals of this study are:

- To illustrate how a multi-criteria optimization approach based on dynamic modelling can help assessing hydrogen supply chains from an economic and environmental impacts perspective;
- To provide insights about the most influencing components regarding cost and environmental emissions breakdown of these hydrogen chains.

We consider a theoretical case study relying on some of the characteristics of the GreenHysland project. This case study (described in Section 2) consists in a hydrogen energy chain comprising a 7.5 MW electrolyzer connected to a local PV plant and to the local electrical grid. The end-use applications consist in five hydrogen fuel cell buses and a flexible hydrogen injection into the natural gas grid. Two hydrogen transport modes are considered (truck trailers and pipeline) for connecting production and end-use applications separated by a distance of 30 km.

The main originality of the work relies in the simultaneous optimization of economic and environmental criteria considering all types of emissions (direct from fuel consumption, indirect from electricity consumption, and indirect from equipment manufacturing) within a dynamic optimization approach.

1.3. Background about optimization of hydrogen energy chains

1.3.1 Evaluating the carbon content of hydrogen

Hydrogen as an energy carrier is widely considered as one of the technologies that could help decarbonizing several energy demand sectors. However, this statement depends on the direct and indirect environmental impacts generated from the primary energy from which hydrogen is produced as well as life cycle impacts of the newly developed technologies over the whole hydrogen supply chains. As an example, water electrolysis is often considered as an environmental-friendly method for hydrogen production. However even though hydrogen produced by electrolysis tends to minimize environmental impact, the impact is not zero since electricity production involves environmental footprints as well as electrolysis and associated processes such as water treatment and desalination [2].

Hence several initiatives are being undertaken at National, European and International levels in order to support ramping-up of clean hydrogen market and related industry in the next years and decades by setting new rules and certification processes. The new version of the European Renewable Energy Directive commonly referred as RED II (2018) defines the global rules and targets for increasing deployment of renewable energies across European Union. Complementary to this directive, a specific Delegated Act recently published (February 2023) establishes a "Union methodology setting out detailed rules for the production of renewable liquid and gaseous transport fuels of non-biological origin" (RFNBO). These rules refer to consideration of additionally (new dedicated renewable power plants associated with hydrogen production plant), temporal correlation (from calendar month basis to hourly correlation basis) and geographical correlation (notion of bidding zone). Another Delegated Act establishes the minimum threshold for greenhouse gas emissions savings of RFNBO fuels at -70% compared to reference process. Complementary to the RED II directive and Delegated Acts, several initiatives (such as CertifHy, IPHE or GH2 standard) have been launched in order to define green or low-carbon hydrogen certification process). For instance, the so-called GH2 standard has been established by the Green Hydrogen Organization which refers to "near-zero greenhouse gas emissions". This standard requires green hydrogen projects to operate at a level of emissions less than or equal to 1 kgCO_{2-eq} per kgH₂, taken as an average over a 12-month period [3]. However, GH2 considers emissions only during hydrogen production, without evaluating them in later stages of the process,

such as in hydrogen transportation, end-use applications, and so on. Therefore, if a study scope includes transportation, the expected emissions might be higher than 1 kgCO_{2-eq} per kgH₂.

Hence, hydrogen stakeholders may be facing a new challenge regarding the appropriate and optimized size and operation of hydrogen equipment to fulfill the GHG requirements while maximizing the profitability of the production plants. Multi-criteria optimization techniques relying on dynamic simulation could help addressing this issue and then providing support to investment decision and daily operation of hydrogen plants. The next sections provide some background information about optimization approaches (section 1.3.2), multi-objective optimization (section 1.3.3) and environmental information in energy system optimization tools (section 1.3.4). Finally, section 1.3.5 presents the PERSEE optimization tool that has been used in the frame of this study.

1.3.2 Optimization approaches

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 and sizing of systems [4]. By including optimization techniques, the design and operation of energy systems can be addressed, resulting in more efficient and cost-effective scenarios [5].

Numerous optimization techniques have been implemented in this area, and one of the most widely used is mixed integer linear programming (MILP) [6]. The main advantage of a MILP Solver method is the accuracy of the solution. If the problem is well defined, 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 [7].

1.3.3 Multi-objective optimization methodology

Energy system optimization inherently involves multiple and conflicting objectives. As way of example, the most efficient energy processes are not necessarily the most economical ones, or a system with low CO_{2-eq} emissions can suppose high investment costs. Therefore, energy system optimization is much 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 giving them an explicit role as objective functions, rather than aggregating them into a single economic indicator objective function [8]. Thus, the problem of optimizing energy systems can be addressed with a multi-objective approach, where the solution vector is not determined by a single technical solution, but by a set of optima. The optimal solution points form what is commonly referred to as a non-dominated set or Pareto optimum. For each of the Pareto arrangements, improving one objective without worsening another is not possible. For the calculation of the Pareto front, the epsilon-constraint method is widely used, especially for cases where there are two objectives. This is due to the fact that it provides high reliability of the results within brief computational time [9].

1.3.4 Environmental information in energy system optimization

Optimization techniques are used in various simulation software packages to plan energy systems. These pieces of software have been developed not only to evaluate the technical and economic potential of energy systems, but also to simplify the design and operation process of systems that include renewable sources maximizing, at the same time, their profitability [10]. Even though the use of software programs seeks to maximize the use of renewable energies and thus, minimize the environmental impact, most of them do not include environmental impact as a decision variable [11]. Moreover when environmental information is considered the impact related to equipment manufacturing is often excluded from the analysis perimeter.

In order to obtain and include environmental information in an optimization problem, a Life Cycle Analysis (LCA) of all components of the energy system must be performed. LCA is a standardized methodology developed to assess the environmental impacts of a product, a process or even a system [12]. 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 [13]. This software has been chosen for this study due to its flexibility for building parametrized environmental impact models (see Section 2.4.2).

1.3.5 PERSEE optimization tool

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 [14]. 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 extrapolate its performance 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 management. 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.

