HYGRID

FLEXIBLE HYBRID SEPARATION SYSTEM FOR H2 RECOVERY FROM NG GRIDS

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WP9 – Environmental LCA and economic assessment

D.9.3
Integrated final environmental life cycle assessment, life cycle costing and business plan

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Table of contents

ACRONYMS and ABBREVIATIONS

CO_2	carbon dioxide
CMSM	Carbon Molecular Sieve Membranes
DALY	disability adjusted life-years
EHP	Electrochemical Hydrogen Purification
FU	functional unit
g	gram
GHG	greenhouse gas
H_2	Hydrogen
H_2O	water
ILCD	International Reference Life Cycle Data System
IPCC	Intergovernmental Panel on Climate Change
ISO	International Organization for Standardization
kg	kilogram
kg CO_2-eq	kilogram of carbon dioxide equivalent
kWh	kilowatt hour
LCA	life cycle assessment
LCC	life cycle costing
LCI	life cycle inventory
LCIA	life cycle impact assessment
m^3	cubic metre
MEA	Membrane Electrodes Assembly
mg	milligram
MJ	megajoule
n/a	not applicable
NOx	nitrogen oxides
O_2	oxygen (gas)
PDF.m^2.y	potentially disappeared fraction per square metre of land per year
PM	particulate matter

PSA	Pressure Swing Adsorption
SOx	sulphur oxides
TBD	to be decided
TSA	Temperature Swing Adsorption
WP	work package
µm	micrometre

1 EXECUTIVE SUMMARY

1.1 Description of the deliverable content and purpose

The objective of the H2020 EU research project HyGrid is the design, scale-up and validation of a novel membrane-based hybrid technology for the direct separation of hydrogen from natural gas grids. This novel technology separates hydrogen through a combination of membranes, electrochemical separation (EHP) and temperature swing adsorption (TSA). The target is to achieve high hydrogen purity at low energy consumption and hence decreased cost of hydrogen separation compared to existing technologies. Moreover, the environmental impacts of hydrogen separation via the HyGrid technology should not be higher than via conventional technologies. A small-scale pilot system with a capacity of 12.6kg hydrogen separated per day was designed, built and tested during the project.

To assess the environmental impacts associated with hydrogen separation via the HyGrid technology compared to the conventional reference technology, pressure swing adsorption (PSA), Quantis had the task to perform an environmental life cycle assessment (LCA). Further, the life cycle costs of the system were determined in an Life Cycle Costing (LCC) analysis.

LCA is an internationally recognized approach that has been standardized by the International Organization for Standardization (ISO) (ISO 14040:2006, ISO 14044:2006) to evaluate and assess the potential environmental and human health impacts associated with products and services throughout their life cycles. LCA is used to identify hotspots and thus opportunities to improve the environmental performance of products or services at all stages along their life cycles. The life cycle costing analysis is an economic analysis aligned in its scope and method with the LCA.

This deliverable present the results obtained for the full LCA and LCC. It builds upon the results of the preliminary screening LCA and LCC which are presented in deliverable D9.2 and which are based on data obtained up to M24 of the HyGrid project. The full LCA assesses the environmental impacts of the HyGrid technology at its latest stage of development within the project. It provides a more in-depth analysis with a particular focus on the environmental hotspots identified during the screening LCA.

The full LCA is based on data collected throughout the entire period of the project. Mostly primary data were provided by various work-packages. In particular, process-design and modelling from WP8 (TUE) provided most of the data related to mass and energy balance of the processes. WP3, Membrane development, WP4 Electrochemical hydrogen separation development and WP5 TSA development provided data related to the manufacturing of the technology's components, their lifetimes and end-of-life.

While the preliminary LCA took a cradle-to-gate approach, meaning that it considered the life cycle stages from the extraction and processing of raw materials through to the separation of hydrogen, the full LCA follows a cradle-to-grave approach. This means, all life cycle stages of both technologies, HyGrid and PSA, including their end-of-life of are considered.

The full LCA is completed with sensitivity analyses (with respect to the main contributors to the environmental impacts) to improve the robustness of the results and manage the possible uncertainty with respect to specific key parameters.

The aim of the full LCA is to identify opportunities for optimized environmental performance and designed of this novel technology to assure a more sustainable solution for hydrogen separation.

The functional unit for this study is:

The recovery of 1kg of hydrogen from an average European natural gas grid

with a purity of at least 99.97%.

As mentioned, primary data have been collected from partners involved in WPs 3, 4, 5, 7 and 8. Each plant design is based on a hydrogen production rate of 12.6 kg H_2/day. All life cycle inventory data are taken from the ecoinvent database v3.7.1.

The peer-reviewed impact assessment method IMPACT 2002+ (vQ2.28) is used for the impact assessment phase of the study, evaluating the impact on the following environmental impact categories:

- Greenhouse gas (GHG) emissions (carbon footprint)
- Water withdrawal (water footprint)
- Ecosystem quality
- Readd depletion
- Human health

The results of the detailed LCA study show that the separation of hydrogen from natural gas is in general more environmentally friendly with the small-scale HyGrid prototype system than with a PSA reference system of comparable size. The operation phase, in particular energy consumption, was identified as the main environmental hotspot for both technologies. The HyGrid technology consumes significantly less energy to separate one kg of hydrogen from the natural gas stream than the PSA comparison case. However, the energy consumption remains also for this system the main hotspot and thus represents the largest potential for improvement in the future development of the system. It is therefore recommended to further reduce the energy consumption, in particular to eliminate the heat demand met with fossil fuels. The remaining energy demand (after efficiency improvements) shall be met with low-impact electricity sources such as wind power to minimize the environmental impacts.

The impacts of system manufacturing become the more relevant the lower the operation impacts become, e.g. when using a low-impact electricity source. The main material hotspot is the use of steel and electronics. Since economies of scale are expected to apply for these, the relative relevance of manufacturing impacts is expected to decrease as the system scale increases to commercial size.

While at this stage of technological development data were not yet available to perform an LCA for a large-scale system, projections of cost data could be obtained for a large-scale system. The life cycle costing analysis was thus performed for a commercial size system of 200kg H_2 per day, providing a range of hydrogen separation cost that is more realistic for commercial application than the analysis of the prototype cost would be. From the LCC it results that the total cost of hydrogen delivery with the HyGrid system likely lies between 1.2 € and 2.4 € per kg H_2. The major cost hotspots are similar to the environmental hotspots: the operation of the system electricity and heat, together with carbon emission costs are the largest contributors; for the manufacturing of the system, the cost for raw materials is dominating.

It can be concluded that both from an environmental as well as from a cost point of view, it is essential to further improve the energy efficiency of the HyGrid system. The recommendations resulting from this study are to further optimize operation conditions for lower energy consumption and to eliminate as far as possible the fossil heat demand. Moreover, material efficiency of the system components shall be increased by optimized design and through the scaling-up to commercial system size. In the future, once an optimized HyGrid system is available at commercial scale and more and more low-impact electricity sources feed into the electricity grids, the system shall ideally be operated with such low-impact energy sources.

1.2 Brief description of the state of the art and the innovation

Since the system under study is currently being developed within the HyGrid project, no LCA results or literature on this specific topic exist. The results of the LCA of the hydrogen recovery systems developed within HyGrid will therefore shed new light on the contributions which these devices can bring in the shift towards more sustainable energy distribution systems.

1.3 Deviation from objectives

No deviation from the objectives.

INTRODUCTION

This deliverable, D9.3, presents the life cycle assessment (LCA) and life cycle costing (LCC) methodology and the scope of the study, the data and the assumptions used, and finally the full LCA and LCC results of the HyGrid technology with a comparison to a reference technology. Moreover, a business plan for the HyGrid technology is presented in this deliverable.

This deliverable builds on D9.2 Preliminary environmental LCA (Itten & Faist Emmenegger, 2018)in which preliminary results for the LCA are presented and on D 9.1 (Itten & Faist Emmenegger, 2017) which specifies the goal and scope of the LCA and LCC study.

1.4 Context and background

Heightened concern around the environmental and social sustainability of society's consumption habits has focused attention on understanding and proactively managing the potential environmental and societal consequences of the production and consumption of products and services. Nearly all major product producers now consider environmental and social impacts as a key decision point in their procurement and product development. Sustainability is a recognized point of competition in many industries.

A leading tool for assessing environmental performance is LCA, a method defined by the International Organization for Standardization (ISO) 14040-14044 standards (ISO 2006a; ISO 2006b). LCA is an internationally recognized approach that evaluates the relative potential environmental and human health impacts of products and services throughout their life cycle, beginning with raw material extraction and including all aspects of transportation, manufacturing, use, and end-of-life treatment.

It is important to note that LCA does not exactly quantify the real impacts of a product or service due to data availability and modelling challenges. However, it allows for estimating and understanding the potential environmental impacts that a system might cause over its typical life cycle, by quantifying (within the current scientific limitations) the likely emissions produced and resources consumed. Hence, environmental impacts calculated through LCA should not be interpreted as absolute, but rather as relative values within the framework of the study. Ultimately, this is not a limitation of the methodology, since LCA is generally used to compare different systems performing the same function, where it is the relative differences in environmental impacts which are key for identifying the solution which performs best.

Among other uses, LCA can identify opportunities to improve the environmental performance of products, inform decision-making, and support marketing, communication, and educational efforts. The importance of the life cycle view in sustainability decision-making is sufficiently strong that over the past several decades it has become the principal approach to evaluate a broad range of environmental problems, to identify social risks and to help make decisions within the complex arena of socio-environmental sustainability.

The aim of the HyGrid project is to develop innovative hydrogen recovery systems based on the combined use of membranes, electrochemical hydrogen purification (EHP) and temperature swing adsorption (TSA). The idea is to use such systems to recover hydrogen from the mixture of gases flowing through the natural gas grid. This would allow for using the existing natural gas grid as a transport and storage system for hydrogen avoiding the construction of a dedicated hydrogen distribution grid and hence avoiding the related costs and impacts.

The aim of WP9 is to perform an environmental LCA and economic LCC assessment of the hydrogen recovery systems developed within HyGrid as well as to make the business case for the commercialization of this novel technology. Further, since the LCA will accompany the research, the idea is to use the LCA work to steer the

development of the systems towards more sustainable solutions. Finally, a comparison will be made between the life cycle performance of the systems developed within HyGrid and the conventional technology currently able to deliver the same service.
This deliverable presents the results of the second step of the LCA analysis (full LCA), following the screening LCA. The model and calculations were revised and extended with updated data and assumptions. Emphasis was set on the process units generating the largest impacts ("hotspots") identified in the screening analysis. The life cycle thinking approach was also extended to the economic perspective by modelling life cycle cost in parallel to the system boundaries and structure of the environmental analysis.

The study at this stage does not comply with all the ISO 14040 requirements to make competitive public statements or marketing claims. While it is not intended to support such purposes, it provides a foundation for additional work aiming at meeting such purposes. Communication of the results presented in this report outside HyGrid should be conducted with caution and accompanied by a statement that the findings are based on an LCA that doesn't support public claims.

1.5 Life cycle assessment and life cycle costing approach

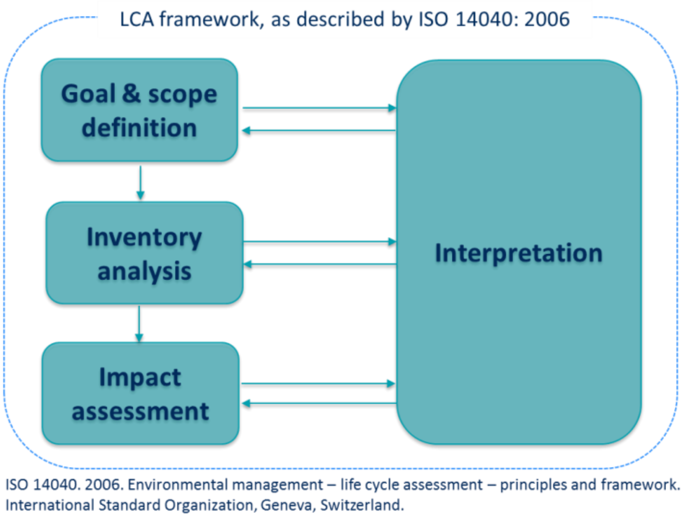
A life cycle assessment (LCA) and a life cycle costing (LCC) are both comprised of four phases as shown in Figure 1 below:

1. **Goal and scope definition:** defining the purposes of the study, determining the boundaries of the system life cycle in question and identifying important assumptions that will be made;
2. **Inventory analysis:** compiling a complete record of the important material and energy flows throughout the life-cycle, in addition to releases of pollutants and other environmental aspects being studied;

3. **Impact and cost assessment**: using the inventory compiled in the prior stage to create a clear and concise picture of environmental and economic impacts among a limited set of understandable impact categories; and
4. **Interpretation**: identifying the meaning of the results of the inventory and impact assessment relative to the goals of the study.

LCA is best practiced as an iterative process, where the findings at each stage influence changes and improvements in the others to arrive at a study design that is of adequate quality to meet the defined goals. The principles, framework, requirements and guidelines to perform an LCA are described by the international standards ISO 14040 series (ISO 2006).

Figure 1: LCA framework (ISO 2006)



2 GOAL AND SCOPE DEFINITION

The goal and scope of the study, along with the methodological framework of the LCA, has been described in D9.1. We copy here the content of D9.1 to facilitate the comprehension of the study and amend/complete where necessary to account for decisions made at the M24 meeting with regards to main assumptions on system configuration, e.g. capacity.

2.1 Objectives

The aim of WP9 is to perform an environmental LCA and economic assessment of the hydrogen recovery systems developed within HyGrid. This will allow understanding what environmental impacts could be caused by the investigated systems and what economic burden will result from their production, use and end-of-life. In order to further assess the advantages and challenges connected to the development of HyGrid's hydrogen recovery systems, the results of the environmental and economic life cycle analysis will be compared against those of the currently available technology typically used for the recovery of hydrogen from a gas mixture mainly comprising natural gas. Finally, by doing an accompanying study which develops together with the findings of the other WPs, the idea is to steer the project towards the realisation of more environmentally friendly hydrogen recovery systems by highlighting, along the way, critical environmental issues which may be optimised.

The hydrogen recovery system developed within HyGrid comprises three successive recovery steps. As schematically shown in Figure 2, the natural gas mixture is first sent through a membrane separation system, then through electrochemical hydrogen purification (EHP). The separated hydrogen is then sent to the temperature swing adsorption (TSA) unit.

Figure 2: Hydrogen recovery system within HyGrid.

The membrane separation system consists of the membranes and of the membrane module. Various membranes are currently being investigated. Particularly, Palladium-based and Carbon Molecular Sieve Membranes (CMSMs) are considered. Regarding the membrane module, the impact on the system's performance of metallic and ceramic supports for the membranes are also analysed.

The life cycle analysis addresses the various subsystems (Membrane separation system, EHP and TSA) as well as the different membrane types and supports in order to identify the most sustainable solutions. Table 1 summarises the key target parameters for the recovery systems addressed within HyGrid (DoW, 2015).

Table 1: Target parameters for HyGrid's hydrogen recovery systems

	P [bar]	T [°C]	H_2 production [kg/day]	H_2 cost [€/kg H_2]	Power consumption [kWh/kg H_2]	Payback time [years]	Lifetime [years]
HyGrid System	0.03-80	T<400	>25	<1.5	<5	<6	>15

2.2 Intended audience

The results of this full LCA and LCC are intended for public disclosure.

2.3 Description of the reference systems

In terms of reference technology, it was identified that the most relevant technology which could deliver a hydrogen recovery service similar to the one provided by HyGrid's systems is 5-bed pressure swing adsorption (PSA) (see also deliverable D9.1). PSA is a mature technology for large-scale applications with high H2 feed concentrations. Its operation at low H2 feed concentration and high H2 purity as it is required for HyGrid comes with challenges but is feasible with certain limitations as outlined in detail in deliverable D2.2. It was therefore decided that 5-bed PSA will be used as reference technology against which the environmental and cost performance of the recovery systems developed within HyGrid will be compared.

2.4 Functional Unit

The functional unit quantifies the performance of a product system and is used as a reference unit for which the life cycle assessment study is performed and the results are presented. It is therefore critical that this parameter is clearly defined and measurable.

The purpose (or function) of the systems developed within HyGrid is the recovery of pure hydrogen from a mixture of gases mainly comprising natural gas and available from the natural gas grid. Moreover, since one potential application of these recovery systems is to use the hydrogen in automotive systems, the recovered hydrogen should be of sufficient purity to be used in fuel cell systems for road vehicles.

The functional unit for the analysis is therefore:

The recovery of 1 kg of hydrogen from an average European natural gas grid with a purity of at least 99.97%

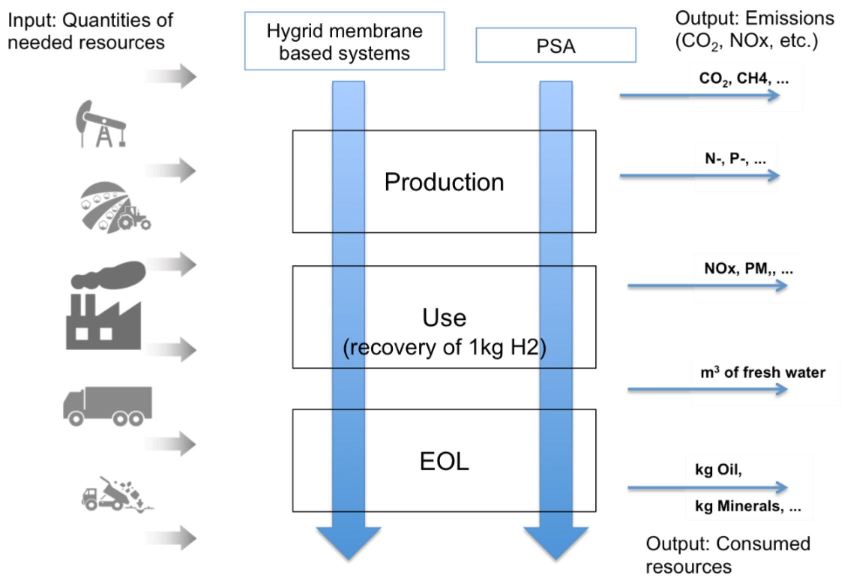
The reference flow is therefore 1 kg of hydrogen with a purity of at least 99.97%.

