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Life Cycle Assessment of a 5 MW Polymer Exchange Membrane Water Electrolysis Plant

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This study performs a cradle-to-grave life cycle assessment of a 5 MW proton exchange membrane water electrolysis plant. The analysis follows a thorough engineering-based bottom-up design based on the electrochemical model of the system. Three scenarios are analyzed comprising a state-of-the-art (SoA) plant operated with the German electricity grid-mix, a SoA plant operated with a completely decarbonized energy system, and a future development plant electrolyzer with reduced energy and material demand, operated in a completely decarbonized energy system. The results display a global warming potential of 34 kg CO2-eq. kg-H_2^{-1} and indicate a reduction potential of 89% when the plant is operated in a decarbonized energy system. A further reduction of 9% can be achieved by the technological development of the plant. Due to the reduced impacts of operation in a completely decarbonized energy system, the operation at locations with large offshore wind electricity capacity is recommended. In the construction phase, the stacks, especially the anode catalyst iridium, bipolar plates, and porous transport layers, are identified as dominant sources of the environmental impact. A sensitivity analysis shows that the environmental impact of the construction phase increases with a decreasing amount of operational full load hours of the plant.

1. Introduction

The transformation of the take-make-dispose economic system toward circular economy and the integration of sectors are two efforts in order to mitigate human pressures on the earth system. The integration of sectors can be achieved with a hydrogen-based economy, whereas the power-to-X (PtX) approach represents a means to integrate renewable energies in other sectors.[1,2] Within this approach, the hydrogen production by means of water electrolysis has been identified as key process for the execution of PtX applications.[2,3] Hydrogen can be produced by several methods, whereas solely 0.04% of the overall production was covered by water electrolysis in 2021.[4] The rest was produced from steam methane reforming (SMR) and coal or oil gasification.[1,2,4] The demand for green hydrogen is expected to increase significantly in the future. The EU as a whole set the target of an installed electrolysis capacity of 40 GW by 2030, supported by national targets and hydrogen roadmaps.[1]

Commercially, there are currently four electrolyzer technologies available, i.e., proton exchange membrane water electrolyzers (PEMWE), alkaline water electrolyzers (AWE), anion exchange membrane water electrolyzers (AEMWE), and solide oxide electrolyzers (SOEC).[1] PEMWE, AWE, and AEMWE are characterized by a comparatively low operation temperature in the order of 40–80 °C. The SOEC technology operates at temperatures above 700 °C. AWE and PEMWE are mature technologies with a respective technological readiness level (TRL) in the order of 8–9. The SOEC and AEMWE technologies are comparatively young with a lower TRL. Furthermore, PEMWE achieves higher efficiencies than AWE along with promising prospects for a large-scale hydrogen production among others due to superior dynamic response and a high turndown ratio.[1,5,6] For these reasons, in this study, the PEMWE technology is assessed. For an exhaustive discussion of the respective technologies refer to the literature.[1,7,8]

The environmental impacts of hydrogen production by water electrolysis depend on a multitude of factors and can be quantified by a detailed life cycle assessment (LCA). In future energy systems, the production of hydrogen by water electrolysis is

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expected to play such a central role, that their large-scale operation influences the energy system and hence the electricity grid mix. This again influences the environmental impact of water electrolysis significantly. Thus, these influences must be considered when conducting prospective LCAs of said systems.[9] In order to identify hot spots due to the materials employed in the system construction, the design of the complete plant, including all relevant balance of plant (BoP) components, must be based on detailed bottom-up electrochemical modeling. To track possible future impact reductions originating from reduced material and energy demands, the technological developments of the system components have to be considered as well. This allows for identifying impact origins in a very detailed manner and guarantees high-quality data. The degradation of the electrolyzer cells significantly increases the energy demand of the system on a life time basis. Hence, this affects the environmental impacts significantly and therefore has to be accounted for. The catalyst-coated membrane (CCM) is a central component of PEMWE, and the catalyst materials are precious metals with high criticality.[6] Therefore, the CCM production must be accounted for and modeled in sufficient detail. The end of life (EoL) of the plant has to be considered in the LCA analysis in order to depict possible circularity potentials. Thus, a comprehensive LCA study of the PEMWE technology must include the previously stated boundary condition.