As regards the multi-optimization criteria, PERSEE software works with the Net Present Value (NPV) and the cumulated greenhouse gases emissions over the entire industrial project lifetime. In order to build the front of optimal solutions, the epsilon-constraint method is currently implemented. 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 maximizing the NPV and/or minimizing CO_{2-eq} emissions.

2. Case study

2.1. System description

As it was mentioned before, the study presented in this paper is based on the GreenHysland hydrogen hub. Some of the characteristics of the GreenHysland project are used as a reference situation from where several scenarios are created. In this section, the overall flowsheet of the theoretical case study is described. Figure 1 shows a schematic representation of the case study general architecture.

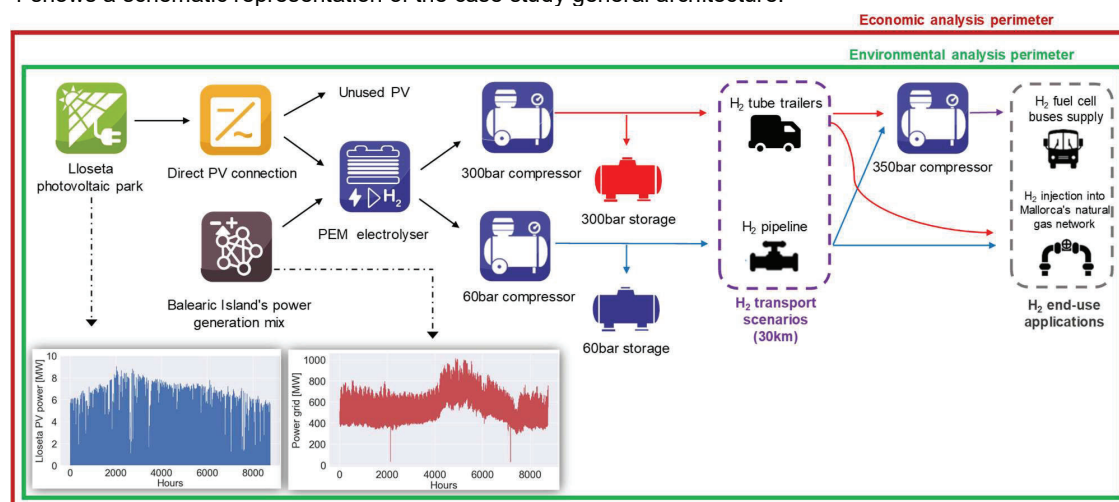


Figure 1. Illustration of the considered hydrogen supply chains and applications.

As it can be seen in Figure 1, hydrogen is produced via water electrolysis. The green hydrogen production facility is placed in the municipality of Lloseta, at almost 30 km northeast from the capital city Palma de Mallorca. The electrolyzer plant mainly includes a 7.5 MW Proton Exchange Membrane (PEM) electrolyzer, compressors, and on-site hydrogen storages to allow desynchronizing hydrogen production and demand. Regarding energy sources, the electrolyzer is coupled to the electricity generation of a photovoltaic park located also in the municipality of Lloseta. This solar farm has a generation capacity of 8.56 MWp [1]. Additional power can be obtained from the Islands' electricity power grid.

Once produced, we assume that the hydrogen is compressed and subsequently transported to Palma de Mallorca to supply two applications: public transport mobility (hydrogen buses) and hydrogen injection into the Mallorca's gas grid.

- In the first end-use application, hydrogen is used as a fuel for a fleet of five fuel cell buses. As the buses refuelling station is placed in Palma de Mallorca, hydrogen must be transported 30 km from Lloseta municipality to the capital city. Each bus has five 350bar hydrogen tanks of 312 liters each, which makes 1,560 liters in total. We assume that this volume is equivalent to a usable capacity of 37.5 kg of hydrogen. It is supposed that all buses are refuelled once a day, hence ~70 tons of hydrogen are needed in a complete year corresponding to an average flowrate demand of 8 kg/h.
- For the second end-use application, green hydrogen is injected into the Mallorca's natural gas network. The injection point is supposed to be also in the capital city, therefore, 30 km hydrogen transport has to be considered. In this case, we consider a maximal allowable hydrogen injection flow rate of 4% of the natural gas volumetric flow.

For both applications, two hydrogen transport modes are considered: truck trailers and hydrogen pipeline.

2.2. Perimeter of economic and environmental evaluations

The environmental impact considered in this study is limited to greenhouse gases (GHG) emissions. As shown in Figure 1 the environmental analysis perimeter comprises the whole direct and indirect emissions of the

hydrogen supply chains. The cumulated emissions E_{GHG} (kgCO_{2-eq}) are calculated considering direct emissions $DE_{t,i}$ during each hour t over year i (e.g. from diesel combustion in truck trailers), indirect emissions $IEG_{t,i}$ related to grid electricity consumption, indirect product emissions IPE_{el} related to manufacturing of element el of the energy system (also referred as “capex-related emissions”) and avoided emissions $AE_{t,i}$ related to substitution of diesel in buses by hydrogen and substitution of natural gas in the grid by hydrogen (this study only compares the avoided emissions in terms of fuel substitution and not the technological equipment involved in the fuel substitution; it is beyond the scope of the study to compare impacts of manufacturing of diesel buses and hydrogen buses). Equation (1) presents the calculation of the cumulated emissions considering a project lifetime of Y years, an annual operating time H of 8760 hours, a number of N elements and annual hydrogen production $M_{H2,i}$ (kgH₂). Then the specific emissions e_{GHG} (kgCO_{2-eq}/kgH₂) are obtained by dividing the cumulated emissions E_{GHG} by the cumulated hydrogen production M_{H2} (kgH₂) over the a Y years.

$$E_{GHG} = \sum_{i=1}^Y \left[\sum_{t=1}^H DE_{t,i} + \sum_{t=1}^H IEG_{t,i} + \sum_{el=1}^N IPE_{el} - \sum_{t=1}^H AE_{t,i} \right] \quad (1)$$