2.5 System boundaries

The system boundaries define what processes will be considered in the analysis. The aim of the environmental and economic assessment in HyGrid is to identify the relevant mechanisms in the life cycle of the hydrogen recovery systems which might impact the environment and to understand its key cost aspects. As such, as far as data availability allows, the target is to try and include all potential main impact and cost contributors. As schematically shown in **Figure 3** for the environmental assessment, this means that all emissions caused and resources consumed by processes such as the production of the raw materials and energy vectors required for the manufacturing, use and end-of-life will be included in the analysis. This includes the impacts deriving from the extraction of the raw materials, production or dismantling infrastructure, all transport services which might be required as well as waste disposal systems or the generation of the needed electricity or fuels. For the life cycle cost analysis, the same approach will be used, only focusing on the cost information for each item considered.

Not included in the system boundaries is the production of hydrogen and natural gas, and their distribution in the natural gas pipeline networks, since this is the same for both systems under comparison, the HyGrid system and the reference technology.

Figure 3: System boundaries in the LCA of the hydrogen recovery systems.



Following the definition of the functional unit, the results will be scaled to the life cycle environmental and cost impacts for the recovery of 1 kg of hydrogen. As already mentioned above, for the recovery systems developed within HyGrid, the analysis will address the various sub-systems (membranes, EHP and TSA) as well as the various membrane types and supports. This will highlight the hot spots of the systems (meaning the sub-processes responsible for the largest environmental impacts and cost contributions) and thereby help to identify the potential for optimisation.

2.6 Allocation methodology

According to ISO, the term allocation refers to the partitioning of the input/or output flows of a process to the product system under study. As there are no co-products, no allocation is necessary in the studied system.

2.7 End-of-life modelling

The end-of-life (disposal and recycling) is modelled using the approach as described in the PEF method (Zampori & Pant, 2019), which allows a consistent description of the burdens and benefits of recycling and disposal. This approach accounts for the status in the recycling market, i.e. if pathways for the recycling of the materials are already well established or not, and distributes in a consistent way the burdens and benefits between the "first" and the "second" life of the material in question. This approach and the circular footprint formula (CFF) are described in detail in (Zampori & Pant, 2019).

2.8 Life cycle inventory

The life cycle inventory (LCI) is an inventory of input/output data that relates to the functional unit of the system being studied.

The foreground processes are based on activity data collected from project partners and literature. For this project a data collection file was prepared and distributed to all partners in order to facilitate the data collection process. Primary data have been collected from WP 3-5 and WP 7-8. The foreground data are described in detail in Section .

The LCI data describing background processes (e.g. electricity generation or natural gas production) are in large part from the ecoinvent database (version 3.7.1), a particularly robust and complete database, both in terms of technological and environmental coverage. This database can be used in ISO-compatible LCAs and it is internationally recognized by experts in the LCA field.

The quality of LCA results is dependent on the quality of data used in the study. It is necessary to utilize, research and implement the most credible and representative information available. Therefore, the data quality has further been improved for the detailed LCA compared to the screening LCA.

The environmental LCA follows the main guidelines of the International Reference Life Cycle Data System (ILCD) Handbook and the ISO norms 14040-14044.

2.9 Environmental impact assessment

The life cycle impact assessment (LCIA) is the step in which the data on the quantities of emissions produced and resources consumed by the life cycle of a system is transformed into information on the damages caused to the environment. The impacts are calculated using characterization factors recommended in internationally recognized impact assessment methods.

In the LCA of the hydrogen recovery systems developed within HyGrid, the IMPACT 2002+ (Humbert et al., 2014) LCIA method is used for this task. The IMPACT 2002+ framework links the emissions caused and resources consumed by the life cycle of a system to five so-called endpoints (damage-oriented) categories (human health, ecosystem quality, climate change, resources, and water withdrawal). It was originally developed at the Swiss Federal Institute of Technology of Lausanne (EPFL), Switzerland. Subsequently, Quantis made some updates to the original IMPACT 2002+ methodology version 2.1[1]. This adapted version is referred to as "IMPACT 2002+ version Q2.30 (adapted by Quantis)". The life cycle assessment focuses on the five IMPACT 2002+ end-point indicators (described in **Table 2** below) over the entire lifecycle of the processes.

[1] The main difference between IMPACT 2002+ v2.1 and IMPACT 2002+ vQ2.30 (adapted by Quantis) are (i) climate change characterization factors are adapted with global warming potentials for a 100 year time horizon, (ii) water withdrawal, water consumption and water turbined are added as the midpoint categories, (iii) aquatic acidification, aquatic eutrophication and water turbined are brought to the damage category ecosystem quality, and (iv) normalization factors are updated.

Table 2: Description of IMPACT 2002+ endpoint indicators

Indicator		Definition
	Greenhouse gas emissions	This indicator measures the potential impact on climate change from greenhouse gas emissions associated with a product, process or organization. It takes into account the midpoint category “global warming". The impact metric is expressed in kg CO_2-eq.
	resource depletion	This indicator measures the potential impact on resource depletion from resource use (e.g. fossil fuels and minerals) associated with a product, process or organization. It takes into account non-renewable energy and mineral extraction. These factors are simply the sum of the endpoint categories non-renewable energy consumption and mineral extraction. The impact metric is expressed in MJ ("measures the amount of energy extracted plus the amount needed to extract the resource itself").
	Water withdrawal	This indicator measures the amount of water withdrawal associated with a product, process or organization. It takes into account water (whether it is evaporated, consumed or released again downstream) excluding turbined water (i.e., water flowing through hydropower generation). It considers drinking water, irrigation water and water for and in industrialized processes (including cooling water), fresh water and seawater. This indicator is actually based and expressed on volumes (m^3) of water withdrawal.
	Human health	This indicator measures the potential impact on human health caused by emissions associated with a product, process or organization. It takes into account human toxicity (carcinogenic and non-carcinogenic), respiratory inorganics, ionizing radiation, ozone layer depletion and respiratory organics. It characterizes disease severity, accounting for both mortality (years of life lost due to premature death) and morbidity (rate of incidence of a disease). The impact metric is expressed in DALY (“disability-adjusted life years”).
	Ecosystem quality	This indicator measures the potential impact on ecosystems (biodiversity, species and their inhabitant) caused by emissions or resource use associated with a product, process or organization. It takes into account aquatic ecotoxicity, terrestrial ecotoxicity, terrestrial acidification & nutrification, aquatic eutrophication, aquatic acidification, water turbined and land occupation. It characterizes the fraction of species disappeared on one m2 surface during one year. The impact metric is expressed in PDF.m^2.y (“potentially disappeared fraction of species over one m^2 and during one year”).

For an additional validation of the robustness of results, a second impact assessment method, the EF 3.0 Method, was applied. The Environmental Footprint (EF) method was developed within an initiative of the European Commission to establish a common methodological approach for quantifying the environmental performance of any good or service throughout its life cycle. We apply version 3.0 of the EF method as released in November 2019.

2.10 Life cycle costing assessment (LCC)

The HyGrid project will further investigate the latest advances in monetary valuation of impacts. The HyGrid framework is an interesting and challenging case for testing the combination of LCA and LCC. In order to ensure consistency between the two methods and to enhance the integrated evaluation of the investigated technologies and products, the LCA and LCC have an equivalent data structure and system boundaries and rely on the same data especially regarding the consumption of raw materials, energy and operating supplies.

The aspect in which LCA and LCC differ in the current study is the scale of the analysed system. For the LCA the current data availability is limited to the prototype system which was developed during the HyGrid project, i.e. a small-scale system of 12.6 kg H_2 per day. For the LCC the cost for commercial-scale hydrogen separation is of interest. Cost data for a large-scale system of 200kg H_2 per day could be obtained. Therefore, the LCC results refer to a large-scale system while the LCA results refer to a small-scale system.

2.11 LCIA limitations

LCIA results present potential and not actual environmental impacts. They are relative expressions, which are not intended to predict the final impact or risk on the natural media or whether standards or safety margins are exceeded. Additionally, these categories do not cover all the environmental impacts associated with human activities. Impacts such as noise, odours, electromagnetic fields and others are not included in the present assessment. The methodological developments regarding such impacts are not sufficient to allow for their consideration within life cycle assessment. Other impacts, such as potential benefits or adverse effects on biodiversity, are also only partly covered by current impact categories.

2.12 Calculation tool

SimaPro 9.1.1 software, developed by PRé Consultants (www.pre.nl) was used to perform the LCA modelling and link the reference flows with the LCI database and link the LCI flows to the relevant characterization factors. The final LCI result was calculated by combining foreground data (intermediate products and elementary flows) with generic datasets providing cradle-to-gate background elementary flows to create a complete inventory of the investigated systems.

3 LIFE CYCLE INVENTORY DATA

3.1 Data availability

Since HyGrid's consortium includes experts in all sub-systems of the hydrogen recovery systems, as far as possible project-specific primary data from project partners has been used, at least regarding the quantities of required input materials, energy and direct emissions occurring for the production and use phase. For the disposal phase, where higher uncertainties about the fate of components during disposal or recycling processes available in the future occur, it is necessary to rely on literature data and experts' feedback. Further, data on the environmental impacts of background processes such as general transport services, the production of the manufacturing infrastructure, the production of the required raw materials or the generation of the necessary fuels are taken from the environmental database ecoinvent. The various data sources used in the project are visualized in Figure 4 and listed in Table 3

Figure 4: Key data sources used for the LCA.

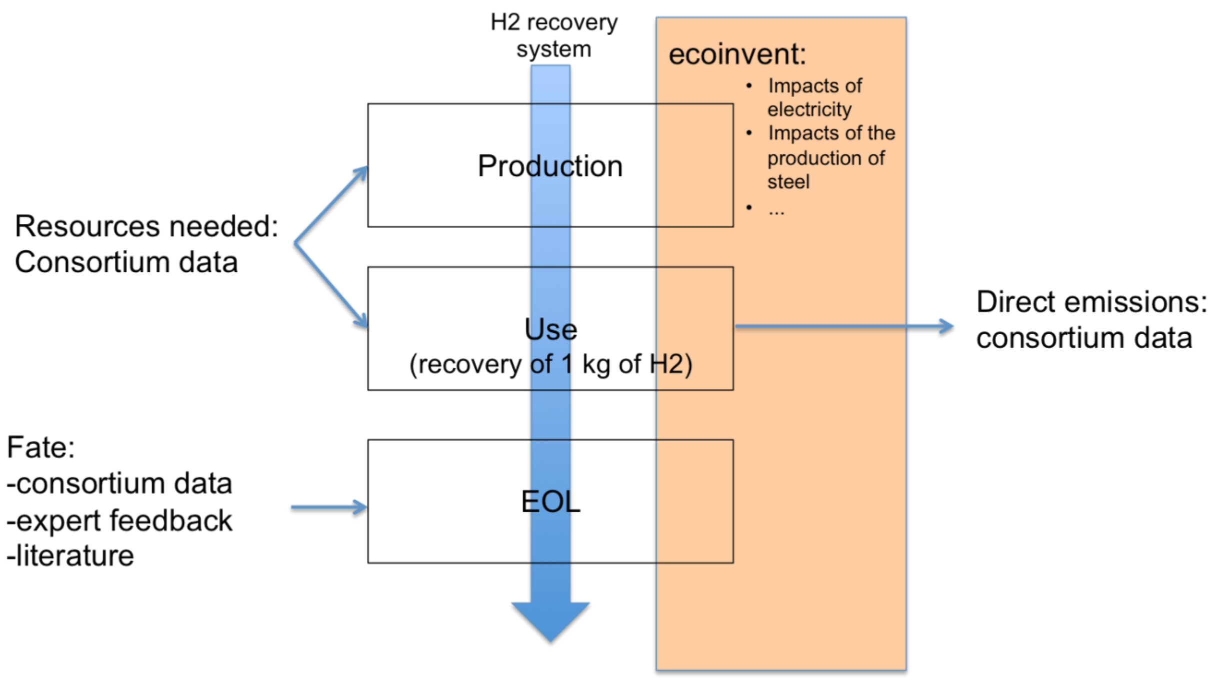


Table 3: Key data sources used for the LCA

	HyGrid	**PSA**
System manufacturing		
Type + amounts of raw material inputs	primary data	Modelled data
Processing of raw materials, e.g. welding of steel	ecoinvent data	ecoinvent data
Production of manufacturing consumables	ecoinvent data	ecoinvent data
Amount + type of energy consumption for manufacturing	primary data	ecoinvent data
Generation of energy used for manufacturing (e.g. electricity mix)	ecoinvent data	ecoinvent data
Transport distance + mode of component to HyGrid assembly site	average based on primary data	
Amounts of manufacturing waste + wastewater, type of waste treatment	primary data	modelled data
System Operation		
Energy consumption (electric & thermal)	primary data	modelled data
Amounts of consumables (water, glycol, equipment with shorter lifetime)	primary data	modelled data
Production of energy + consumables for operation	ecoinvent data	ecoinvent data
System End-of-life (EOL)		
EOL treatment + recycling processes	ecoinvent data	ecoinvent data

The data availability and therefore the management of the data collection (including coordination, preparation of data collection templates, definition of a time plan, etc.) are key for Quantis to be able to perform the assessments. Quantis encouraged interactive dialogue throughout the project, by means of regular actions, teleconferences and discussions during meetings.

The collected inventory data for the manufacturing of the four HyGrid components are confidential and are therefore omitted from this report.

3.2 Key assumptions

The main data and hypotheses used in this study are detailed below.

End-of-life modelling

As described in section 2.7 the approach of the PEF method is applied to consistently model burdens and benefits of material recycling and disposal. We developed datasets applying the circular footprint formula. The formula's parameters applied for each material and end-of-life scenario are documented in Table 12 in ANNEX I of this report.

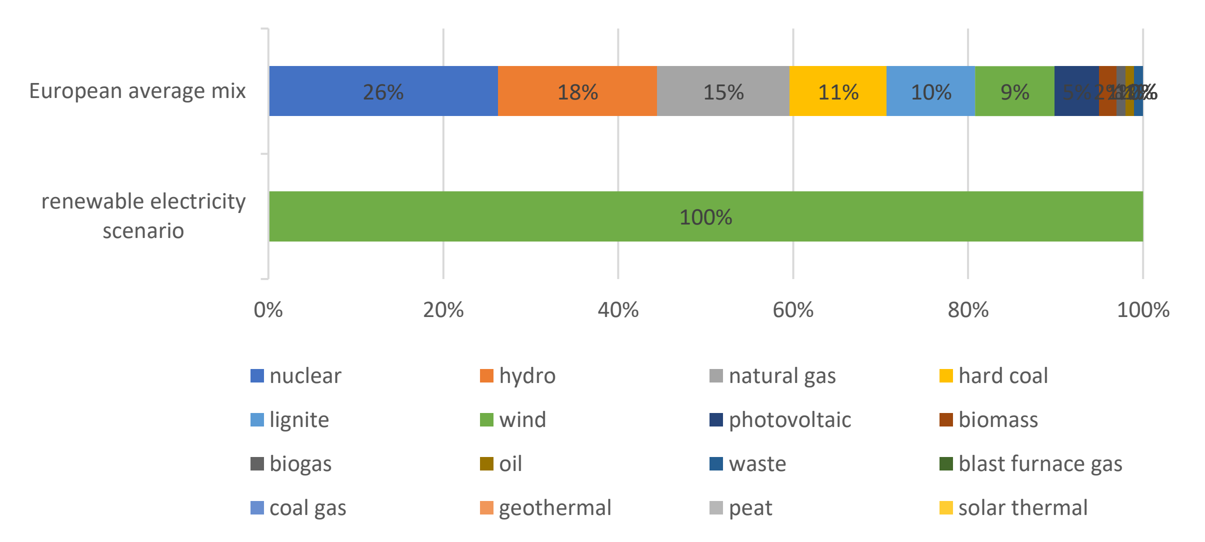
Electricity mix

The major part of the electricity consumption occurs in the operation phase of the HyGrid technology. It is a major contributor to the life cycle results. For this reason, scenarios with different electricity sources in the operation phase were analysed. No country-specific electricity mixes were considered since the aim of this LCA is to assess the HyGrid technology in general, rather than a specific supply chain. By default, we consider the average European electricity mix, which is modelled as the average over all electricity supplied in the grid region of the European Network of Transmission System Operators for Electricity (ENTSO-E) in the year 2017 as available in the ecoinvent dataset "Electricity, low voltage {ENTSO-E}| market group for | Cut-off, U" (ecoinvent database v3.7.1, 2020b). The alternative scenario models an exemplary renewable and low-impact electricity source, off-shore wind power in the Netherlands, as represented in the dataset "Electricity, high voltage {NL}| electricity production, wind, 1-3MW turbine, offshore | Cut-off, U" (ecoinvent database v3.7.1, 2020a).

Electricity consumption occurring in the manufacturing stage is modelled with the average European mix, regardless of the operation scenario.

The composition of the European mix is shown by generation technology in Figure 5.

Figure 5: Electricity scenarios: Composition of average European electricity mix (ENTSO-E) by generation technology.



Water Balance

Input, treatment, disposal and evaporation of water are considered. Where no primary information was available regarding evaporation, the typical assumption was applied that 20% of the water evaporates while 80% is treated in a wastewater treatment plant (or according to the local technological standard).

Consumables

Consumables are material needs that have a much smaller lifetime than the overall system, such as lubricating oil. Here, no assumptions had to be made.

Transport

Specific transports are included where data was provided. Otherwise, standardized transport is included where relevant.

3.3 Considered scenarios

3.3.1 Operation scenarios

In the screening LCA (see deliverable D9.2) it was identified that the operation of the system (use phase) is the major determinant of environmental impacts per kg of hydrogen separated. In particular, the energy consumption (heat and electricity) dominates the results. However, the actual heat and electricity consumption of the system is not constant. It depends on a variety of parameters such as the hydrogen feed concentration and the operating temperature. Given the high relevance and variability of energy consumption for the environmental impacts, we consider multiple operation scenarios in the full LCA. They are defined in
Table 4.
All scenarios represent the operation of the prototype size, i.e. small-scale, system of 12.6 kg H_2 separated per day as specified in
Table 4.

Table 4: Overview of considered operation scenarios. Heat and electricity consumption depends on operating temperature and H2 feed concentration.