In this study, a fully transparent bottom-up cradle-to-grave LCA of a 5 MW PEMWE plant based on electrochemical modeling considering the above stated implications is conducted. As deduced, in an increasingly decarbonized energy system, the environmental impact due to the electricity supply decreases and the share of the construction phase increases. Furthermore, especially for the PEMWE technology, critical raw materials are required for the construction.[6,10,11] Due to this fact, the necessity for tracking the required materials and their environmental impact for the construction of the plant as well as the possible reduction of their demand in the future is of central importance. To the best of the authors' knowledge, no analysis considering all of the previously stated implications has been conducted so far.

Previously conducted LCA studies[12–17] reveal that the electricity supply in the use phase of the electrolysis plant is the main source of environmental impacts. The remaining paragraphs of this section present a literature review of recent LCA studies of hydrogen production by electrolyzers along with the respective derivations for this study.

Cetinkaya et al.[12] analyzed five hydrogen production technologies, i.e., steam reforming of natural gas, coal gasification, water electrolysis via wind and solar, and thermochemical water splitting with a Cu–Cl cycle. The authors quantify the global warming potential (GWP) and the energy equivalents for a hydrogen fueling station. The case study comprises the construction and decommissioning of the plant, natural gas production and transport, electricity generation, and the plant operation. They conclude that the hydrogen production via electrolysis from wind is the environmentally most benign option followed by electrolysis from Photovoltaic (PV). The study does, however, not give details regarding the material demand for the system construction. Furthermore, the electrolyzer plants are operated with electricity from one single source which will not be the case in an integrated electricity grid. Consequently, the study at hand accounts for the plant construction as well as the operation of the plant in a fully integrated electricity grid.

Dufour et al.[13] conduct an LCA for the hydrogen production from water photosplitting, solar two-step thermochemical cycles and auto maintained methane composition and compare the results to the production of hydrogen from water electrolysis from grid electricity, wind and PV electricity. The authors quantify the GWP, the cumulative energy demand (CED), and the cumulative exergy demand (CExD). They conclude that photo splitting shows high potentials for environmentally benign hydrogen production and that wind and PV-based electrolysis produce almost completely renewable hydrogen. Anon, it becomes evident that the operation of the plant in a fully integrated decarbonized electricity grid is essential for further studies.

Valente et al.[14] perform an LCA for the hydrogen production at off-peak hours via electrolysis from run-off river electricity as an energy management solution. They assess nine impact categories, among others GWP, abiotic resource depletion (ADP) and CED. They compare the results to the ones from SMR and conclude that hydrogen from electrolysis shows a favorable life cycle environmental performance when compared to the fossil counterparts. The construction and decommission of the electrolyzer plant are not integrated in this study, thus no assertions regarding the material demand can be made.

Koj et al.[15] assess the environmental impacts of industrial hydrogen production by AWE. They analyze several midpoint indicators among others the GWP, ADP, and eutrophication potential (EP). The authors conclude that the most significant share of the environmental impact originates from the operation of the plant. They give a thorough overview over the plant layout and the material demand for the construction, however, lack in transparency for its derivation. Therefore, a transparent plant design and LCA model are fundamental for further studies.

Bareiß et al.[16] conduct an LCA of PEMWE in future energy systems. The authors assess among others the GWP, metal depletion, and ozone depletion and compare the results to SMR. They conclude that the system construction plays a minor role regarding the potential environmental impacts of the system and the main source stems from the plant operation. Furthermore, they identify that the operation of PEMWE as an alternative to conventional SMR production in the future. In the study, the plant operation for the complete life cycle is assumed with a cell voltage commonly associated to the beginning-of-life (BoL) of the electrolyzer cells, not considering degradation phenomena. Thus, the results potentially underestimate the environmental impact of the plant operation. They do give an overview over the material demand for the stack and the BoP along with expected potential material reductions for the stack in the future. However, no conclusions on the implemented LCA model architecture can be drawn. Thus, for complete transparency, a detailed presentation of the model and an engineering-based derivation of the material demand is required.