As shown in Figure 1 the same perimeter has been considered for the economic analysis. PERSEE minimizes the total cost function $f(x)$ presented in Eq. (2) which is the opposite of the Net Present Value. This equation shows that the cost of each element el of the energy system is computed considering specific capital expenditures CA (€ per unit size) and size S (in the present study, only the sizes of 60bar and 300bar stationary hydrogen storage systems are optimized) as well as yearly operational expenses comprising direct operation and maintenance costs OP (€/year), energy buying costs BC (computed from hourly grid electricity price data in our case) and selling price SP (hydrogen prices for mobility application and gas grid injection application). These operational expenses are computed considering hourly dynamic flux over each year of operation.

$$f(x) = \sum_{el=1}^N \left[CA * S + \sum_{i=1}^Y \frac{OP + BC * Flux * Dt - SP * Flux * Dt}{(1 + k)^i} \right] \quad (2)$$

2.3. Optimization approach

2.3.1 Scenarios

In the present study a multi-criteria optimization of three hydrogen supply scenarios is addressed:

- [Truck scenario]: We assume that tube trailers are 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 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 kg/h). Therefore, the capital cost and embedded Greenhouse Gases (GHG) emissions of the pipeline are adjusted, being divided by 10.

2.3.2 Optimization variables

Table 1 provides an overview of the optimization variables considered in this study.

Table 1. Optimization variables

Type of optimization variables	Variables	Units
Size of components	300bar stationary storage capacity (Truck scenario)	kg
	60bar stationary storage capacity (Pipeline scenarios)	kg
Power or mass flow management (dynamic optimization of operation)	PV electricity consumption	MW
	PV electricity injection to electrical grid	MW
	Grid electricity consumption	MW
	PEM electrolyzer production	kg/h
	H ₂ injection in NG grid at 4%vol max	kg/h

2.3.3 Multi-criteria optimization method

The optimization of the energy system is performed by using the economic objective function and restrictions on total CO_{2-eq} emissions. In order to build the Pareto front, two mono-objective optimizations are performed. In the first one, NPV is maximized without applying any CO_{2-eq} emissions restrictions. In the second one, CO_{2-eq} emissions are minimized. This allows to obtain the extreme points of the Pareto front. Afterwards, the internal points in the front are determined by selecting 10 equidistant CO_{2-eq} emissions values between the two extreme points (highest and lowest CO_{2-eq} emissions cases). Each of them is fixed as a CO_{2-eq} emissions constraint in subsequent mono-objective optimization problems, where the NPV is maximized. This means that 10 NPV optimization runs are generated for each hydrogen transport scenario, in which a restriction value of maximum CO_{2-eq} emissions is set.

2.3.4 Project lifetime and discount rate

We assume a project lifetime of 20 years. However, as it is explained in the following section, data series are based only on information of the year 2019. For this reason, each time series is replicated over the years in order to guarantee the optimization over the 20-years period. The Net Present Value optimization is performed considering a discount rate of 7%.

2.4. Data sources and assumptions

A summary of all numerical assumptions is given in Appendix of this paper. In the following paragraphs, we provide more details about the sources and construction of input temporal data and environmental data.

2.4.1 Temporal data

The Table 2 provides the list of temporal data used in the present study.

Table 2. Input temporal data considered in the study

Type of temporal data	Units	Sources and characteristics
PV production	MW	PVGIS platform (Lloseta location)
Grid electricity price and emissions	€/MWh & CO _{2-eq} /MWh	UIB personal communication and additional calculations related to emissions from HVDC mainland connexion
Maximal allowable hydrogen injection	kg/h	4%vol of natural gas (NG) consumption NG consumption approximated from electrical production
Hydrogen demand for fuel cell buses	kg/h	Considered constant 8kg/h

Data of the hourly power generation mix and its CO_{2-eq} emissions in 2019, as well as the hourly electricity spot price in 2019 in the Balearic Islands were provided by the Industrial Engineering Department of the University of the Balearic Islands. 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. As it was mentioned before, hydrogen demand for the mobility application is fixed at 8 kg/h. This constant value might not be representative of the real hourly hydrogen demand profile due to the fact that demand can vary, for instance, from summer to winter when the amount of tourists visiting the Islands is considerably lower. However this value represents a fixed constraint which forces the system to produce hydrogen to supply the demand. Thanks to this constraint, in the optimization problem there is at least one constant hydrogen demand to fulfil. In the case of hydrogen demand for injection into the natural gas network, a maximum constraint of 4% in volume of the existing natural gas flow is considered. As no information regarding real consumption of natural gas could be found, a roughly estimation is performed. It is supposed that all the natural gas sent to the Island is used exclusively for power generation. Figure 2 represents the maximum hydrogen mass flow that can be injected in to the natural gas grid.

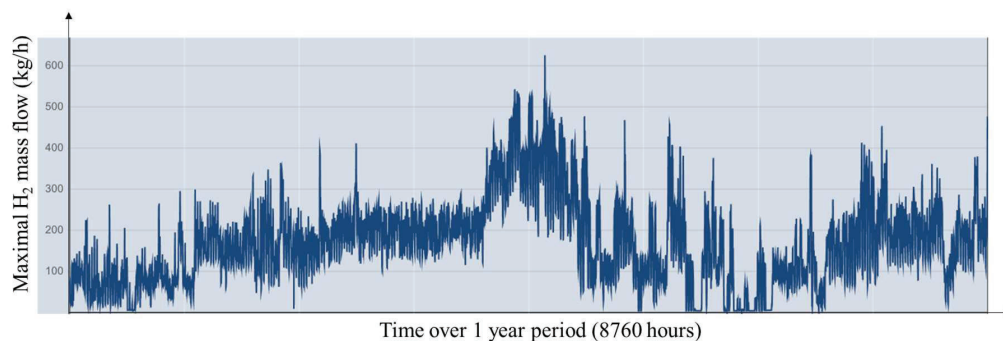


Figure 2. Illustration of the yearly maximal hydrogen mass flowrate injection considering a limit of 4%vol of hydrogen in natural gas.