Scenario No.	Scenario Name	T [C]	HRF [%]	electricity consumption [kWh/kg H_2]	purity %	Heat consumption [kWh/kg H_2]
1	TUe_Temp_400 (Default)	400	65	4.69	99.85	6.64
2	TUe_Temp_500	500	75	4.82	99.86	5.78
3	TUe_Temp_350	350	60	4.32	99.84	7.21
Scenario No.	**Scenario Name**	**H2 concentration [%]**	**HRF [%]**	**electricity consumption [kWh/kgH2]**	**purity %**	**Heat consumption [kWh/kgH2]**
4	TUe_H2concentr_10%	10	65	4.69	99.85	6.64
5	TUe_H2concentr_15%	15	71	3.00	99.89	4.06
6	TUe_H2concentr_5%	5	57	6.74	99.79	10.64

Scenarios No. 1-6 are theoretical operation scenarios resulting from the modelling performed by TUE in WP 8.They were calculated for the original prototype scale of 25 kg H_2/day. According to discussions with the consortium partners from WP 2-5 and 7 they can be assumed equally applicable to the scale of 12.6 kg H_2/day which we considered for the full LCA. Scenario 1 (TUe_Temp_400 (Default)) with an operating temperature of 400°C and a hydrogen recovery factor of 65% are considered the most likely operation conditions and was therefore defined as default. If not specified otherwise in the following chapters, results refer to the default scenario. Results for the other scenarios were generated as part of the sensitivity analysis.

3.3.2 Parameters in system manufacturing

The contribution of the system manufacturing plays a smaller role compared to system operation. Given that the Technological Readiness Level (TRL) of the HyGrid system is still low at the end of the project, there is a number of parameters regarding the manufacturing/configuration of the system which are not yet definite, and which potentially influence the LCA results.

Table 5 lists the identified parameters related to the system manufacturing and the considered values. The default values are highlighted in bold. If not specified otherwise in the following chapters, results reflect default values.

As part of a sensitivity analysis, we analysed what relevance these parameters have on the environmental performance of the system. The results are described in section 5.4 Detailed results – system manufacturing.

Table 5: Parameters considered for system manufacturing.

Parameters: configuration/manufacturing	Considered values
Lifetime of PdAg Membranes	**2** / 5 / 10 years
Number of Membranes in EHP Module	144 / **288** membranes
Lifetime of MEA[2] components in EHP	3 / **4** / 5 years
Platinum recovery rate at EOL of EHP membranes	**85%**
End-of-life scenario of major material fractions (steel, aluminium , copper, polyethylene)	Average treatment mix / **100% Recycling**

[2] MEA = Membrane Electrodes Assembly. It is a part of the EHP module and includes 3 components: Membranes (modeleld as Nafion membranes) + GDL (Gas diffusion layer) + Platinum catalyst

4 LIFE CYCLE COST DATA

4.1 System configuration

The LCC assesses a commercial size system of 200 kg H_2 recovered per day.

4.2 Data availability

As for the LCA, project-specific primary cost data were collected from the consortium partners as far as possible. For the cost for material and component inputs, for labour, for maintenance, dismantling and required certifications primary data were provided by WP 3-7. Due to their confidentiality, these costs will not be disclosed in this report.

Prices for fuels (natural gas), electricity, green electricity certificates (so called Guarantees of Origin, GoO) and the carbon emission price were taken from statistics and literature.

For other minor cost components such as water, propylene glycol and transport services, prices were taken from the environmental database ecoinvent.

For the reference technology, PSA, no primary cost information could be provided by the consortium partners. Therefore, the overall life cycle cost per kg hydrogen recovered with the HyGrid system will be compared against literature data for the PSA technology.

An overview of the used cost data and their sources is provided in Table 6.

Table 6: Key cost data and data sources used

cost item	cost	unit	source	comment
EHP module	confidential		primary data	projected cost for a 200 kg H_2/day system
Membrane separation system	confidential		primary data	projected cost for a 200 kg H_2/day system
TSA module	confidential		primary data	projected cost for a 200 kg H_2/day system
System BOP	confidential		primary data	projected cost for a 200 kg H_2/day system
electricity price, average grid mix	0.11	€/kWh	(European Commission, 2021a)	5 year average electricity price for non-household consumers in the EU-27 between 2015-2020 (EUROSTAT)
price premium renewable el., GoO in 2020	0.001	€/kWh	(ECOHZ, 2019)	2020 price for GoO mentioned to be around 1€/MWh, expected to rise to 2-2.5€/MWH by 2030

price premium renewable el., GoO in 2030, estimate	0.0025	€/kWh	(ECOHZ, 2019)	2021 price for GoO mentioned to be around 1€/MWh, expected to rise to 2-2.5€/MWH by 2030
natural gas price	0.040	€/kWh	(European Commission, 2021b)	5 year average (2015-2020) natural gas price for non-household consumers in the EU
carbon price in 2020	0.045	€/kg	(Reuters, 2021)	May 2021 EU ETS prices reached 45€/t, expected to rise further to 55 and higher in 2022
carbon price in 2030, estimate	0.1	€/kg	(Reuters, 2021)	May 2021 EU ETS prices reached 45€/t, expected to rise further to 55 and higher in 2022; assumption: 100€/t in 2030
tap water price	0.0004	€/Kg	ecoinvent database, v3.6	
propylene glycol price	1.12	€/kg	ecoinvent database, v3.6	
transport	0.021	€/tkm	ecoinvent database, v3.6	

4.3 Considered scenarios

Operation cost, i.e. primarily electricity, natural gas and carbon cost, play a key role in the life cycle cost of the HyGrid system. Since these are traded commodities with high variability in their price over time and depending on the market location, we considered three scenarios: a default scenario, a lower price estimate and an upper price estimate.

Default scenario

In the default scenario, the current (2020) prices are applied to the energy consumption as defined in the default operation scenario (TUe_Temp_400 (Default)) described in Table 4.

Lower cost scenario

In the scenario estimating the lower boundary of the price range, we apply the current price for renewable electricity (average electricity price plus 2020 price premium), the average natural gas price and the 2020 carbon price to the operation scenario with the lowest heat and electricity demand (TUe_H2concentr_15%).

Upper cost scenario

In the scenario estimating the upper boundary of the price range, we apply the price for average heat and electricity price, the 2030 estimate for the carbon price to the operation scenario with the highest heat and electricity consumption (TUe_H2concentr_5%).

5 LCA RESULTS

This section presents final LCIA results for the PSA reference case and the HyGrid system in its latest configuration. The goal is to identify and understand the hotspots contributing to the overall comparative LCA results.

5.1 Overall LCA Results

The life cycle impacts per kg of hydrogen recovered with the HyGrid prototype and with the PSA reference case are presented in Table 7 and visualized in Figure 6. It can be seen that 1 kg oh H_2 recovered with the HyGrid prototype has lower impacts across all five assessed indicators than 1 kg of H_2 recovered with the PSA reference technology. This is true for the default operation scenario and the other scenarios described in Table 4. The absolute results for the default scenario are shown in Table 7 and visualized by the blue bars in Figure 6. The error bars in Figure 6 show the variability of results between the operation scenario with minimal impacts (MIN) and maximal impacts (MAX). The scenario parameters defining these two scenarios are documented in Table 14 in ANNEX II of this report.

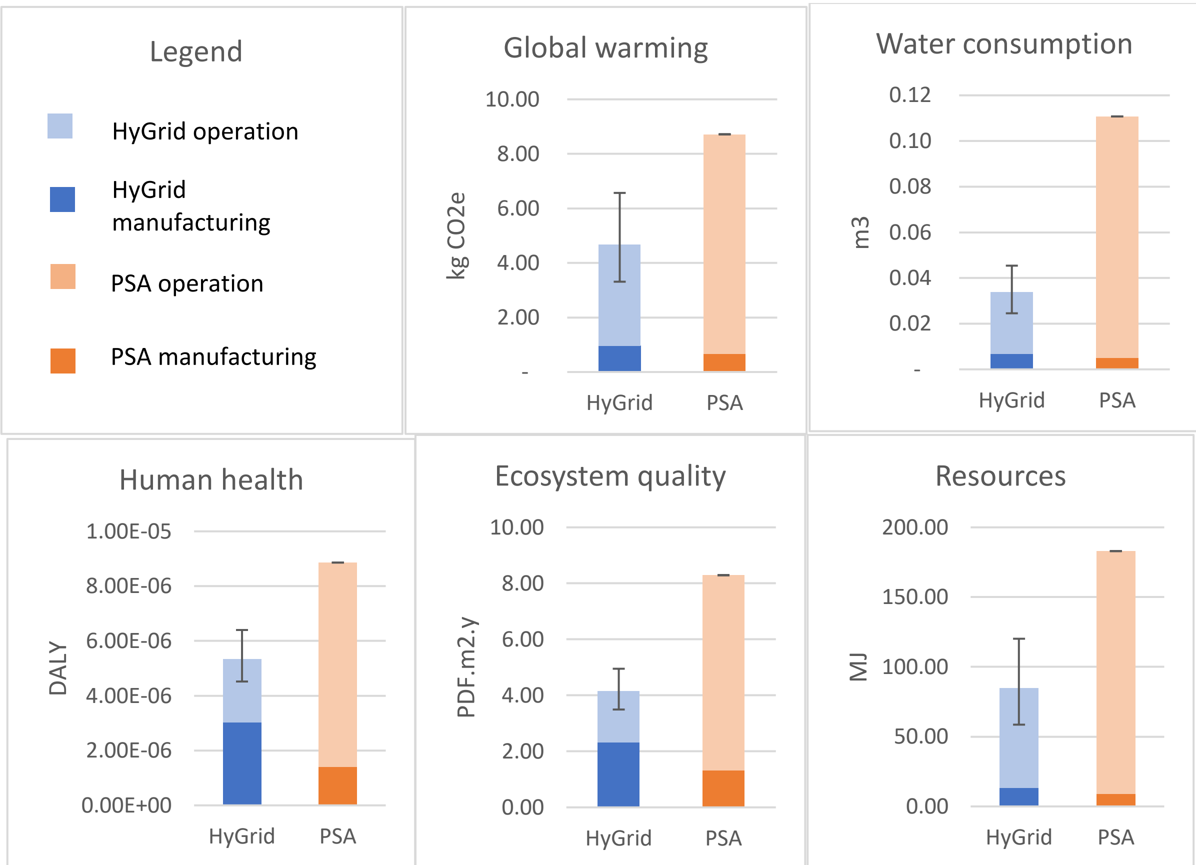
A detailed comparison between HyGrid and the reference technology, considering further scenarios is presented in section 5.5 of this report.

Table 7 and Figure 6 also show how much of the overall impacts per kg H_2 are associated with the manufacturing versus the operation of the systems. Generally, manufacturing impacts are (significantly) lower than operation impacts. This effect can be expected to become more pronounced once the HyGrid technology is scaled up to commercial size, i.e. manufacturing impacts will be distributed over a larger volume of H_2 separated during the system's lifetime. A more detailed contribution analysis breaks down manufacturing and operation further into individual contributors and is presented in the next report section, 5.2.

Table 7: Absolute LCA results HyGrid prototype (default operation scenario and manufacturing parameters) and PSA reference case per kg H_2 recovered

	HyGrid	thereof manufacturing	thereof operation	PSA	thereof manufacturing	thereof operation
Global warming [kg CO2e]	**4.7**	1	3.7	**8.7**	0.7	8
Water consumption [m3]	**0.03**	0.01	0.03	**0.11**	0.01	0.11
Human health [DALY]	**5.3E-06**	3E-06	2.3E-06	**8.9E-06**	1.4E-06	7.5E-06
Ecosystem quality [PDF.m2.y]	**4.1**	2.3	1.8	**8.3**	1.3	7
Resource depletion [MJ]	**84.7**	13.4	71.3	**183**	9.1	173.9

Figure 6: Absolute LCA results HyGrid prototype, (default operation scenario and manufacturing parameters) and PSA reference case per kg H_2 recovered. Error bars represent the range between the Min and Max operation scenario as documented in Table 14 in ANNEX II.



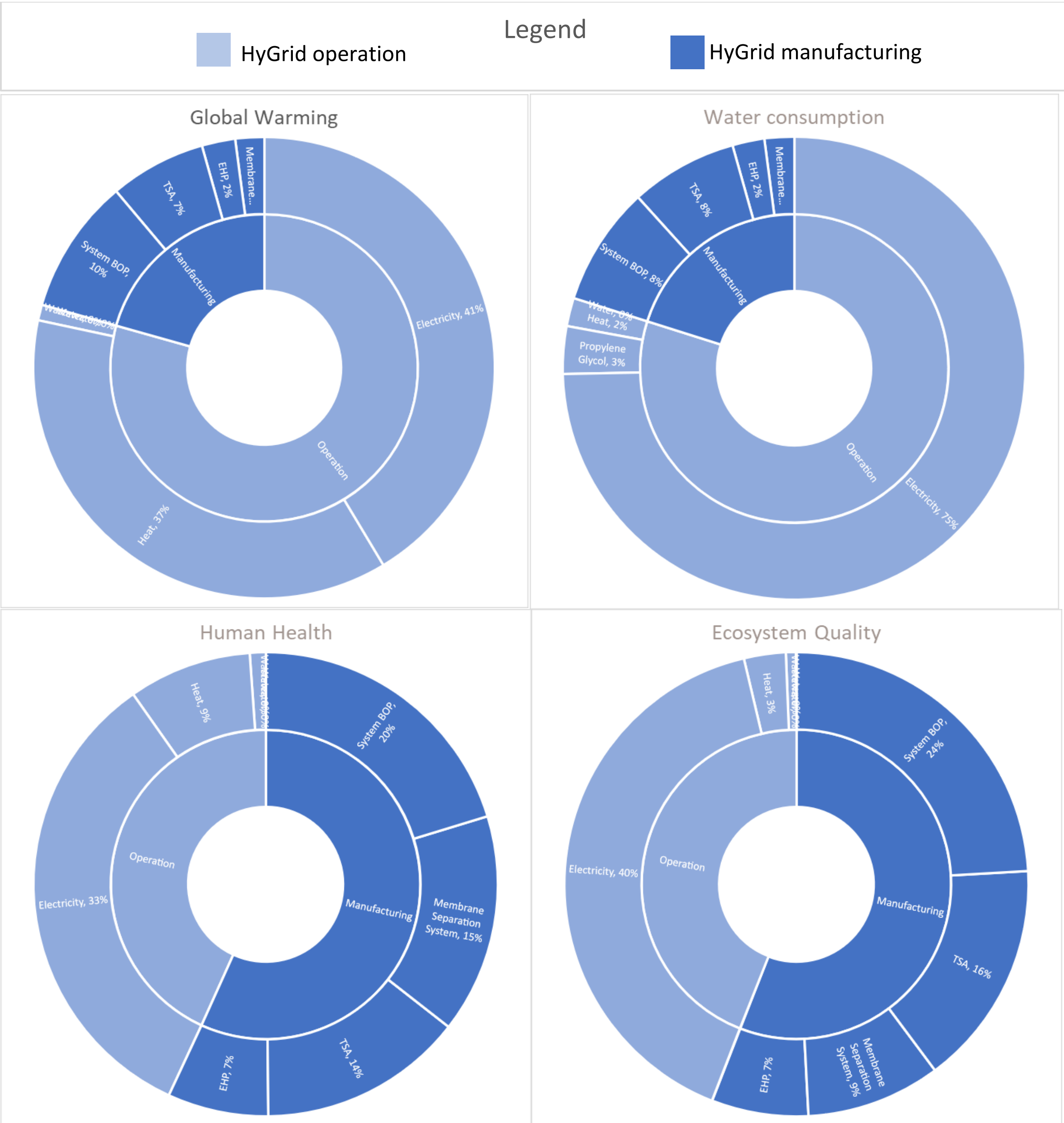
5.2 Identification of environmental hotspots

A breakdown of the overall results into individual contributors allows identifying which elements of the system's manufacturing and operation are the main drivers of environmental impacts, i.e. the hotspots. Figure 7 shows this breakdown for the five considered indicators.

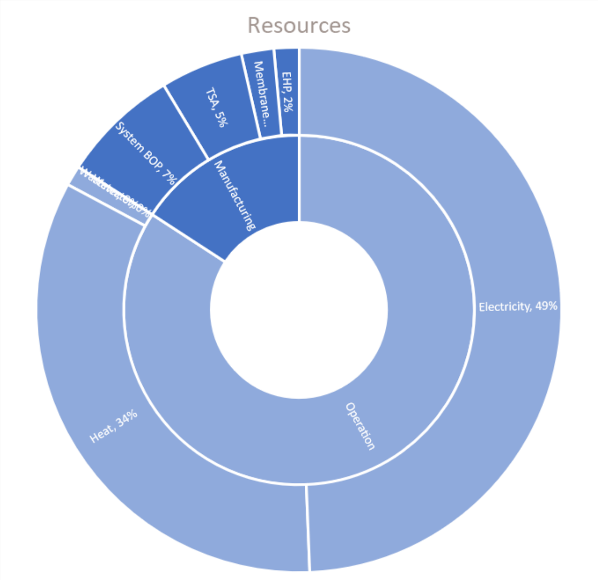
The relative contribution shows different proportions for different indicators: The indicators water consumption and resources follow the pattern of the indicator global warming potential, i.e. impacts are dominated by operation, with the main hotspots being electricity and heat consumption. The indicators human health and ecosystem quality, however, do not follow this pattern. The results of these two indicators are dominated by the manufacturing impacts, in particular the manufacturing of the EHP module and the system balance of plant drive these impacts. The reason is that human health and ecosystem quality impacts associated with the provision of raw materials such as steel are higher than those of energy generation, i.e. system operation. However, the manufacturing impacts will become proportionately less relevant once the prototype system is scaled up to commercial size. Therefore, it can be expected that human health and ecosystem quality impacts of a large-scale system will also be dominated by the system's operation.

Thus, we identify the main environmental hotspots of the HyGrid technology to be the operation phase, in particular energy (heat and electricity) consumption.