Schropp et al.[17] conduct a cradle-to-gate prospective LCA for the production of hydrogen with PEMWE. They analyze a 1.25 MW state-of-the-art (SoA) plant and develop three prospective scenarios, each for 2030 and 2050, combining parameters for the system efficiency, the cell lifetime and the material demand based on rough specifications. They conclude that 6 out of 12 impact categories decrease over time, while the remaining impact categories, all regarding the resource depletion except the depletion of fossils, do not. They do not give further discussion regarding the reasons for the diverging trends. They conduct an additional analysis regarding the impacts in the GWP and depletion of mineral and metal resources (RDP) impact categories concluding that the GWP decreases with increasing renewable electricity, while the RDP shows opposite trends indicating a burden shifting. As stated earlier, the model is based on rough specifications regarding central parameters for the plant. Furthermore, in order to pinpoint and quantify potential reduction potentials, a detailed discussion of the results of ever life cycle phase is required. Hence, for full transparency, all plant specifications need to be derived from a detailed bottom-up electrochemical system model, so that each system component can be designed and the results can be interpreted accordingly in sufficient detail.

In view of the existing literature, further detailed analysis with an emphasis on the transparency of both the plant design as well as the implemented LCA model is required. Here, especially the potential reduction of the material demand for the plant construction, based on a thorough bottom-up modeling of the plant as well as the integration of the plant operation in a fully decarbonized electricity grid in the future, has to be depicted along with a thorough and detailed interpretation of the results.

2. Preliminary Considerations

In this chapter, preliminary considerations in the bottom-up cradle-to-grave LCA of a 5 MW PEMWE plant are provided in four segments. First of all, the LCA methodology is introduced. Second, a technical system description of the 5 MW PEMWE plant follows. Third, the origin of input data for the LCA model is specified. The chapter closes with a description of the electrochemical model of the plant and the underlying energy system model that provide the input data for the LCA model.

2.1. Life Cycle Assessment Methodology

LCA is a standardized methodology for assessing the potential environmental impacts of products, services, or processes throughout their complete life cycle. The methodology aims to reveal potential environmental impacts and hotspots of the analyzed systems and tries to prevent a burden shifting from one life cycle phase to another.[18] According to the ISO standards 14040 and 14044, the methodology comprises four phases: 1) goal and scope definition; 2) life cycle inventory (LCI); 3) life cycle impact assessment (LCIA); and 4) interpretation.[19,20]

Central characters of the methodology are the definition of a functional unit (fU) and the assessment of the complete life cycle ("cradle-to-grave") of a process or product.[21] In the first phase, the goal of the study along with the fU and the reference flow is defined unambiguously and the system boundary for the analysis is set. In the second phase, all relevant mass and energy flows of the system are quantified. These flows are then classified and assigned to environmental impact categories in the third phase. In the concluding phase, the results are interpreted. A further characteristic feature of the methodology is the iterative manner of the conduct of the phases giving space for potential adjustments of important parameters if necessary.[21] For hydrogen applications, detailed guidelines such as the FC HyGuide have been elaborated in order to guarantee a high quality of studies and comparability of the results.[22,23]

The goal of this study is the conduct of a detailed bottom-up LCA for the production of green hydrogen in a 5 MW PEMWE plant operated in the current energy system as well as in a completely decarbonized energy system in order to determine possible impact reduction potentials. Furthermore, a particular emphasis on the construction phase of the plant is made enabling a detailed tracking of the material demand. Thus, in order to conduct a meaningful and detailed LCA, a comprehensive system description including the mass, material, and energy balances for each system component in every stage of the life cycle (construction, operation, and EoL) is required. To this end, a discussion of the 5 MW PEMWE plant and the deduction of the input data for the LCA follows.