2.4.2 Environmental data

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. In addition, the environmental impact category selected for the Life Cycle Impact Assessment (LCIA) is the Global warming potential of the EV3.0 method. Ecoinvent 3.8 database [15,16] 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 is given to Spain data in the database. If there is no Spain reference, European data (RER) is selected and, if the latter is not available, "global" (GLO) and "rest of the world" (RoW) data is chosen. In the next paragraphs a description of the environmental aspects of some elements of the system is presented (all other input data are available in the Appendix).

2.4.2.1 Compressor

In the case of the compressor, in order to obtain the CO_{2-eq} emissions values, the study published by Ghandehariun and Kumar [17] is used. Since the assumptions between the literature and the studied system are different, particularly the system capacity, the exponential rule in Eq. (3) is applied for the calculation of energy and material inputs. In this way, the mass of the components and the energy required for compressor manufacturing are adapted to the system size, based on the study reported by Lee et al. [18].

$$m_{1,BOP} = m_{2,BOP} \times \left(\frac{P_1}{P_2}\right)^f \quad (3)$$

Where m is the mass (or energy input), P the system capacity and f the scale factor.

This equation is used for the different components of the Balance of Plant (BOP) for electrolyzers. However, information must be adjusted in such a way that it can be added to the MILP optimization problem. Therefore, the value of the environmental impact, expressed in kgCO_{2-eq}, has been calculated for different compressor capacities and a linear regression was made resulting in the linear function expressed in Eq. (4) where $IPE_{compressor}$ refers to indirect production emissions (kgCO_{2-eq}) of compressor manufacturing and $P_{compressor}$ refers to compressor electrical power (MW).

$$IPE_{compressor} = 258027 * P_{compressor} + 24217 \quad (4)$$

2.4.2.2 Hydrogen Storages and Pipeline transportation

Equations 5, 6 and 7 provide the considered linear functions for calculating indirect product emissions $IPE_{product}$ (kgCO_{2-eq}) related to the manufacturing of type I tank for 60bar storage, type II tank for 300bar storage and hydrogen pipeline respectively. Variables $C_{storage60bar}$ and $C_{storage300bar}$ refer to storage capacity (kgH₂) and variable $L_{pipeline}$ refers to the length of the pipeline (km). Numerical coefficients are based on data from Ecoinvent [15,16] and [19] from which a dedicated environmental model has been built.

$$IPE_{storage60bar} = 310 * C_{storage60bar} \quad (5)$$

$$IPE_{storage300bar} = 350 * C_{storage300bar} \quad (6)$$

$$IPE_{pipeline} = 80000 * L_{pipeline} \quad (7)$$

2.4.2.3 PEM Electrolyzer

The PEM electrolyzer inventories used in this study are updated from the study published by Sharma et al. [20]. CO_{2-eq} emissions for the production phase of the PEM system have been calculated for 10 system capacities, since some components of the PEM do not increase in a linear way. The information obtained must be 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 Eq. (8) where $IPE_{electrolyzer}$ refers to indirect production emissions (kgCO_{2-eq}) of electrolyzer manufacturing and $P_{electrolyzer}$ refers to electrolyzer electrical power (MW).

$$IPE_{electrolyzer} = 261351 * P_{electrolyzer} + 45156 \quad (8)$$

2.4.2.4 Mallorca Grid Data

Since the objective of the study is to optimize the hydrogen production, including the environmental impact, CO_{2-eq} emissions of the Balearic Islands' electricity grid is required. Different sources such as Ecoinvent [15, 16] provide an average value of CO_{2-eq} emissions resulting from the overall Spain electricity grid. Other

sources, such as ENTSOE [21] and REE [22] give hourly, monthly and yearly average values of CO_{2-eq} emissions. However, this data correspond to the CO_{2-eq} emissions of the energy generation mix in the Balearic Islands, without taking into account the energy import from Spain Mainland. Therefore, in order to know the CO_{2-eq} emissions of the electricity consumed in the Balearic Islands, emissions from energy imports need to be taken into account.

For this purpose, ENTSOE and REE emission data of power generation in Spain Mainland were weighted, averaged and added to the CO_{2-eq} emissions database provided by the Industrial Engineering Department of the University of the Balearic Islands. An emission factor of 590 kgCO_{2-eq}/MWh was obtained for our reference year 2019. In addition, we considered a reduction of carbon intensity of the electrical grid based on the scenario proposed by the Ministry for Ecological Transition and the Demographic Challenge of the Balearic Islands [23] and assuming an emission factor below 160 kgCO_{2-eq}/MWh for year 2039. This hypothesis implies a Balearic generation mix composed of 65% renewables and 35% of energy imports from the Peninsula. Thus, a reduction coefficient was implemented in PERSEE in order to take into account this decrease in grid CO_{2-eq} emissions over the supposed 20 years of the project.

3. Optimization results & Discussion

3.1. Pareto Front

As it was explained in the section 2.2, a Pareto front is generated for each hydrogen transport scenario. Figure 3a shows the NPV and cumulated emissions over the 20 years project time. It can be noted that, as avoided CO_{2-eq} emissions are being considered, the three scenarios present negative values of CO_{2-eq}, when the emissions are being exclusively optimized. We observe that all scenarios adopt negative values of NPV, meaning that the system is not economically profitable when environmental aspects are being exclusively optimized given our set of assumptions (see Appendix). Besides, in terms of emissions, tube trailer (truck) scenario and pipeline scenario do not considerably differ. In other words, for this study case, these two means of H₂ transportation produce similar amount of CO_{2-eq} emissions. However, in economic terms, they present great differences, being the scenario of pipeline with reduced CAPEX the most profitable.