Figure 7: Contribution analysis HyGrid prototype (default operation scenario and manufacturing parameters)



Legend
HyGrid operation
HyGrid manufacturing
Global Warming
Operation
Manufacturing
Electricity, 41%
Heat, 37%
System BOP, 10%
TSA, 7%
EHP, 2%
Membrane...
Water consumption
Operation
Manufacturing
Electricity, 75%
Propylene Glycol, 3%
Heat, 2%
System BOP, 8%
TSA, 8%
EHP, 2%
Membrane...
Human Health
Operation
Manufacturing
Electricity, 33%
Heat, 9%
System BOP, 20%
Membrane Separation System, 15%
TSA, 14%
EHP, 7%
Ecosystem Quality
Operation
Manufacturing
Electricity, 40%
Heat, 3%
System BOP, 24%
TSA, 16%
Membrane Separation System, 9%
EHP, 7%

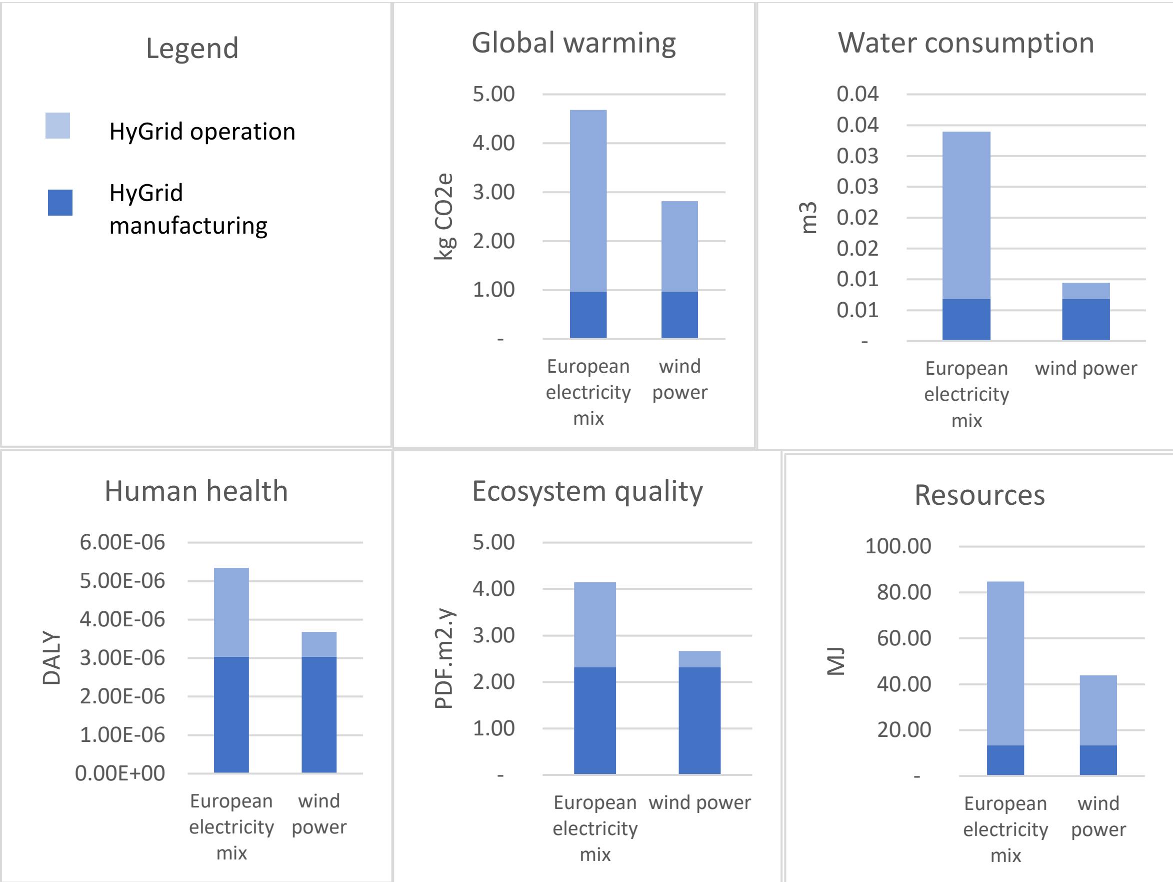


5.3 Detailed LCA results - system operation

As identified in the previous section of this report, the main drivers of operation impacts are the electricity and heat consumption of the HyGrid system. In the prototype configuration, the heat demand is associated with the heating of the PdAg membranes to their required operating temperature. It is met by the combustion of natural gas from the feed stream. The remaining energy demand is met with electricity from the grid. In the default operation scenario, the average European electricity mix is applied. The composition of this mix by primary energy source is described in section 3.2.

Given the high relevance of electricity for the overall LCA results per kg H_2 recovered, we also analysed a scenario using a low-impact electricity source, namely wind power. Under this scenario, the impacts associated with electricity consumption are minimized. The remaining operation impacts are dominated by the heat demand supplied from natural gas. Figure 8 shows how the absolute results for each indicator compare between the two electricity source scenarios. The use of wind power significantly reduces the overall environmental impacts per kg H_2 separated.

Figure 8: LCA results for the HyGrid prototype (default operation scenario and default manufacturing parameters) per kg H2 recovered depending on the electricity mix – average European mix vs. wind power



5.4 Detailed LCA results - system manufacturing

5.4.1 Absolute Results

Table 8 shows the absolute results of the impact assessment for the four system components as well as for the sum of the entire system. Default values were considered for the manufacturing parameters described in section 3.3.2. The variability of these results depending on the parameters is described in the following sections on the individual components, membrane separation system, EHP, TSA and system Balance of Plant (BOP) (sections 5.4.2.2 - 5.4.2.5).

Table 8: Absolute LCIA results for the manufacturing of the system components (default parameters).

	Membrane Separation System	EHP	TSA	System BOP	**TOTAL Hygrid system**

	piece	piece	piece	piece	**piece**
Global warming [kg CO2e]	6.2E+03	7.2E+03	2.1E+04	2.9E+04	**6.3E+04**
Water consumption [m3]	4.6E+01	5.0E+01	1.7E+02	1.9E+02	**4.5E+02**
Human health [DALY]	5.0E-02	2.0E-02	5.0E-02	7.0E-02	**2.0E-01**
Ecosystem quality [PDF.m2.y]	2.5E+04	1.8E+04	4.3E+04	6.5E+04	**1.5E+05**
Resource depletion [MJ]	1.1E+05	8.6E+04	2.8E+05	4.0E+05	**8.8E+05**

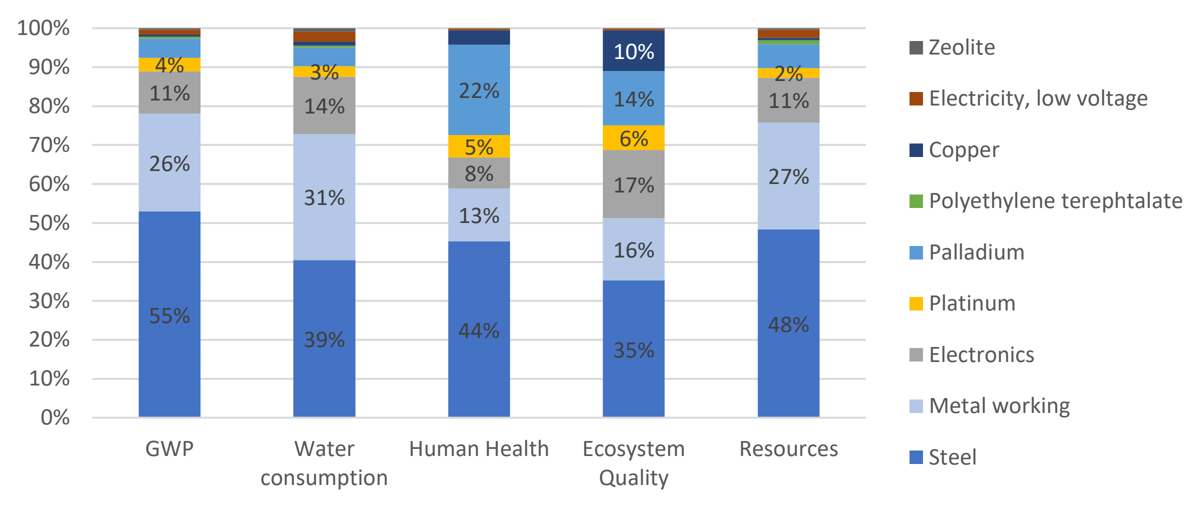
For all indicators the system BOP contributes the most to the overall manufacturing impacts (35-46%), followed by the TSA (25-37%), the membrane separation system (10-25%) and the EHP (10-12%).

5.4.2 Contribution Analysis

5.4.2.1 By Material

Figure 9 shows which raw materials contribute the most to the impacts of the HyGrid infrastructure. Steel together with “metal working” are the major contributors across all indicators. “Metal working” represents the processes needed to get the steel and other relevant metal components (e.g. copper) into their required shape. This includes for example welding, (laser) cutting, machining and hot rolling. Also of significant relevance for all impact categories are the electronic components such as control units. For the indicators of human health and ecosystem quality palladium, platinum and copper are of relevance as well. Palladium is used in the silver-palladium (PdAg) membranes of the membrane separation system. Platinum is used in the EHP system. Copper is mostly used in the EHP, TSA and the System BOP.

Figure 9: Contribution analysis of system manufacturing by type of raw material.



5.4.2.2 Membrane Separation System

Contribution Analysis

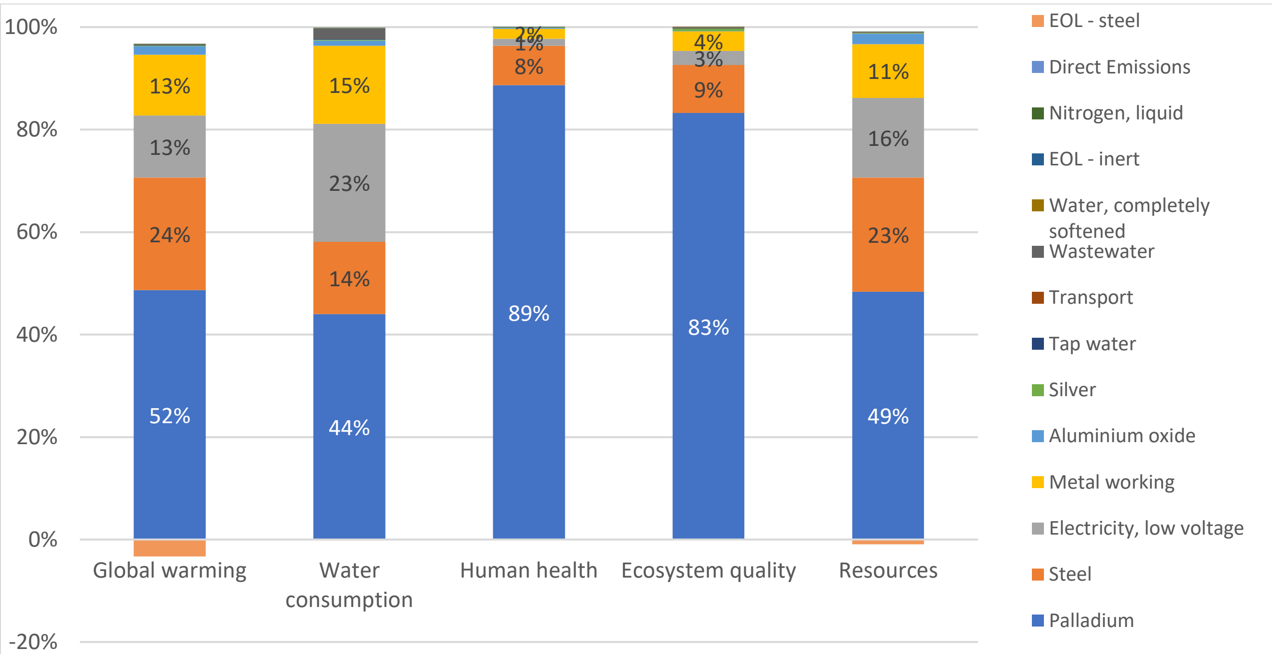
Figure 10 shows which materials contribute by how much to the manufacturing impacts of the membrane separation system. It can be seen that the largest contributor, i.e. the major hotspot, across all indicators is the palladium used in the PdAg membranes. The amount of palladium required per m^2 of membrane is small, however the specific impacts for the extraction and refining of 1kg of palladium are large. The specific impacts per kilogram differ largely between different countries (and with that processes) of palladium extraction and refining. For example, the global warming potential for palladium from South Africa is around 24,000 kg CO_2e / kg palladium (ecoinvent database v3.7.1, 2020c) while that from Russia is around 3,800 kg CO_2e / kg palladium (ecoinvent database v3.7.1, 2020d).

Human health and ecosystem quality impacts are particularly dominated by palladium.

It shall be noted that at the project end Tecnalia is already developing a way to recycle the palladium at the end of the membrane's lifetime. However, these developments were not yet mature enough to provide data that could be modelled in the LCA. For this reason, the recycling of palladium is not considered in the LCA. The impacts associated with the palladium in the prototype are therefore likely overestimated once the recycling solution is in place and the system is scaled up.

Other hotspots in the membrane separation system, namely steel and metal working, are consistent with the hotspots for the overall HyGrid system (see section 5.4.2.1). Moreover, a significant amount of electricity required for the baking of the PdAg membranes shows of relevance for the global warming potential, for water consumption and for resource depletion.

Figure 10: Membrane separation system - contribution analysis of manufacturing impacts (default lifetime of PdAg membranes of 2 years)



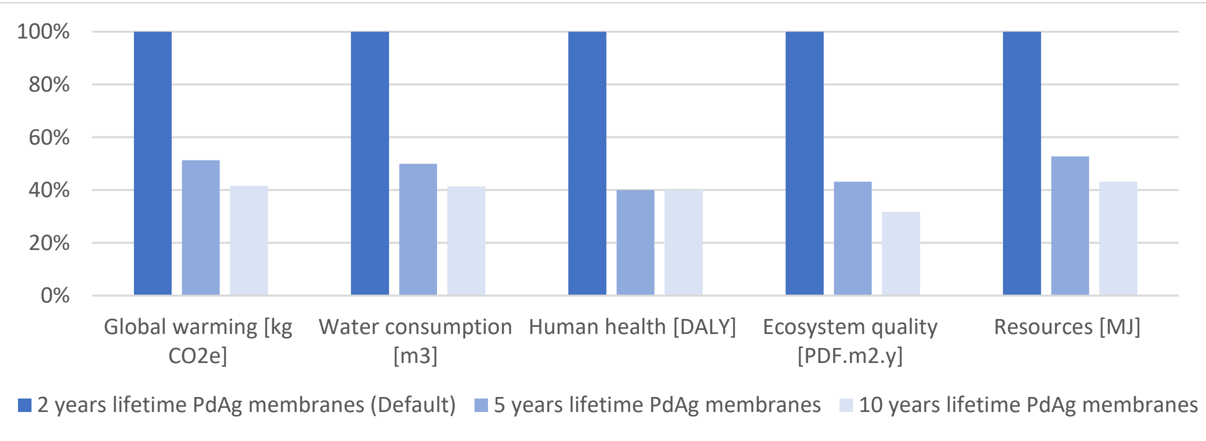
Sensitivity analysis

The membrane separation system consists of the membranes and the membrane module. The membrane module fulfils the function of encasing the membranes themselves. The membranes themselves are palladium-silver membranes in the HyGrid prototype, they are supported by components made of aluminium oxide and steel.

The variable parameter in the manufacturing of the membrane separation system with relevant influence on the environmental performance is the lifetime of the PdAg membranes. It is shorter than the lifetime of the entire membrane separation system and the entire HyGrid system (both 15 years). The longer the lifetime of the membranes is, the less often they need to be exchanged and hence the less palladium is needed, which is the major impact driver.

The actual lifetime of the membranes is yet uncertain, by default 2 years were considered (see absolute results in section 5.4.1). As part of the sensitivity analysis, 5 years and 10 years were analysed. Figure 11 shows that the impacts of the membrane separation system could be reduced by more than half with a membrane lifetime of 5 or even 10 years.

Figure 11: Membrane Separation System - Sensitivity analysis on the lifetime of the PdAg membranes (2, 5 and 10 years).



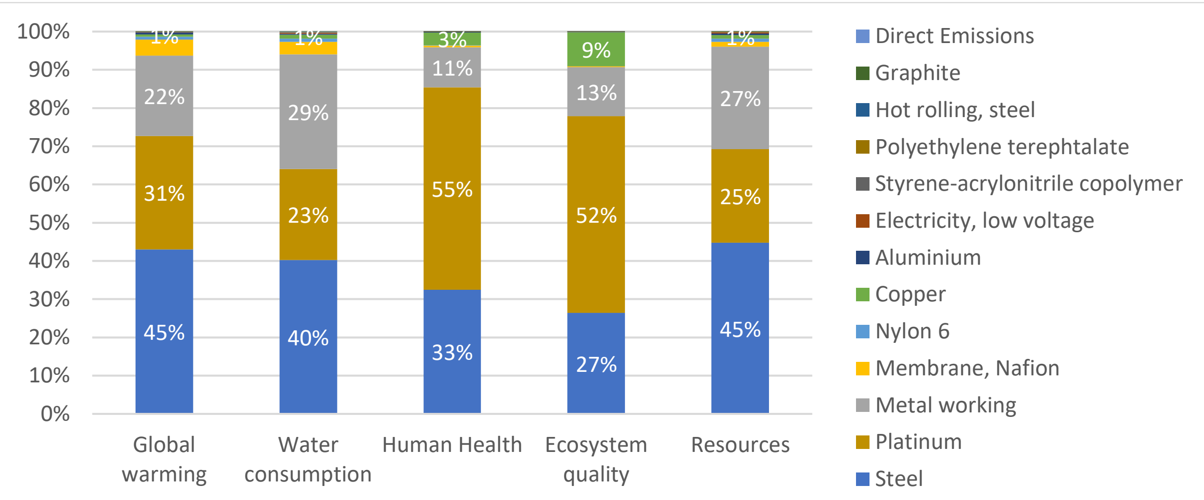
5.4.2.3 EHP Module

<u>Contribution Analysis</u>

Figure 12 shows which materials contribute by how much to the manufacturing impacts of the EHP module. It can be seen that the largest contributor, i.e. the major hotspot, is steel and its associated metal working processes. Moreover, the platinum used as a catalyst is a significant contributor, even dominating impacts for the indicators of human health and ecosystem quality. The amount of platinum required per MEA component is small, however the specific impacts for the extraction and refining of 1 kg of platinum are large. The specific impacts per kg differ largely between different countries (and with that processes) of platinum extraction and refining. For example, the global warming potential for platinum from South Africa is around 88,000 kg CO_2e / kg platinum (ecoinvent database v3.7.1, 2020c) while that from Russia is around 14,000 kg CO_2e / kg platinum (ecoinvent database v3.7.1, 2020d).