2.2. Technical System Description

In a PEMWE plant, hydrogen is produced from water and electricity. The flowsheet of the PEMWE plant under consideration is given in **Figure 1**. Core of the plant are the Proton Exchange Membrane (PEM) electrolyzer stacks (component E). As shown in the flowsheet, the system requires BoP equipment (i.e., circulating (component C) and feed pumps (component A), gas water separators (components B and G), a cooling system (components D, I, K, and L), product processing (components H and J)), and power electronics (PE) (component F) in order to function. Note that the required water purification system is not shown in this flowsheet.

As stated earlier, the electrolyzer stacks are the core of the system, where the reaction takes place. The stack comprises a number of separate cells where water is split into hydrogen and oxygen. The energy demand for the propagation of the chemical reaction is provided by a direct current. Each cell consists of a cathode and an anode compartment, which are separated by a membrane (for a detailed discussion of the cell and stack setup including required materials refer to Supporting Information 1, Section S4). Water is fed on the anode side where it is split into oxygen and hydrogen ions. The hydrogen ions permeate through the membrane to the cathode side and recombine to form molecular hydrogen. The hydrogen ions do, however, not cross the membrane exclusively. A small amount of water is dragged along to the cathode side and part of the formed oxygen crosses over the membrane from anode side to cathode side as well. Furthermore, some of the generated hydrogen crosses the membrane, back to the anode side. Thus, the hydrogen product stream on the cathode side contains impurities that need to be removed subsequently, and some of the generated hydrogen is "lost" by crossover to the anode side. The produced oxygen is usually vented from the system.[1,8,24,25]

Due to thermodynamic limitations, the provided electricity cannot be transformed into hydrogen completely. Part of the electricity is converted into heat that has to be rejected from the stack in order to prevent overheating. The waste heat is removed by means of surplus water circulation through the stack