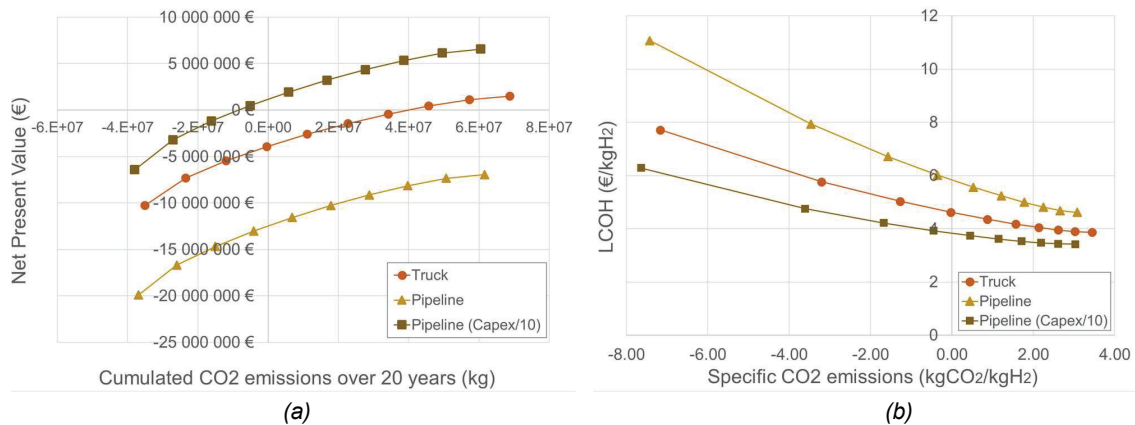
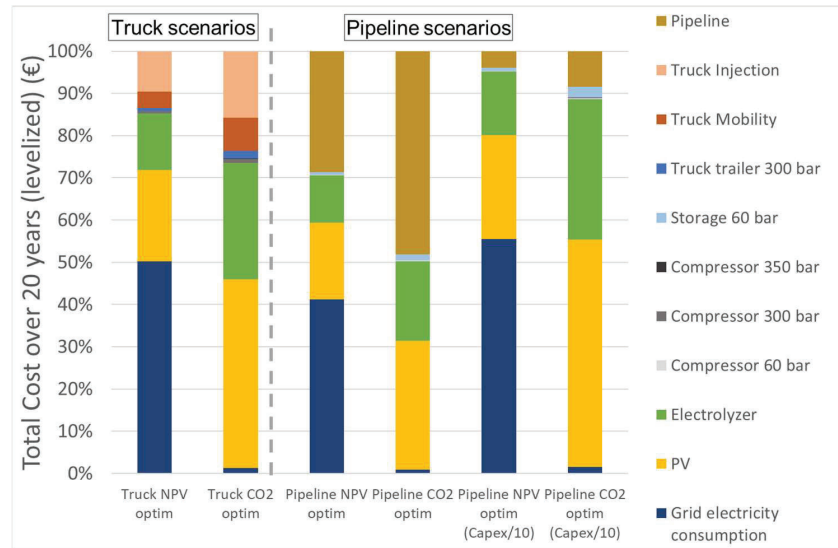


Figure 3. a) Pareto Front obtained for each of the three scenarios, b) Levelized Cost of Hydrogen compared with Specific CO_{2-eq} emissions.

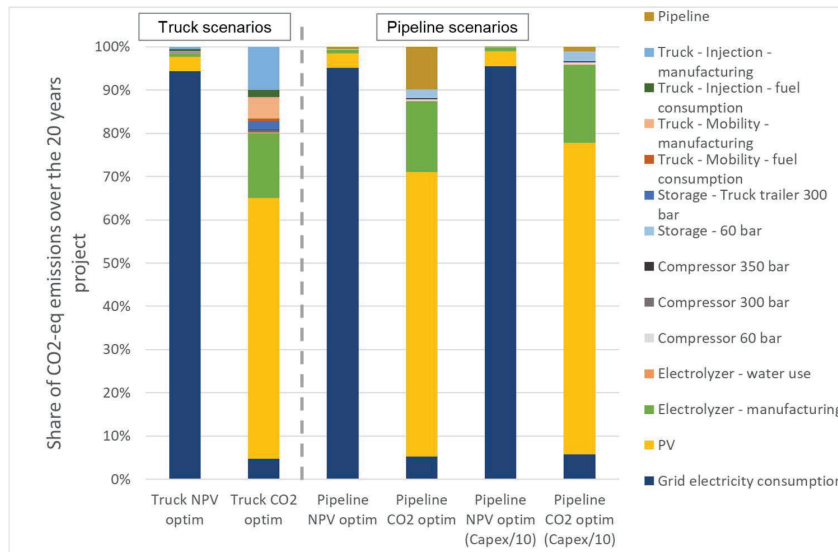
Figure 3b illustrates the Levelized Cost of Hydrogen and the specific emissions, expressed in kilograms of CO_{2-eq} per kilogram of hydrogen. It can be seen from the Figure that, when the NPV is being exclusively optimized, the pipeline with reduced CAPEX scenario presents the lowest LCOH value, accounting for ~3.4€/kgH₂. It is then followed by the tube trailer scenario (~3.9€/kgH₂) and the original pipeline scenario (~4.6€/kgH₂). For each scenario, the reported LCOH values determine the minimum H₂ averaged sell price from which the system is profitable. In addition, 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.

3.2. Cost and emissions structure

In the present section, the cost and emissions breakdown analysis of the projects is performed. Figure 4a depicts the components relative contribution to the cost, while Figure 4b shows their relative contribution to the emissions.



(a)



(b)

Figure 4. Structure of each scenario considering: a) relative cost, b) relative emissions

For the NPV optimization cases, it can be observed that the electrical grid is responsible for the highest percentage of costs and CO_{2-eq} emissions. This proves that, in this case, energy extraction from the grid takes the highest shares. For the CO_{2-eq} optimization cases it can be seen that the photovoltaic farm is responsible for most of the costs and emissions. In this optimization case, the use of the grid is minimized in order to reduce overall CO_{2-eq} emissions. Even though an emission reduction factor is assigned to the energy extracted from the grid, it seems that, environmentally speaking, it is better to reduce energy grid extraction anyway.