Human health and ecosystem quality impacts are particularly dominated by platinum.

Figure 12: EHP – contribution analysis of manufacturing impacts (default lifetime of MEA components of 4 years, 288 MEAs, 85% platinum recovery rate)

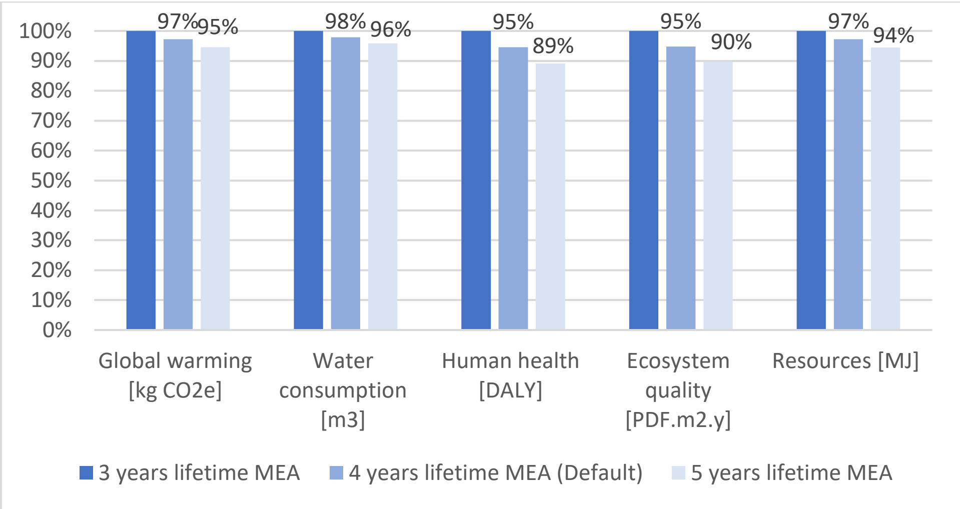


Sensitivity analysis

The electrochemical hydrogen separation (EHP) module consists of the EHP stack, tubing, instrumentation and equipment. The EHP module overall has a lifetime of 15 years, equal to that of the entire HyGrid system.

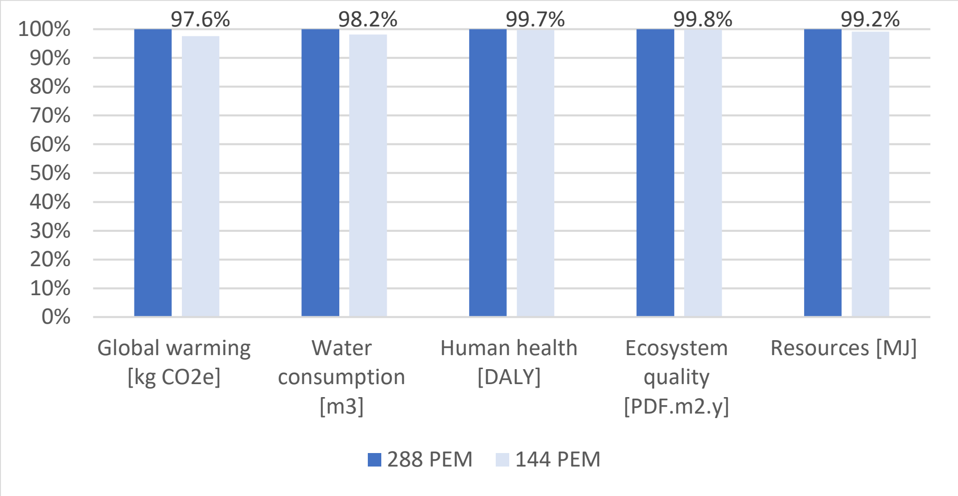
Part of the EHP stack is the Membrane Electrode Assembly (MEA). An MEA consists of three components, namely a proton exchange membrane (PEM), a gas diffusion layer (GDL), and a platinum catalyst. The MEA components have a shorter lifetime than the overall EHP module. The actual lifetime will be known once a system has been in operation long enough for empirical experience and hence remains uncertain at project closure. The expected lifetime ranges between 3 years and 5 years. Therefore, a lifetime of MEA components of 3, 4 (default) and 5 years was considered in the sensitivity analysis. Figure 13 shows that a higher lifetime of the MEA components from 3 years to 4 or 5 years leads to an impact reduction by a few percentage points. A 5 years lifetime reduces impacts compared to a 3 years lifetime by 6% (global warming, water consumption and resource depletion) to 11% (human health).

Figure 13: EHP - sensitivity analysis on the lifetime of the MEA components (3, 4 and 5 years)



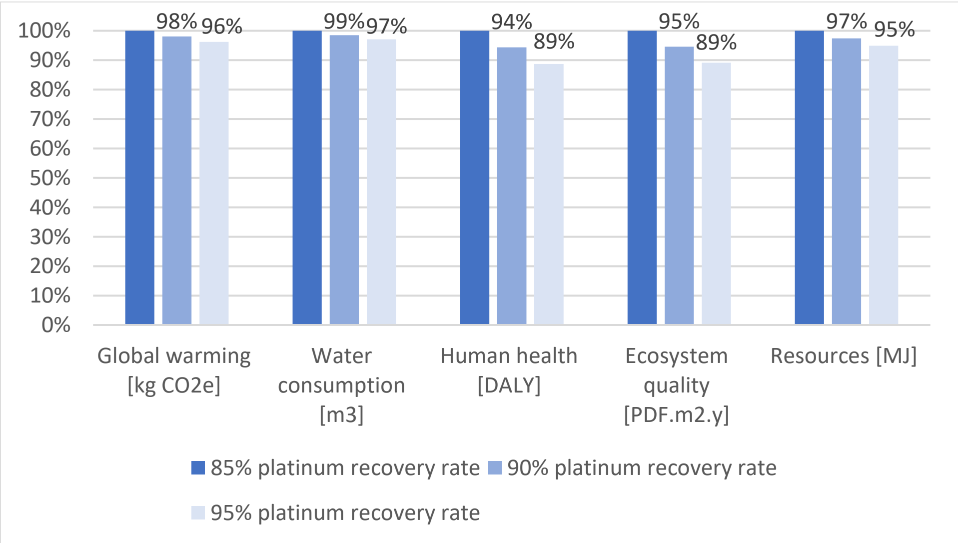
A second variable considered in the sensitivity analysis is the number and of proton exchange membranes in the EHP module, which was considered to be either 144 membranes at a reduced thickness or 288 membranes at a standard thickness (default). Figure 14 shows that the impact reduction associated with reducing the number of membranes to half and reducing their thickness is minor, i.e. less than 3% across indicators.

Figure 14: EHP – sensitivity analysis on the number of proton exchange membranes (144 membranes 30 µm thick, 288 membranes 50 µm thick)



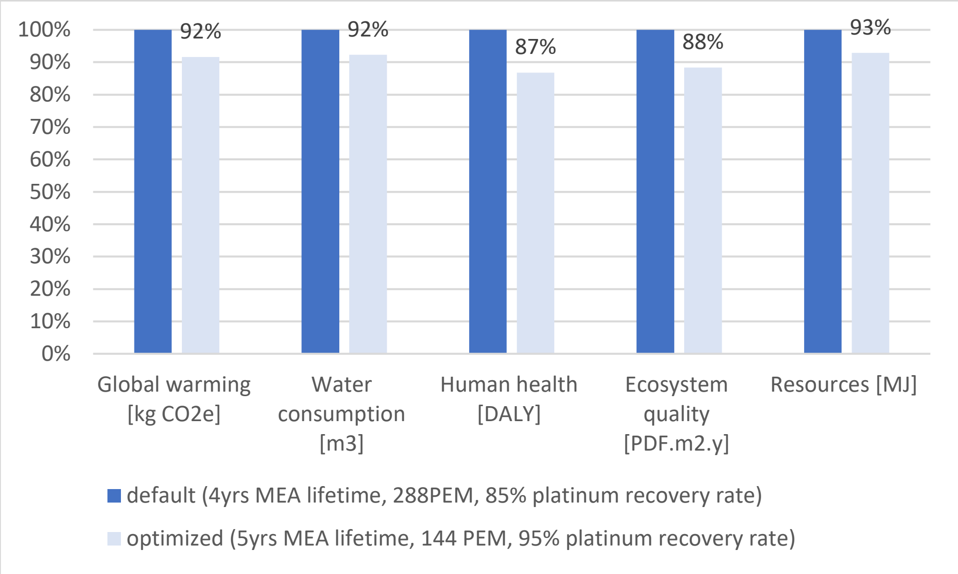
The third variable considered in the EHP sensitivity analysis is the recovery rate of the platinum which serves as a catalyst in the MEA component. It is expected to range between 85% and 95%. Figure 15 shows that the considered increase of recovery rate leads to an impact reduction by a few percentage points. A 95% recovery rate reduces impacts between 4% (global warming, water consumption) and 11% (human health) compared to an 85% recovery rate.

Figure 15: EHP - sensitivity analysis on the recovery rate of platinum in the platinum catalyst.



Optimizing for all three of the above variables results in an impact reduction of the EHP module of 8% (global warming, water consumption) to 13% (human health) as shown in Figure 16.

Figure 16: EHP - sensitivity analysis on system design optimized by the 3 parameters identified for sensitivity analysis (MEA lifetime, number of proton exchange membranes, platinum recovery rate)



5.4.2.4 TSA Module

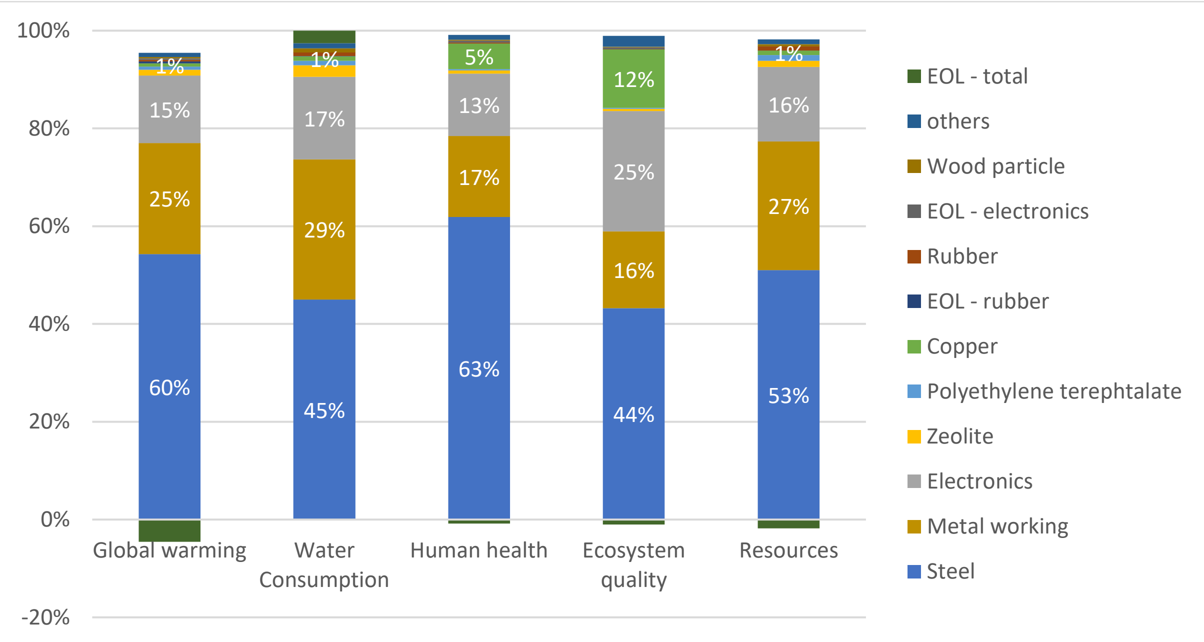
Contribution analysis

The TSA module is encased in a 10 ft container and has a total weight of more than 2.5 tonnes. In terms of its material composition, the largest part (more than three quarters) of this overall mass is steel. The remaining fractions are much smaller amounts of copper, wood (for pallets), electronics, polyethylene, rubber, zeolite and other minor fractions. Unlike the membrane separation system or the EHP module the TSA module does not require raw materials of particularly high specific (per kg) environmental burdens, as is the case for palladium and platinum in the membrane separation system and EHP, respectively.

The expected lifetime of the TSA module is with 15 years equal to the lifetime of the entire HyGrid system. No relevant replacements are expected prior to that.

Figure 17 shows which materials contribute by how much to the manufacturing impacts of the TSA module. It can be seen that the largest contributor, i.e. the major hotspot, is steel and it is associated metal working processes. Also, electronic components play a relevant role for all indicators. Copper contributes significantly to ecosystem quality and human health scores with 16% and 17% respectively.

Figure 17: TSA – contribution analysis of manufacturing impacts (incl. EOL recycling)

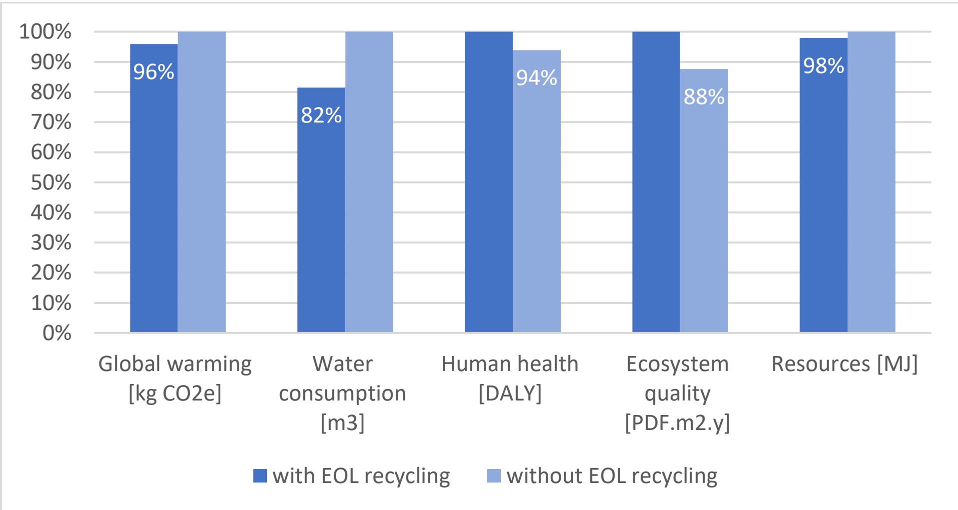


Sensitivity analysis

As shown in the contribution analysis, the major determinant of the TSA's environmental impact is associated with the material steel. In the inventory data collection with WP5, stainless steel (18/8) was chosen to be the most appropriate modelling choice for all steel components. We apply the circular footprint formula (CFF) as developed by the European Union within the PEF method (Zampori & Pant, 2019) in the modelling of steel inputs and end-of-life steel treatment. Two scenarios were considered. In the first scenario, the steel (as well as the copper and PET fractions) is fully dismantled and 100% recycled at the module's end-of-life. In the second scenario 0% of these materials are recycled. It shall be noted that applying the CFF modelling approach means that the user of recycled material is responsible for a part of the primary material production. In particular, in the case of steel this means that the credits for recycling are limited, because the demand of the recycled material is high and primary material production can thus not be avoided completely.

As a result, the difference between the recycling and the non-recycling scenario is not large. Figure 18 shows that end-of-life recycling reduces the global warming potential by 4%, water consumption by 18% and fossil resource consumption by 2%. For human health and ecosystem quality the impacts of the recycling scenario exceed that of the scenario without recycling. Hence the impact reduction potential of EOL recycling is limited.

Figure 18: TSA - sensitivity analysis on the EOL scenario of steel, copper and PET (recycling vs. no recycling)



5.4.2.5 System Balance of Plant

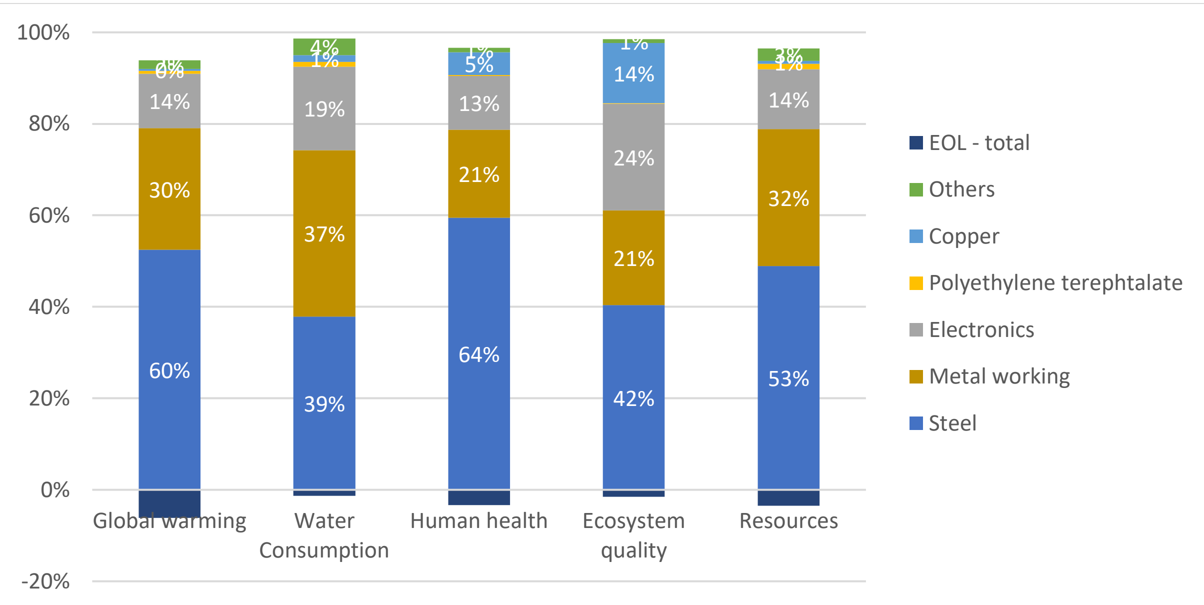
Contribution analysis

The system balance of plant represents the part of the HyGrid system which allows for the integration of all other components (EHP, TSA and membrane separation module) into one functional system. It is encased in a 20 ft steel container of more than 3.5 tonnes. In terms of its material composition, the largest part (more than 85%) of this overall mass is steel. The remaining fractions are much smaller amounts of copper, wood (for pallets), electronics, polyethylene, rubber, and other minor fractions.