Finally, 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. 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.

4. Conclusions and perspectives

In this paper a multi-criteria optimization approach based on dynamic modelling has been implemented for evaluating the economic performance and greenhouse gases emissions of a PV based hydrogen energy chain.

We considered a theoretical case study relying on some of the characteristics of the GreenHysland EU project deployed in Mallorca, Spain. This case study consisted in a hydrogen energy chain comprising a 7.5 MW electrolyzer connected to a local PV plant and to the local electrical grid. The end-use applications consisted in mandatory refuelling of five hydrogen fuel cell buses and a flexible hydrogen injection into the natural gas grid up to 4%_{vol}. Hydrogen truck trailers and hydrogen pipeline were both considered for connecting production and end-use applications. The optimization was conducted over 20 years plant lifetime and considering one year of data at a timestep of one hour. The two optimization criteria were the Net Present Value and the cumulated greenhouse gases emissions including direct (fuel combustion), indirect (capex-related and from grid electricity) and avoided emissions (substitution of diesel buses and natural gas).

Several fronts of non-dominated solutions were obtained using the epsilon-constraint method. These fronts show that the cumulated greenhouse gases emissions could become negative mainly due to the greenhouse gas emission savings from substitution of natural gas by hydrogen in the natural gas grid. The structure of costs and emissions was also analysed. It was shown that when maximizing the Net Present Value, the grid electricity consumption takes the greatest share of cost breakdown and CO_{2-eq} emissions for all scenarios, as the optimizer tends to maximize the utilization rate of the electrolyzer for minimizing the costs.

On the contrary, when the cumulated CO_{2-eq} emissions are being minimized, the optimizer prefers using direct production from the local PV plant, which in turns reduces the utilization rate of the electrolyzer and increases the costs. Hence, in this case 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 emissions, the photovoltaic production involves the biggest contribution for all scenarios. However, the optimal solution shows that 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.

Hence, this study emphasizes the potential interest of such dynamic multi-criteria optimization approach to support impact assessment in pre-design phases of hydrogen projects complying with current and future GHG savings 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 relevant dynamic multi-criteria optimization approaches.

Several perspectives can be envisaged for increasing the robustness of these approaches. In terms of environmental inventory information, a comprehensive study of the waste management of the system should be carried out, i.e. the end-of-life analysis of all components. Besides, in the LCA section, several other impact categories, such as water consumption and land use, could be added to the optimization problem. Future studies should focus on how to perform a complete environmental optimization study, considering several environmental indicators as objective functions. Finding the optimal solution in an optimization problem involving more than two objectives constitutes a challenge in terms of resolution time and appropriate algorithms should be investigated to reach this objective. Uncertainties regarding all types of inputs should also be included and handled in energy system optimization problems. Including them would ensure the derivation of more robust conclusions useful for investment decision-making process and daily optimal operation. However, such methods and tools do not substitute to stakeholders investment decisions which may depend on additional local and global considerations such as regulation, market readiness, business model, social acceptance or political support.

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Appendix

Table 3. Technical, economic and environmental assumptions considered.

Component	Parameters	Units	Data	References
Lloseta PV park	Installed peak power	MWp	8.56	[1]
	Solar production	MW/MWp	PV production time series. Lloseta location	[24]
	CAPEX	EUR/kWp	1,000	Assumption
	OPEX	EUR/kWp	1% of investments costs	Assumption

	Embedded emissions ¹	kgCO _{2-eq} /MWh	26	[25]
Balearic islands power mix	Power production	MW	Hourly power time series.	[26]
	Extraction price	EUR/MWh	Hourly energy sport price time series.	[26]
	Grid emissions	kgCO _{2-eq} /MWh	Hourly CO _{2-eq} emissions time series.	[26]
PV connection	Efficiency	%	84.2	[27]
PEM Electrolyzer	Nominal power	MW	7.5 ²	[1]
	H ₂ mass flow rate	kg/h	135 ³	[28]
	Efficiency	%	61.7	[28]
	Lifetime	years	20	Assumption
	CAPEX	EUR/MW	500,000	[29]
	OPEX	EUR/MW	1.8% of investments costs	[29]
	Emissions for water use	kgCO _{2-eq} /kgH ₂	0.0044	[15,16]
Embedded emissions	kgCO _{2-eq}	261351 x P _{electrolyzer} + 45156	[6]	
300bar compressor	Inlet H ₂ pressure	bar	30	Assumption
	Outlet H ₂ pressure	bar	300	Assumption
	H ₂ mass flow rate	kg/h	135 ⁴	Assumption
	Embedded emissions	kgCO _{2-eq}	258027 x P _{compressor} + 24217	Assumption
	CAPEX	EUR/MW	700,000	[29]
OPEX	EUR/MW	7% of investments costs	[29]	
60bar compressor	Inlet H ₂ pressure	bar	30	Assumption
	Outlet H ₂ pressure	bar	60	Assumption
	H ₂ mass flow rate	kg/h	135 ⁴	Assumption
	Embedded emissions	kgCO _{2-eq}	258027 x P _{compressor} + 24217	Assumption
	CAPEX	EUR/MW	700,000	[29]
OPEX	EUR/MW	7% of investments costs	[29]	
300bar storage tank	Storage capacity	kgH ₂	Optimized	-
	Embedded emissions	kgCO _{2-eq} /kgH ₂	350 (type II H ₂ storage tank)	[19]
	CAPEX	EUR/kgH ₂	550	[29]
OPEX	EUR/kgH ₂	0% of investments costs	Assumption	
60bar storage tank	Storage capacity	kgH ₂	Optimized	-
	Embedded emissions	kgCO _{2-eq} /kgH ₂	310 (type I H ₂ storage tank)	[19]
	CAPEX	EUR/kgH ₂	550	[29]
OPEX	EUR/kgH ₂	0% of investments costs	Assumption	
Tube trailers for mobility and H ₂ injection	Distance	km	30 ⁵	-
	Fuel consumption	Kg _{diesel} /km	0.4	Assumption
	Max speed	km/h	60	Assumption
	Total capacity	KgH ₂	462	Assumption
	Usable capacity	kgH ₂	370 ⁶	-
	CO _{2-eq} (fuel use)	kgCO _{2-eq} /km	0.79 ⁷	[15,16,30,31]
	Embedded emissions	kgCO _{2-eq} /kgH ₂	350	[15,16,19]
	CAPEX	EUR/kgH ₂ ⁸	550 ⁹	[29]
OPEX	EUR/kgH ₂ ⁸	0.153 ¹⁰	Assumption	
H ₂ pipeline	H ₂ max mass flow rate	kg/h	1350 (Scenario 1); 135 ⁴ (Pipeline Scenario 2)	Assumption
	Efficiency	%	100 ¹¹	Assumption
	Embedded emissions	kgCO _{2-eq} /km	80,000	[15,16]
	CAPEX ₃ ¹²	EUR/km	1,000,000	[32]
	CAPEX ₀ ¹³	EUR/km	500,000	[32]
OPEX	EUR/km	0% of investments costs	Assumption	
350bar compressor	Inlet H ₂ pressure	bar	60	Assumption
	Outlet H ₂ pressure	bar	350	[1]
	H ₂ mass flow rate	kg/h	8	Assumption
	Embedded emissions	kgCO _{2-eq}	258027 x P _{compressor} + 24217	Assumption
	CAPEX	EUR/MW	700,000	[29]
OPEX	EUR/MW	7% of investments costs	[29]	
H ₂ demand for buses	H ₂ fixed flow rate	kg/h	8	Assumption
	Avoided CO _{2-eq}	kgCO _{2-eq} /km	1.222 ¹⁴	[15,16]
	H ₂ sell price	EUR/kgH ₂	4	Assumption