Figure 19 shows which materials contribute by how much to the manufacturing impacts of the system balance of plant. It can be seen that the largest contributor, i.e. the major hotspot, is steel and its associated metal working processes. Also, electronic components play a relevant role for all indicators. Copper contributes significantly to ecosystem quality and human health scores with 14% and 5% respectively.

Results for the System BOP are hence directly proportional to use of the mentioned materials. This means that optimizing the system design for a reduced use of these materials as well as material recycling at the end-of-life will lead to reduced impacts and reduced contribution to the overall results per kg H_2 separated.

Figure 19: System BOP – contribution analysis of manufacturing impacts (incl. EOL recycling)



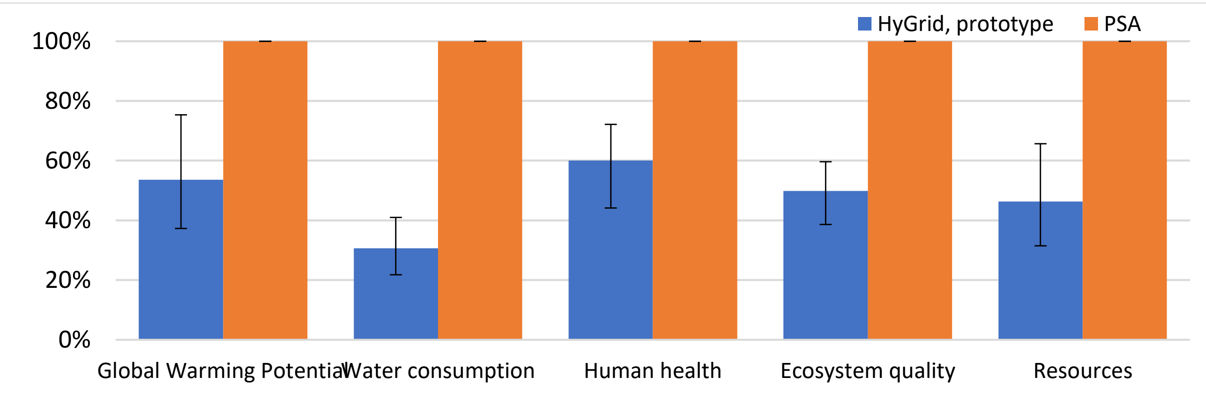
5.5 Comparison HyGrid and PSA

When comparing the environmental impacts of 1 kg H_2 separated with the HyGrid technology to 1 kg H_2 separated with the reference technology PSA it depends on the operation scenario, in particular on the consumed electricity mix, which technology performs better than the other.

When the average European electricity grid mix is used for the operation of both technologies, HyGrid performs better than the PSA reference case for all environmental indicators. This is shown in Figure 20. The blue bar represents the impacts of the HyGrid prototype with its default configuration. The error bars indicate the variability of results which depend most prominently on the operation scenario (i.e. the amount of electricity & heat consumption in turn depending on T [°C] and H_2%) and to a lesser extent on the lifetime of components and other manufacturing parameters previously described.

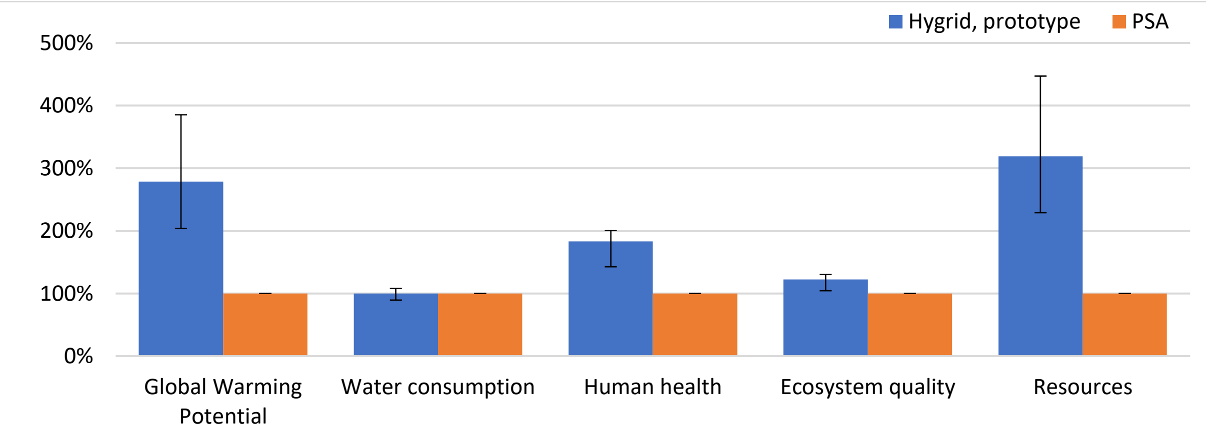
When operated with the average European electricity mix, even the most impactful scenarios for the HyGrid prototype perform better than the PSA reference case.

Figure 20: Comparison HyGrid vs. PSA per kgH$_2$ recovered – average European electricity mix



When assuming electricity consumption for both technologies to be met from a low-impact energy source such as wind power, HyGrid no longer performs better than the PSA. Figure 21 shows the results for the HyGrid default scenario (blue bars) and their variability (error bars) normalized against the PSA results, both running on wind power. The reason for HyGrid's relatively higher impacts here, is the heat demand for heating the PdAg membranes to the operation temperature (of 350°C – 500°C) which is met with natural gas directly taken from the separated gas stream. Natural gas, as fossil heat source, is associated with much higher environmental impacts than wind power. The energy demand of the PSA reference case is fully met with wind power.

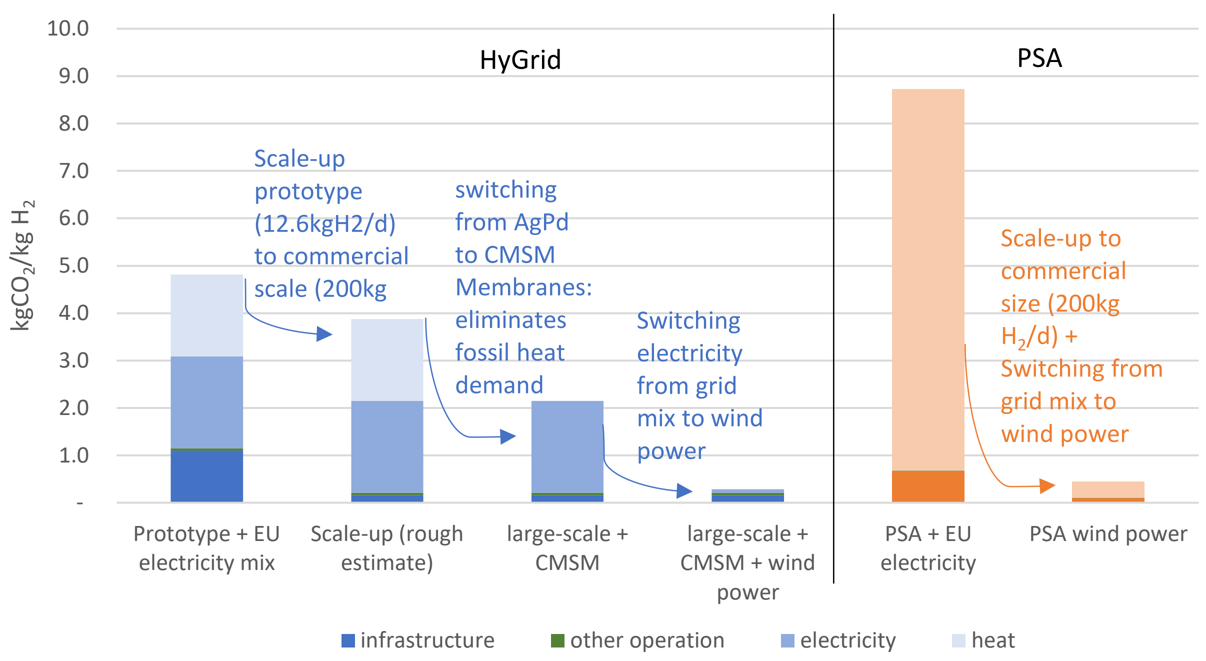
Figure 21: Comparison HyGrid vs. PSA per kgH_2 recovered - electricity from wind power



As can be seen, the environmental performance of the HyGrid system varies greatly depending on a multitude of parameters and scenarios. Under most, however not under all scenarios HyGrid performs better than that the PSA reference case. The impact intensity (per kg H_2) of the current small-scale prototype is high.

This leads to the question of how the HyGrid system can be optimized further to assure minimal environmental impacts and better performance than the PSA system under all conditions Figure 22 outlines the pathway identified for a low carbon (global warming potential) system development. No major trade-offs between carbon and other environmental indicators are expected. Hence, we consider this pathway leading to an overall low-impact system design.

Figure 22: Low-carbon system design pathway



In the first optimization step in Figure 22, the HyGrid infrastructure is scaled-up from the current prototype to a commercial size system (200 kg H_2/day). Since no inventory data were available on the actual commercial size system the following equation (Gerber et al., 2011) is used for adjusting the scale difference for both the HyGrid and the PSA system.

Equation 1 for adjusting scale difference

$$\frac{LCA_2}{LCA_1} = \left(\frac{A_1}{A_2}\right)^b$$

Whereby:

LCA1: *environmental impact of component 1 (known)*

LCA2: *environmental impact of component 2 (unknown)*

A1: *the scale of component 1*

A2: *scale of component 2*

b: *scaling factor, "cost capacity factor". The generic scaling factor of 0.7 is assumed.*

The scale-up reduces manufacturing impacts per kg H_2 produced, leading to a reduction potential of roughly 20%.

HyGrid's heat demand is associated with the use of the PdAg membranes in the membrane separation module, which requires an operation temperature of around 400 °C. A different type of membrane, the carbon molecular sieve membrane (CMSM), operates at ambient temperature. Replacing the PdAg membranes with CMSM would thus eliminate the heat demand and with that the impacts associated to the combustion of natural gas, which corresponds to a reduction potential of about 45% in a second optimization step in Figure 22. It hast to be noted tough, that this reduction potential does not account for changing impacts in the membrane manufacturing.
Detailed data for the manufacturing of the CMSM alternative were not yet available. According to first estimates by WP3, the required membrane area is likely to be larger in the case of CMSM membranes than in the case of PdAg membranes. A first rough assessment of the manufacturing impacts of the CMSM membranes shows that impacts per m^2 of CMSM membrane exceed those of PdAg membranes for some environmental indicators (global warming potential, resources and water consumption). The single largest contributor to CMSM membranes is the electricity consumption during manufacturing. This could further be reduced and/or met with lower-impact sources in the future to avoid potential trade-offs when replacing PdAg membranes with CMSM. Nonetheless, potential trade-offs shall be analysed in more detail once more precise CMSM manufacturing data are available.

In the third step displayed in Figure 22 the electricity source is switched from the average European grid mix to wind power. This step reduces emissions from the remaining energy consumption significantly, with an estimated reduction potential of about 87%.

All optimization steps combined results in a minimal carbon footprint of the HyGrid technology (less than 0.3 kg CO_2/kg H_2, which corresponds to an overall reduction potential of over 90% based on the current prototype operated under default conditions (4.7 kg CO_2/kg H_2). The estimated carbon emissions of the optimized HyGrid system are lower than the estimated emissions of a large-scale PSA system running on wind power (more than 0.4 kg CO_2/kg H_2). Given the uncertainty of those estimates, it can be said that carbon emissions of both systems are in a similar range, however only under the condition that both systems are based on renewable energy sources. Given the fact that renewable energy provision is not unlimited, the HyGrid system would still be preferable. A detailed assessment could be conducted once actual data for commercial size systems are available.

5.6 Sensitivity LCIA method

To validate the robustness of the presented results we applied a second LCIA method, EF method version 3.0. It can be seen that the conclusions we can draw from the results based on the IMPACT 2002+ method also hold when we apply the EF method. This is firstly that the HyGrid system performs better than the PSA system across the observed indicators (default scenario, operated with average European grid mix) as seen in Figure 23. The only exception is the EF indicator “human toxicity, cancer”. However, given the high uncertainty underlying this indicator, we evaluate the difference between PSA and HyGrid of about 10% not to be significant.

Secondly, Figure 24 shows that the impacts of the HyGrid system are dominated by its operation phase, in particular for the indicators related to climate change, water use and fossil resource use. For human health and ecosystem related indicators (e.g. human toxicity, particulate matter, ecotoxicity) system manufacturing makes up a relevant contribution similarly to the results with the method IMPACT 2002+.

Figure 23: Sensitivity analysis of comparison HyGrid vs. PSA with EF 3.0 LCIA method

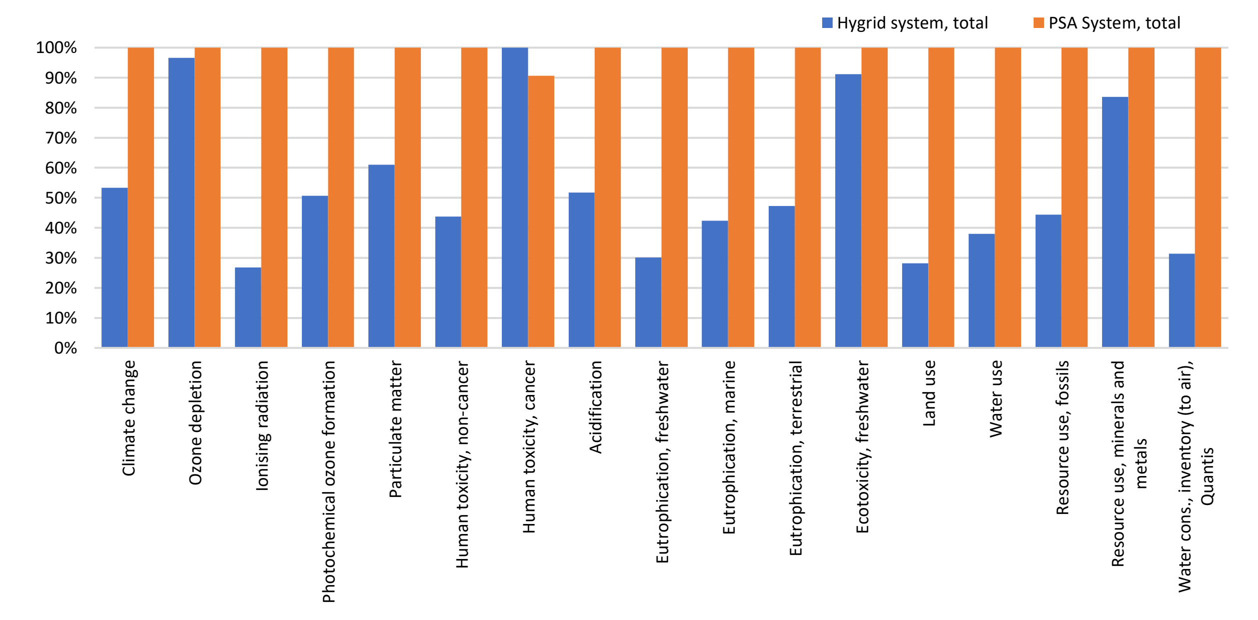
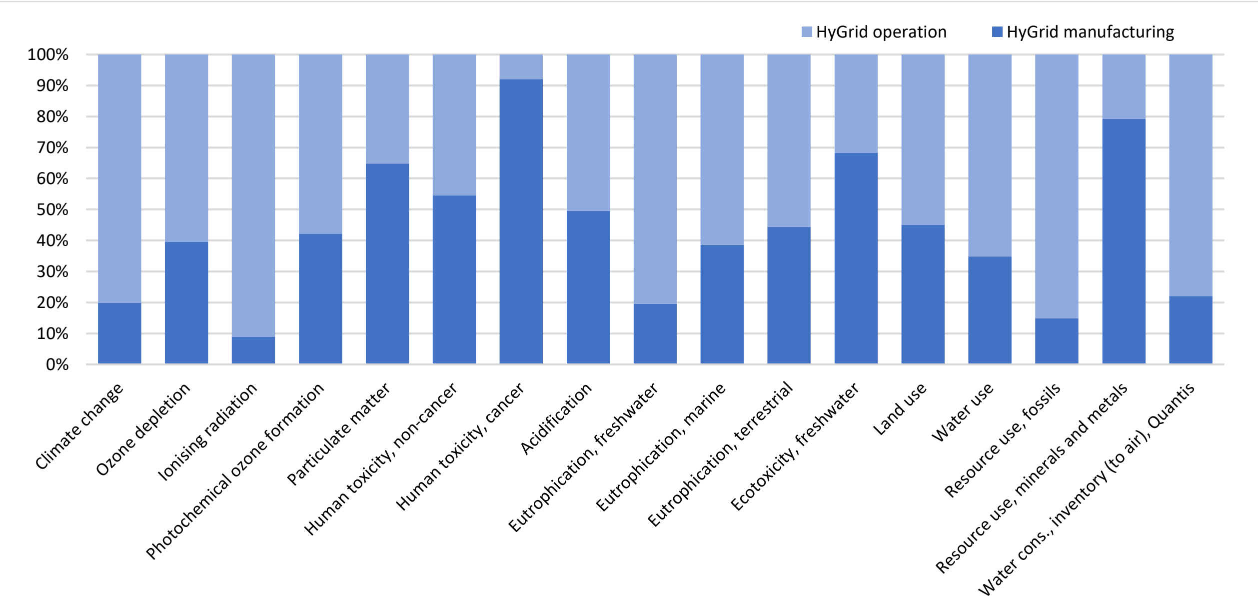


Figure 24: Sensitivity analysis of HyGrid contribution of operation vs. manufacturing with EF 3.0 LCIA method



6 LCC RESULTS

6.1 Overall LCC results

As described in section 4.3, three scenarios were considered for the life cycle costing analysis to reflect the high variability in energy and carbon prices. This also allows to determine the expected range of life cycle costs and is more robust than relying on a single scenario. All scenarios represent the hydrogen separation cost for a commercial-size system of 200 kg hydrogen recovered per day.