¹ Refers to CO_{2-eq} emissions

² Three 2.5 PEM electrolyzers.

³ Hydrogen production: 1080 kgH₂/day, which is 45 kgH₂/h. Considering three 2.5 MW electrolyzers, this gives 135 kgH₂/h.

⁴ Based on the three-electrolyzer production.

⁵ Lloseta – Palma de Mallorca distance

⁶ Assuming a discharge equilibrium pressure of 60bar, hence usable capacity of 300bar trailer assumed at 80% of total capacity

⁷ Two were considered for H₂ transportation (while one refuels, the other delivers). Calculation:

$$0.3 \frac{L_{diesel}}{km} \times 0.85 \frac{kg_{diesel}}{L_{diesel}} \times 1.55 \frac{kg_{CO_2}}{kg_{diesel}} \times 2 = 0.79 \frac{kg_{CO_2}}{km}$$

⁸ EUR per transported H₂

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

¹⁰ Calculation : $0.4 \frac{kg_{diesel}}{km} \times \frac{1}{0.85} \frac{L_{diesel}}{kg_{diesel}} \times 2 \frac{EUR}{L_{diesel}} = 0.94 \frac{EUR}{km} \rightarrow 0.94 \frac{EUR}{km} \times 60km = 56.47EUR \rightarrow \frac{56.47EUR}{370 kg_{H_2}} = 0.153 \frac{EUR}{kg_{H_2}}$

¹¹ No head losses are considered for the pipeline

¹² Amortized in 20 years

¹³ Amortized in 40 years

¹⁴ CO_{2-eq} emissions of a diesel bus

H ₂ demand	Max H ₂ flow rate	kg/h	Timeserie	[1]
NG grid	Avoided CO ₂ -eq	kgCO ₂ -eq/kgH ₂	8.43 ¹⁵	[15,16]
injection	H ₂ sell price	EUR/kgH ₂	4	Assumption (same price as mobility)

Nomenclature

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
H ₂	Hydrogen
HVDC	High Voltage Direct Current
LCA	Life Cycle Assessment
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
UIB	Universitat de les Illes Balears

References

- [1] GreenHysland project. – Available at: <<https://greenhysland.eu/>> [accessed 15.03.2023].
- [2] A. Valente, D. Iribarren, and J. Dufour, "Life cycle assessment of hydrogen energy systems: a review of methodological choices," *The International Journal of Life Cycle Assessment*, vol. 22, no. 3, pp. 346–363, 2017.
- [3] T. G. H. Organisation, "The Green Hydrogen Standard," 2022, [Online]. Available: <https://gh2.org/our-initiatives/gh2-green-hydrogen-standard>
- [4] E. Iturriaga, Á. Campos-Celador, J. Terés-Zubiaga, U. Aldasoro, and M. Álvarez-Sanz, "A MILP optimization method for energy renovation of residential urban areas: Towards Zero Energy Districts," *Sustainable Cities and Society*, vol. 68, p. 102787, 2021.
- [5] O. Hafez and K. Bhattacharya, "Optimal planning and design of a renewable energy based supply system for microgrids," *Renewable Energy*, vol. 45, pp. 7–15, 2012.
- [6] E. Cuisinier, C. Bourasseau, A. Ruby, P. Lemaire, and B. Penz, "Techno-economic planning of local energy systems through optimization models: a survey of current methods," *International Journal of Energy Research*, vol. 45, no. 4, pp. 4888–4931, 2021.
- [7] C. Haikarainen, F. Pettersson, and H. Saxen, "An MILP model for distributed energy system optimization," *Chemical Engineering Transactions*, vol. 35, pp. 295–300, 2013.
- [8] H. Ren, W. Zhou, K. Nakagami, W. Gao, and Q. Wu, "Multi-objective optimization for the operation of distributed energy systems considering economic and environmental aspects," *Applied Energy*, vol. 87, no. 12, pp. 3642–3651, Dec. 2010, doi: 10.1016/j.apenergy.2010.06.013.
- [9] P. J. Copado-Méndez, C. Pozo, G. Guillén-Gosálbez, and L. Jiménez, "Enhancing the ϵ -constraint method through the use of objective reduction and random sequences: Application to environmental problems," *Computers & Chemical Engineering*, vol. 87, pp. 36–48, Apr. 2016, doi: 10.1016/j.compchemeng.2015.12.016.
- [10] S. Sinha and S. S. Chandel, "Review of software tools for hybrid renewable energy systems," *Renewable and Sustainable Energy Reviews*, vol. 32, pp. 192–205, 2014, doi: <https://doi.org/10.1016/j.rser.2014.01.035>.