Table 9 shows the cost range between the lower estimate of 1.2 €/kg H_2 and the higher cost estimate of 2.4 €/kg H_2. The separation cost for the default operation scenario, using the average electricity mix and the average energy price lies between the lower and the upper limit, at 1.6 €/kg H_2. Hence it is feasible to meet the initially defined target for hydrogen separation cost of 1.5 €/kg H_2 (Table 1). The following section outlines in more detail the cost drivers and thus optimization potential.

Table 9: Overview HyGrid life cycle cost results

	Lower cost scenario		Default scenario		Upper cost scenario	
	€/kg H_2 recovered	%	€/kg H_2 recovered	%	€/kg H_2 recovered	%
CAPEX	0.6	48%	0.6	36%	0.6	23%
OPEX	0.6	52%	1.0	64%	1.9	77%
Total cost of delivery	1.2		1.6		2.4	

6.2 Identification of cost hotspots

The absolute capital cost (CAPEX) of 0.6 €/kg H_2 recovered is equal across the three cost scenarios. Depending on the operation scenario, capital cost's contribution is up to half of the total life cycle costs. Hence it is relevant to break the capital cost down further and identify the cost hotspots.

As shown in Figure 25, within the CAPEX, costs are almost evenly distributed over three system components: 32% of CAPEX are associated with the membrane separation system, 31% with the EHP module, 24% with the balance of plant, while the contribution of the TSA module is proportionally lower with 13%. Zooming in one level further, it can be seen that the major cost factor for the manufacturing of all four components and hence of the HyGrid system as a whole are the cost for the material inputs. Labour for development, engineering, construction and maintenance as well as other smaller cost factors such as certifications and transport are less relevant. Material costs make up 81% of the CAPEX.

Operation costs dominate the overall cost of hydrogen delivery, especially in the default and higher cost scenario. Three cost hotspots can be identified in the OPEX: the cost for electricity, the cost for heat (i.e. natural gas) and the cost for the externality of carbon emissions which result from system manufacturing and operation. All three of these commodities are exchange-traded and highly variable in their price, both time-wise and location-wise. To make our analysis more robust against this variability, we consider i) a five-year average (2015-2020) of the electricity and natural gas price and ii) an expected future price increase for the carbon price and decreases for renewable electricity price premiums. Future developments of electricity and gas price are more controversial and are not considered here.

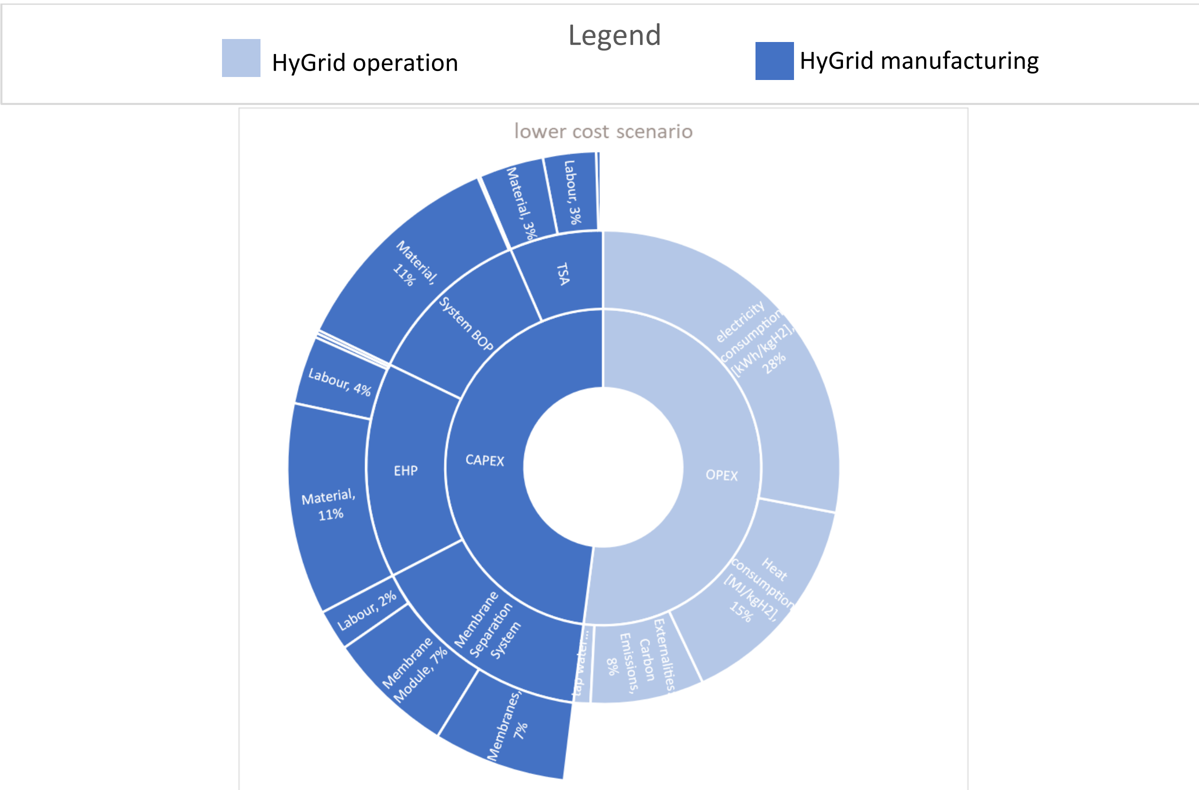
The relative contribution of the three operation cost hotspots depends on two factors. Firstly, the amount of electricity and heat vary with the operation scenarios. As a result, also carbon emissions from energy generation vary accordingly. Secondly, the considered market prices vary. The low-cost scenario uses renewable electricity, i.e. comes with an additional cost for the purchase of Guarantees of Origin (GoO), which reduces the amount of carbon emission certificates to be purchased. Under this scenario, electricity cost constitutes 54%, heat 29% and carbon cost 15% of OPEX. The rest is other small cost components, e.g. consumables and water.

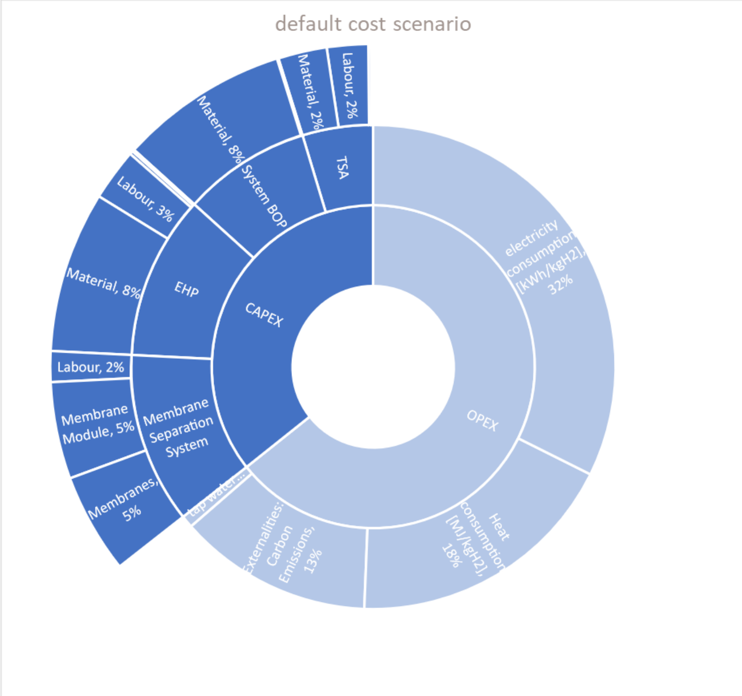
The default cost scenario operates at the most likely conditions (hydrogen concentration, operation temperature) for the HyGrid system, i.e most likely energy consumption. The average European electricity grid mix and its associated carbon emissions are assumed. This results in 50% of the OPEX stemming from electricity cost, 28% from natural gas cost and 20% from carbon cost.

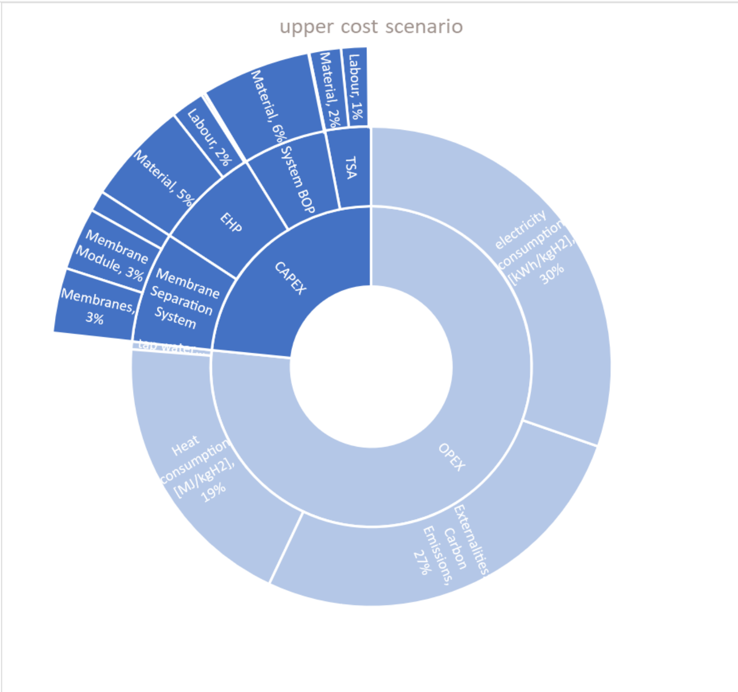
The relevance of the carbon cost increases with the high-cost scenario in which not only an energy-intensive operation scenario (low hydrogen concentration) is considered but also with the assumption of a future price increase of the carbon cost from 45€ per tonne in 2021 to 100€ per tonne in 2030. In this case, electricity makes up 40%, carbon cost 35% and natural gas 25% of the OPEX.

Regardless of the operation scenario, it can be said that the system operation dominates life cycle cost, whereby energy and carbon price are the hotspots. In addition, the material costs for system manufacturing are an important contributor as well.

Figure 25: Detailed cost contribution analysis for the lower, default and upper cost scenario







6.3 Comparison HyGrid and PSA

Since no cost data were available to perform a detailed LCC for the PSA system, literature data were used for the comparison to the HyGrid system. Table 10 shows the expected cost ranges for the separation of 1 kg hydrogen with the HyGrid technology, with PSA as well as the cost for hydrogen production. It can be seen that the separation cost overlaps between the two compared technologies, whereby the upper cost estimate for PSA (7.1 €/kg H2) is more than twice as high as the upper estimate for HyGrid (2.4 €/kg H2). It shall be noted that this comparison is only an indication and of limited robustness, because the price range from literature may be based on different assumptions (e.g. energy price) than the assumptions applied in our LCC study.

Table 10: Life cycle cost range for HyGrid, PSA and hydrogen production

	Min [€/kg H_2]	Max[€/kg H_2]
HyGrid	1.2	2.4
PSA at natural gas distribution pipeline**,** 10% H_2 conc., 80% recov. rate, 100-1000kg H_2 /day, USA (Melaina et al., 2010)	2.8	7.1
H_2 production (Min = from natural gas via steam reforming, USA; Max = green H_2) (Dagdougui et al., 2018)	1.06	6.0

6.4 Study limitations

The LCA results presented here are limited to the objectives, goal and scope defined beforehand. This study is based on available primary data combined with generic data from existing commercial databases or best estimates. There are, therefore, some important limitations to the outcomes of this study. The main limitations of the LCA include the following:

- These LCA results were developed for a system with a low TLR and low output. Accordingly, the efficiency of the system can be expected to increase with its scale.
- Unlike environmental risk assessment conducted in a regulatory context, which uses a conservative approach, LCA seeks to provide the best possible estimate

(Udo de Haes et al. 2002). In other words, the LCIA tries to represent the most probable cause in that the models (of transport and fate of contaminants in the environment and toxic effects on biological receptors) do not attempt to maximize exposure and environmental damage, the worst-case scenario approach.

- This study is an attributional LCA study, not a consequential LCA. In short, it focuses only the environmentally relevant flows to and from the systems studied, and not on any marginal perturbations of those flows as a result of changes in the life cycle (Ekvall & Weidema, 2004).
- LCIA methodologies such as IMPACT 2002+ do not and cannot characterize the wide array of emissions released to soil, air and water from processes. However, it does characterize the most well-known pollutants and in doing such, provides the best estimate to evaluate environmental impact.
- LCIA results present potential and not actual environmental impacts. They are relative expressions, which do not predict impacts on category endpoints, the exceeding of thresholds, safety margins or risks. Additionally, these categories do not cover all the environmental impacts associated with human activities. Impacts such as noise, odours, electromagnetic fields and others are not included in the present assessment. The methodological developments regarding such impacts are not sufficient to allow for their consideration within life cycle assessment. Other impacts, such as potential benefits or adverse effects on biodiversity, are also only partly covered by current impact categories.

The main limitations of the LCC analysis include:

- As mentioned in the LCC results section, the main cost contributors (i.e. electricity, natural gas and carbon price) depend on the development of commodity markets, hence they show a high temporal and geographical variability. To reduce the uncertainty, we considered five-year average prices for electricity and gas. For the less mature yet rapidly developing carbon market, we judge the past five years to be a less appropriate approximation and therefore consider the current (2021) carbon price and an estimate for the future (2030) based on literature.

- It is also important to mention that the cost data for the system manufacturing are projected costs as provided by the other work packages. They are not primary data. However, the major cost contributors are the material components, for which the price is not expected to change a lot with the system scale-up. Some quantity discounts may apply.
- The cost comparison between HyGrid and PSA has limited validity due to the very different data sources and possible system boundaries applied.

When this study is communicated to stakeholders, the magnitude and nature of the limitations should be communicated at the same time.

7 CONCLUSIONS

7.1 System Operation

The main environmental hotspot for the HyGrid technology was identified to be the system's operation (see section 5.3 of this report). For the analysed prototype configuration the operation impacts are associated with electricity consumption from the grid and heat consumption from natural gas boilers. The operation is expected to be of even higher relevance once the system will be scaled up to commercial size because the relative contribution of the system's manufacturing per kg of H_2 output will decrease. Thus, for the system's optimal environmental performance it is essential to minimize the impacts associated with energy consumption, first by optimizing the energy efficiency of the system, secondly by sourcing electricity from a low impact source such as wind power. The impact of the heat demand, however, is harder to reduce through a fuel switch since it has practical and cost reasons to meet it with natural gas from the feed stream.

Although the energy efficiency of the PSA system is significantly lower than of the HyGrid system (i.e. the PSA system has an overall higher energy demand per kg H_2 separated than the HyGrid system) the PSA system it requires only electric energy which can easily be switched to a low-impact source.

HyGrid's heat demand is associated with the use of the PdAg membranes in the membrane separation module. Replacing the PdAg membranes with CMSM, which operate at ambient temperature, would thus eliminate the heat demand and with that the impacts associated to the combustion of natural gas. While the membrane switch leads to a significant reduction of operation impacts, the effect on membrane manufacturing impacts are less clear at this stage. Potential trade-offs shall be analysed with better data availability.

It can be concluded that the system scale-up, the use of a low-impact electricity source and the minimization of the fossil heat demand would lead to optimized environmental performance of the HyGrid system in terms of climate impacts.

7.2 System Manufacturing

7.2.1 Materials

For the three main contributors, namely steel, metal working and electronics it can be expected that economies of scale apply once the system is scaled up from the small-scale prototype to a large-scale, commercial size system. For example, the number of control units (electronics) required in the small system is likely close to if not equal to the number needed in a large system. Also, for steel components their size would not need to increase (linearly or at all, depending on the component) in a large-scale system.

Hence, it can be concluded that the relative contribution of the infrastructure to the impacts per kg of hydrogen recovered by a commercial size system will be much lower than is the case for the prototype.

7.2.2 Membrane Separation System

Following we outline the identified hotspots and optimization potential for the PdAg membranes (namely palladium, steel, metal working and electricity). Moreover, we recommend to consider switching PdAg membranes with CMSM membranes to decrease the system's operation impacts. Potential trade-offs related to the manufacturing of CMSM membranes shall therefore be identified as data become available.

Palladium: As platinum-group metal, palladium belongs to the group of precious metals. Both its high price and high environmental impacts suggest to minimize the required amounts of palladium. As mentioned above, Tecnalia already addresses this aspect by developing a recycling solution for the palladium at the end of the membranes' life (which is shorter than that of the Membrane Module and of the entire HyGrid system).

Moreover, considering that environmental impacts of palladium production differ largely between different countries of origin, we recommend to establish procurement criteria, assuring that palladium is sourced from environmentally and socially favourable sources.

Steel and metal working: As outlined above (5.2.3.1) it can be expected that the amount of steel used in proportion to the system size, i.e. H_2 output, will significantly decrease with the scale-up of the system to commercial size.

Electricity: significant reduction in the electricity consumption required for the baking during membrane manufacturing could already be realized throughout the project. Where further reductions are feasible this should be considered.

7.2.3 EHP Module

The identified hotspots (namely steel, metal working and platinum) also constitute the largest improvement potential in the manufacturing of the EHP module. The sensitivity analysis showed that prolonging the lifetime of the MEA components, reducing the number of MEAs and increasing the platinum recovery rate leads to reduced environmental impacts. Moreover, we recommend considering the following aspects to further optimize the system for environmental performance:

Platinum: Both, its high price and high environmental impacts suggest to minimize the required amounts of platinum. HyET already addresses this aspect by recovering platinum at the end of the life of the MEA component as mentioned above. The same procurement criteria are recommended as for the membrane separation system (see chapter 7.2.2)

Steel and metal working: As outlined above it can be expected that the amount of steel used in proportion to the system size, i.e. H_2 output, will significantly decrease with the scale-up of the system to commercial size.

7.2.4 TSA Module

The identified hotspots (namely steel, metal working, electronics and copper) constitute the largest improvement potential in the manufacturing of the TSA module. Impacts per kg H_2 separated for these hotspots are expected to decrease in relevance with the scale-up of the system. The sensitivity analysis showed that the impact reduction potential associated with EOL recycling of the materials is limited. We therefore conclude, that the focus should be on reducing the absolute amount of materials used in the first place as far as possible.

7.2.5 System Balance of Plant

The identified hotspots are the same as for TSA, namely steel, metal working, electronics and copper. The same recommendations therefore apply as well in this case.

7.3 Overall Conclusions & Recommendations

Drawing upon the results presented in this study, it can be said that the separation of hydrogen from natural gas is more environmentally friendly with the small-scale HyGrid prototype system than with a PSA reference system of comparable size.

For both technologies the operation phase is dominating the impacts, whereby HyGrid operates with significantly higher energy efficiency than the PSA system, i.e. consumes less energy per kg hydrogen separated.

To ensure that this advantage over the reference technology persists with scale-up to commercial size and to further improve the HyGrid technology for environmental performance, we identified four main recommendations for the further development of the HyGrid technology beyond the end of this project. Our recommendations along with an indication of their impact on the life cycle costs are summarized in Table 11.

Table 11: Recommendations for the future improvement of the HyGrid technology's environmental performance

Recommendations to improve HyGrid's environmental performance	**expected impact on life cycle costs**
Reduce energy consumption: largest improvement potential	↓
Reduce heat demand: Investigate CMSM membrane option	→
Material efficiency of infrastructure & scale-up	↘
System operation: **low-impact electricity** sources	↗

Firstly, the largest benefits both in environmental as well as in cost terms can be achieved by further reducing the energy consumption per kg H_2 separated. Secondly, it should be investigated further if the part of the energy consumption associated with the heat demand for the operation of the PdAg membranes can be eliminated by using a different type of membrane (e.g. CMSM). Potential trade-offs due to the required membrane surface area likely being larger for CMSM membranes than for PdAg membranes shall be assessed carefully with more detailed data on the CMSM production. According to a first estimate by partners from WP3 the membrane change does neither lead to relevant increase nor decrease of the life-cycle-costs. Precise cost data shall further be evaluated once they are available.

Thirdly, material efficiency of the system components can be expected to improve significantly with the system's scale-up to commercial size and shall further be optimized beyond that. More detailed recommendations for each system component are provided in section 7.2 above.

Our final recommendation regards the operation phase, i.e. goes beyond the technological development of the system and hence becomes relevant to the system user once the system available for commercial installation. This is to meet the energy demand with low-impact electricity sources.

Note that the above conclusions and recommendations come with the study limitations outlined in section 6.4. In particular, recommendations are based on the assessment of the HyGrid prototype which is of low technological readiness level (TLR) compared to an already commercialized system.

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9 ANNEX I

Table 12 in Annex I documents the parameters applied for the end-of-life modelling with the circular footprint approach described in section 2.7 of this report.

Table 12: Documentation of parameters applied in CFF datasets

Circular Footprint Formula (CFF) datasets		
parameter	**parameter value**	**parameter description**
Polyethylene terephtalate PET, 0% recycling, incl. collection and transport, RER, Circular Footprint Formula (CFF)		
A	0.5	Allocation factor of burdens and credits between supplier and user of recycled materials according to Annex C_Guidance 6.2.xlsx
R2	0	Recycling rate at EOL according to Annex C_Guidance 6.2.xlsx. R2 is 0.42 for PET bottles
Qsout	0.9	Quality of the recycled material outgoing the system at the point of substitution. Default value is 1 for common applications but can be lower if contaminated. Qsout is 0.9 for PET mechanical recycling and 1 for PET SSP recycling according to Annex C_Guidance 6.2.xlsx
Qp	1	Quality of the primary material, i.e. quality of the virgin material. Qp is 1 for steel packaging according to Annex C_Guidance 6.2.xlsx
B	0	Allocation factor of energy recovery processes: it applies both to burdens and credits. Equals to 0 as default according to Annex C_Guidance 6.2.xlsx
LHV	22.95	Lower Heating Value of the material in the product that is used for energy recovery. ecoinvent dataset for PE incineration
Stainless Steel, 0% recycling, incl. collection and transport, RER, Circular Footprint Formula (CFF)		
A	0.2	Allocation factor of burdens and credits between supplier and user of recycled materials according to Annex C_Guidance 6.2.xlsx
R2	0	Recycling rate at EOL according to Annex C_Guidance 6.2.xlsx. R2 is 0.74 for packaging, 0.9 for appliances sheets, 0.95 for building sheet and pipes (for galvanized steel pipes), 0 when mixed in copper alloys in building fittings, when in photovoltaic pannels or for water supply pipes in PPSU fittings.
Qsout	1	Quality of the recycled material outgoing the system at the point of substitution. Default value is 1 for common applications but can be lower if contaminated. Qsout is 1 for steel packaging according to Annex C_Guidance 6.2.xlsx
Qp	1	Quality of the primary material, i.e. quality of the virgin material. Qp is 1 for steel packaging according to Annex C_Guidance 6.2.xlsx
B	0	Allocation factor of energy recovery processes: it applies both to burdens and credits. Equals to 0 as default according to Annex C_Guidance 6.2.xlsx
LHV	0	Lower Heating Value of the material in the product that is used for energy recovery. Based on ecoinvent report no 13 - part 1, section 4.4.1, "No net energy is generated as the energy consumption to

		process the waste is larger than the gross energy that is produced from 2 MJ/kg waste".
Copper, 0% recycling, incl. collection and transport, RER, Circular Footprint Formula (CFF)		
A	0.2	Allocation factor of burdens and credits between supplier and user of recycled materials according to Annex C_Guidance 6.2.xlsx
R2	0	For info, recycling rate at EOL according to Annex C_Guidance 6.2.xlsx are 0.8 is for electronic or mechanical applications, 0.95 is for building applications (pipes, sheets) or electrical (cables). For photovoltaic pannels components, R2=0
Qsout	1	Quality of the recycled material outgoing the system at the point of substitution. Default value is 1 for common applications but can be lower if contaminated.
Qp	1	Quality of the primary material, i.e. quality of the virgin material.
B	0	Allocation factor of energy recovery processes: it applies both to burdens and credits. Equals to 0 as default according to Annex C_Guidance 6.2.xlsx
LHV	0	Lower Heating Value of the material in the product that is used for energy recovery. Based on ecoinvent report no 13 - part 1, section 4.4.1, "No net energy is generated as the energy consumption to process the waste is larger than the gross energy that is produced from 2 MJ/kg waste".
Wood particle board, average secondary production, RER, Circular Footprint Formula (CFF)		
R1	0.2	Proportion of secondary material in the input. According to Annex C_Guidance 6.2.xlsx, R1=0 for pallets,
A	0.8	Allocation factor of burdens and credits between supplier and user of recycled materials.
Qsin	1	Quality of the secondary material used as input. Default value is 1 for common applications but can be lower if contaminated.
Qp	1	Quality of the primary material that is substituted. Default value is 1 for common applications but can be higher for specific high-quality applications.
Steel, low-alloyed, average secondary production, RER, Circular Footprint Formula (CFF)		
R1	0.18	Proportion of secondary material in the input. According to Annex C_Guidance 6.2.xlsx, R1 for building - sheet = 0.18 According to Annex C_Guidance 6.2.xlsx; This material group was chosen as closest proxy for the input of stainless steel to the HyGrid system because the components in this system are assumed to be highly specialized and requiring specific material characteristics for which the recycled material content is assumed rather low
A	0.2	Allocation factor of burdens and credits between supplier and user of recycled materials.
Qsin	1	Quality of the secondary material used as input. Default value is 1 for common applications but can be lower if contaminated. 1 for packaging
Qp	1	Quality of the primary material that is substituted. Default value is 1 for common applications but can be higher for specific high-quality applications.
Steel, chromium, average secondary production, RER, Circular Footprint Formula (CFF)		
R1	0.18	Proportion of secondary material in the input. According to Annex C_Guidance 6.2.xlsx, R1 for building - sheet = 0.18 According to Annex C_Guidance 6.2.xlsx; This material group was chosen as closest proxy for the input of stainless steel to the HyGrid system

		because the components in this system are assumed to be highly specialized and requiring specific material characteristics for which the recycled material content is assumed rather low.
A	0.2	Allocation factor of burdens and credits between supplier and user of recycled materials.
Qsin	1	Quality of the secondary material used as input. Default value is 1 for common applications but can be lower if contaminated. 1 for packaging
Qp	1	Quality of the primary material that is substituted. Default value is 1 for common applications but can be higher for specific high-quality applications.
Polyethylene terephtalate PET, average secondary production, RER, Circular Footprint Formula (CFF)		
R1	0	Proportion of secondary material in the input. According to Annex C_Guidance 6.2.xlsx, R1=0 for HDPE in buildings and constructions and for other plastic applications according to Annex_C_V2.1_May2020_EoL_MP.xls
A	0.5	Allocation factor of burdens and credits between supplier and user of recycled materials.
Qsin	0.9	Quality of the secondary material used as input. Default value is 1 for common applications but can be lower if contaminated. 0.9 for packaging with mechanical recycling, 1 for packaging with SSP recycling
Qp	1	Quality of the primary material that is substituted. Default value is 1 for common applications but can be higher for specific high-quality applications.
Copper, average secondary production, RER, Circular Footprint Formula (CFF)		
R1	0.79	Proportion of secondary material in the input. According to Annex C_Guidance 6.2.xlsx, R1=0.3 for electrical cables, 0.44 for PV pannels, 0.72 for electronic applications, 0.79 for building sheets and pipes, mechanical applications, water supply pipes.
A	0.2	Allocation factor of burdens and credits between supplier and user of recycled materials.
Qsin	1	Quality of the secondary material used as input. Default value is 1 for common applications but can be lower if contaminated.
Qp	1	Quality of the primary material that is substituted. Default value is 1 for common applications but can be higher for specific high-quality applications.
Aluminium, average secondary production, RER, Circular Footprint Formula (CFF)		
R1	0	Proportion of secondary material in the input. According to Annex C_Guidance 6.2.xlsx, R1=0 for Aluminium building - sheet according to Annex_C_V2.1_May2020_EoL_MP.xls
A	0.2	Allocation factor of burdens and credits between supplier and user of recycled materials.
Qsin	1	Quality of the secondary material used as input. Default value is 1 for common applications but can be lower if contaminated.
Qp	1	Quality of the primary material that is substituted. Default value is 1 for common applications but can be higher for specific high-quality applications.
Stainless steel, 100% recycling, incl. collection and transport, RER, Circular Footprint Formula (CFF)		

A	0.2	Allocation factor of burdens and credits between supplier and user of recycled materials according to Annex C_Guidance 6.2.xlsx
R2	1	Recycling rate at EOL according to Annex C_Guidance 6.2.xlsx. R2 is 0.74 for packaging, 0.9 for appliances sheets, 0.95 for building sheet and pipes (for galvanized steel pipes), 0 when mixed in copper alloys in building fittings, when in photovoltaic pannels or for water supply pipes in PPSU fittings.
Qsout	1	Quality of the recycled material outgoing the system at the point of substitution. Default value is 1 for common applications but can be lower if contaminated. Qsout is 1 for steel packaging according to Annex C_Guidance 6.2.xlsx
Qp	1	Quality of the primary material, i.e. quality of the virgin material. Qp is 1 for steel packaging according to Annex C_Guidance 6.2.xlsx
B	0	Allocation factor of energy recovery processes: it applies both to burdens and credits. Equals to 0 as default according to Annex C_Guidance 6.2.xlsx
LHV	0	Lower Heating Value of the material in the product that is used for energy recovery. Based on ecoinvent report no 13 - part 1, section 4.4.1, "No net energy is generated as the energy consumption to process the waste is larger than the gross energy that is produced from 2 MJ/kg waste".
Polyethylene terephtalate PET, 100% recycling, incl. collection and transport, RER, Circular Footprint Formula (CFF)		
A	0.5	Allocation factor of burdens and credits between supplier and user of recycled materials according to Annex C_Guidance 6.2.xlsx
R2	1	Recycling rate at EOL according to Annex C_Guidance 6.2.xlsx. R2 is 0.42 for PET bottles
Qsout	0.9	Quality of the recycled material outgoing the system at the point of substitution. Default value is 1 for common applications but can be lower if contaminated. Qsout is 0.9 for PET mechanical recycling and 1 for PET SSP recycling according to Annex C_Guidance 6.2.xlsx
Qp	1	Quality of the primary material, i.e. quality of the virgin material. Qp is 1 for steel packaging according to Annex C_Guidance 6.2.xlsx
B	0	Allocation factor of energy recovery processes: it applies both to burdens and credits. Equals to 0 as default according to Annex C_Guidance 6.2.xlsx
LHV	22.95	Lower Heating Value of the material in the product that is used for energy recovery. ecoinvent dataset for PE incineration
Copper, 100% recycling, incl. collection and transport, RER, Circular Footprint Formula (CFF)		
A	0.2	Allocation factor of burdens and credits between supplier and user of recycled materials according to Annex C_Guidance 6.2.xlsx
R2	1	For info, recycling rate at EOL according to Annex C_Guidance 6.2.xlsx are 0.8 is for electronic or mechanical applications, 0.95 is for building applications (pipes, sheets) or electrical (cables). For photovoltaic pannels components, R2=0
Qsout	1	Quality of the recycled material outgoing the system at the point of substitution. Default value is 1 for common applications but can be lower if contaminated.
Qp	1	Quality of the primary material, i.e. quality of the virgin material.

B	0	Allocation factor of energy recovery processes: it applies both to burdens and credits. Equals to 0 as default according to Annex C_Guidance 6.2.xlsx
LHV	0	Lower Heating Value of the material in the product that is used for energy recovery. Based on ecoinvent report no 13 - part 1, section 4.4.1, "No net energy is generated as the energy consumption to process the waste is larger than the gross energy that is produced from 2 MJ/kg waste".
Aluminium, more than 90 µm, 100% recycling, incl. collection and transport, RER, Circular Footprint Formula (CFF)		
A	0.2	Allocation factor of burdens and credits between supplier and user of recycled materials according to Annex C_Guidance 6.2.xlsx
R2	1	Recycling rate at EOL according to Annex C_Guidance 6.2.xlsx
Qsout	1	Quality of the secondary material that is used for substitution. Default value is 1 for common applications but can be lower if contaminated.
Qp	1	Quality of the primary material that is substituted. Default value is 1 for common applications but can be higher for specific high-quality applications.
B	0	Allocation factor of energy recovery processes: it applies both to burdens and credits. Equals to 0 as default according to Annex C_Guidance 6.2.xlsx
OxiRate	0.15	The share of oxidized aluminium during incineration is the following (according to European Aluminium Association (PEF-OEF_EOL DefaultData_V1.2_uploaded.xlsx)): o Thick section aluminium packaging 90-900 micron (beverage cans, closures and aerosols) is oxidised at a rate of 10-20% --> use 15% as oxyrate o Small pieces (aluminium trays) 50-90 micron is oxidised at a rate of 20%. --> use 20% as oxyrate o Thin alufoil and foil laminates eg household foil, laminated plastic wrappers with alufoil and pouches with alufoil (and beverage cartons) with a thickness of 6-50 micron, between 50% to 60% is oxidised --> use 55% as oxyrate. These values are used identically for the remelting process.

10 ANNEX II

Table 13 shows the scenario defining parameters and the respective LCIA results for the six considered HyGrid operation scenarios. Table 14 shows the defining parameters and LCIA results for what we identified as the operation scenario of the small-scale prototype resulting in minimal and maximal LCIA results. It also shows the results for the small-scale PSA comparison case, as well as the carbon emission estimates for an optimized HyGrid and PSA system in the future.

Table 13: Scenario parameters and LCIA results for the six considered HyGrid operation scenarios

Scenario Name	**TUe_Temp_400 (Default)**	**TUe_Temp_500**	**TUe_Temp_350**	**TUe_H2concentr _10%**	**TUe_H2concentr _15%**	**TUe_H2concentr _5%**
kg H_2/day	12.6	12.6	12.6	12.6	12.6	12.6
T [C]	400	500	350			
H_2 concentration				10	15	5
HRF [%]	65	75	60	65	71	57
electricity consumption [kWh/kgH2]	4.69	4.82	4.32	4.69	3.00	6.74
purity %	99.85	99.86	99.84	99.85	99.89	99.79
Heat consumption [kWh/kgH2]	6.64	5.78	7.21	6.64	4.06	10.64
Membrane (PdAg) lifetime [yr]	2	2	2	2	2	2
electricity mix	ENTSO-E	ENTSO-E	ENTSO-E	ENTSO-E	ENTSO-E	ENTSO-E
EHP number of membranes	288	288	288	288	288	288
lifetime MEA components [yr]	4	4	4	4	4	4
Platinum recovery rate [%]	85%	85%	85%	85%	85%	85%
Global warming [kg CO2e]	4.70E+00	4.50E+00	4.70E+00	4.70E+00	3.30E+00	6.60E+00
Water consumption [m3]	3.40E-02	3.50E-02	3.20E-02	3.40E-02	2.50E-02	4.50E-02
Human health [DALY]	5.30E-06	5.30E-06	5.20E-06	5.30E-06	4.50E-06	6.40E-06
Ecosystem quality [PDF.m2.y]	4.10E+00	4.20E+00	4.00E+00	4.10E+00	3.50E+00	5.00E+00
Resources [MJ]	8.50E+01	8.20E+01	8.40E+01	8.50E+01	5.90E+01	1.20E+02

Table 14: Scenario parameters and LCIA results for the minimum, maximum and estimated optimized HyGrid system as well as for the small-scale and optimized estimate of the PSA system.

Scenario Name	HyGrid MIN	HyGrid MAX	HyGrid optimized (estimate)	PSA small-scale	PSA optimized (estimate)
kg H_2/day	12.6	12.6	200	12.6	200
T [C]					
H_2 concentration	15	5			
HRF [%]	71	57			
electricity consumption [kWh/kgH2]	3.00	6.74		19.41	19.41
purity %	99.89	99.79			
Heat consumption [kWh/kgH2]	4.06	10.64	0.00	0.00	0.00
Membrane (PdAg) lifetime [yr]	10	2			
electricity mix	ENTSO-E	ENTSO-E	wind	ENTSO-E	wind
EHP number of membranes	144	288			
lifetime MEA components [yr]	5	3			
Platinum recovery rate [%]	90%	80%			
Global warming [kg CO2e]	3.20E+00	6.60E+00	2.80E-01	8.70E+00	4.40E-01
Water consumption [m3]	2.40E-02	4.50E-02		1.11E-01	
Human health [DALY]	3.90E-06	6.50E-06		8.90E-06	
Ecosystem quality [PDF.m2.y]	3.20E+00	5.00E+00		8.30E+00	
Resources [MJ]	5.80E+01	1.20E+02		1.83E+02	