¹⁵ Natural gas emission factor times LHV_{H₂}

- [11] H. Sharma, É. Monnier, G. Mandil, P. Zwolinski, and S. Colasson, "Comparison of environmental assessment methodology in Hybrid energy system simulation software," *Procedia CIRP*, vol. 80, pp. 221–227, 2019.
- [12] I. O. for Standardization (ISO), "ISO 14040: 2006 Environmental Management–Life Cycle Assessment–Principles and Framework (2)." International Organization for Standardization Geneva, 2006.
- [13] B. Steubing, D. de Koning, A. Haas, and C. L. Mutel, "The Activity Browser—An open source LCA software building on top of the brightway framework," *Software Impacts*, vol. 3, p. 100012, 2020.
- [14] É. Cuisinier, P. Lemaire, B. Penz, A. Ruby, and C. Bourasseau, "New rolling horizon optimization approaches to balance short-term and long-term decisions: An application to energy planning," *Energy*, vol. 245, p. 122773, Apr. 2022, doi: 10.1016/j.energy.2021.122773.
- [15] G. Wernet, C. Bauer, B. Steubing, J. Reinhard, E. Moreno-Ruiz, and B. Weidema, "The ecoinvent database version 3 (part I): overview and methodology," *The International Journal of Life Cycle Assessment*, vol. 21, no. 9, pp. 1218–1230, 2016.
- [16] B. Steubing, G. Wernet, J. Reinhard, C. Bauer, and E. Moreno-Ruiz, "The ecoinvent database version 3 (part II): analyzing LCA results and comparison to version 2," *The International Journal of Life Cycle Assessment*, vol. 21, no. 9, pp. 1269–1281, 2016.
- [17] S. Ghandehariun and A. Kumar, "Life cycle assessment of wind-based hydrogen production in Western Canada," *International Journal of Hydrogen Energy*, vol. 41, no. 22, pp. 9696–9704, Jun. 2016, doi: 10.1016/j.ijhydene.2016.04.077.
- [18] Y. D. Lee, K. Y. Ahn, T. Morosuk, and G. Tsatsaronis, "Environmental impact assessment of a solid-oxide fuel-cell-based combined-heat-and-power-generation system," *Energy*, vol. 79, pp. 455–466, 2015.
- [19] H. W. Langmi, N. Engelbrecht, P. M. Modisha, and D. Bessarabov, "Chapter 13 - Hydrogen storage," in *Electrochemical Power Sources: Fundamentals, Systems, and Applications*, T. Smolinka and J. Garche, Eds. Elsevier, 2022, pp. 455–486. doi: 10.1016/B978-0-12-819424-9.00006-9.
- [20] H. Sharma, G. Mandil, É. Monnier, E. Cor, and P. Zwolinski, "Sizing a hybrid hydrogen production plant including life cycle assessment indicators by combining NSGA-III and principal component analysis (PCA)," *Energy Conversion and Management: X*, vol. 18, p. 100361, Apr. 2023, doi: 10.1016/j.ecmx.2023.100361.
- [21] A. ENTSO-E, "ENTSO-E transparency platform," URL <https://transparency.entsoe.eu>, 2017.
- [22] Red Eléctrica de España (REE), "REData API," <https://www.ree.es/es/apidatos>, 2022.
- [23] Ministerio Para la Transición Ecológica y el Reto Demográfico, "Plan Nacional Integrado de Energía y Clima (PNIEC) 2021–2030," 2019.
- [24] JRC Photovoltaic Geographical Information System (PVGIS) - European Commission. Available at: < https://re.jrc.ec.europa.eu/pvg_tools/en/ > [accessed 02.02.2023].
- [25] Live 24/7 CO₂ emissions of electricity consumption. - Available at:< <https://app.electricitymaps.com/zone/ES>>[accessed 02.02.2023].
- [26] Industrial Engineering Department, University of the Balearic Islands. Hourly datasheet from 2019.
- [27] Tecnicos consultores. Parque solar fotovoltaico Lloseta: Proyecto: Power to Green Hydrogen. Balearic Islands, Spain. - Available at: <https://www.caib.es/sites/normativaindustria/f/282195> [accessed 05.02.2023].
- [28] HyLYZER® WATER ELECTROLYZERS datasheet. - Available at < <https://mart.cummins.com/imagelibrary/data/assetfiles/0070330.pdf> >. [accessed 05.01.2023].
- [29] FCH 2 JU - MAWP Key Performance Indicators (KPIs). Available at: < https://www.clean-hydrogen.europa.eu/knowledge-management/strategy-map-and-key-performance-indicators/fch-2-ju-mawp-key-performance-indicators-kpis_en > [05.03.2023].
- [30] International Council of Clean Transportation. Fuel Consumption Testing of Tractor-Trailers in The European Union and the United States. - Available at <https://theicct.org/wp-content/uploads/2021/06/EU_HDV_Testing_BriefingPaper_20180515a.pdf> [accessed 10.03.2023].
- [31] Speight, J.G, 2-Production, properties and environmental impacts of hydrocarbon fuel conversion. In: *Advances in Clean hydrocarbon Fuel Processing*. United States: Woodhead Publishing Series in Energy. 2011.p.54-82.
- [32] IEA, The Future of Hydrogen. Paris, France. 2019 Jun. Report prepared by the IEA for the G20.