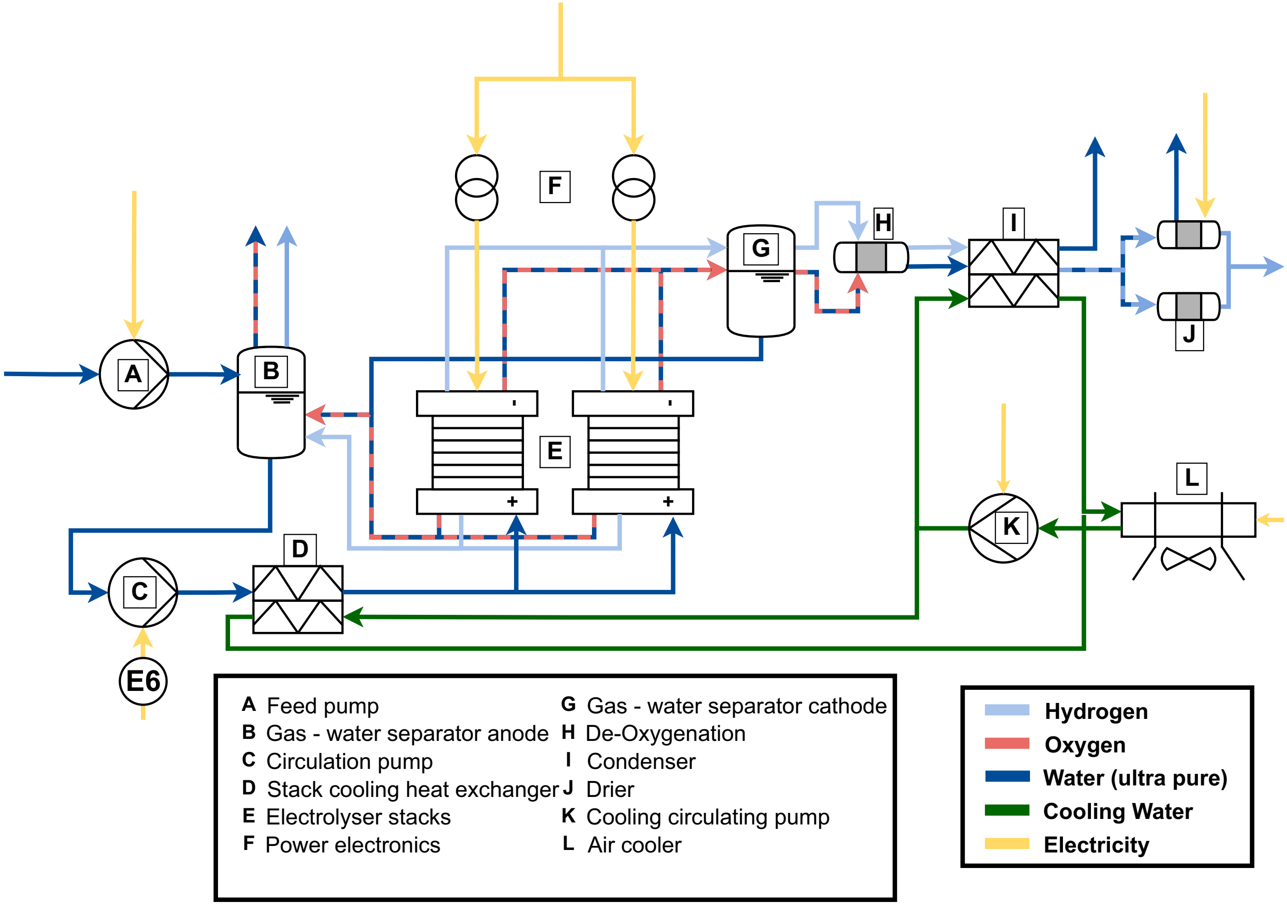

Figure 1. Flowsheet of the proton exchange water electrolysis (PEMWE) plant under consideration—required water purification system not shown in this depiction.

and conveyed out of the system in a separate cooling cycle. The cooling duty is typically provided by an air cooled dry-cooling unit. Feed and circulation pumps elevate the water to system pressure and overcome pressure losses.

The produced hydrogen is purified in a deoxygenation stage where part of the product stream reacts with the remaining oxygen to form water. Anon, a part of the product stream is "lost". The generated water is subsequently removed in a dryer, providing a purified product stream. During operation, the cells are prone to degradation phenomena that increase the required cell voltage and thus the energy demand of the system over its lifetime. This in turn affects the environmental impact of the system. Hence, the cell degradation needs to be accounted for. As the stacks operate on direct current, PE that convert the alternating current from the grid are required. Furthermore, the plant requires a control system for operation as well as housing and a foundation (not shown in Figure 1). Housing is typically provided by standard shipping containers.

2.3. Data

In order to conduct the LCA study, two sets of input data, hereafter referred to as key performance indicators (KPIs), are required. The KPIs of the PEMWE technology are subdivided into operational KPIs (see **Table 1**) and construction KPIs (see **Table 2**).

As stated earlier, the demand for green hydrogen is expected to increase significantly in the future. To estimate the environmental impact of hydrogen production from plants that are constructed in the future to meet that demand, the technological development of the plant has to be accounted for. For this reason, the production of hydrogen from a SoA plant and the production in a future development plant electrolyzer are assessed in this study. Table 1 gives an overview over the employed operational KPIs of the system for a SoA and a future development plant electrolyzer that are fed into the PEMWE model. As can be seen, the stack scaling is expected to increase significantly (stack power and active cell area) together with a decrease of the required energy demand (further details later) due to increased current density of the cell along with a decreased cell voltage.

Table 2 gives an overview of a chosen set of construction KPIs for the PEMWE stack that are employed in the LCI phase for the determination of the material demand in the system construction. A detailed discussion regarding the construction including a list of the material demand for every system component is

Table 1. Operational KPIs of the proton exchange water electrolysis (PEMWE) stack/input data for the PEMWE model.

Parameter	Unit	State-of-the-art plant	Future development plant	References
Stack scaling	MW	2.5	10	[1,8]
Cell voltage beginning of life	V	1.8	1.7	[38]
Cell degradation	$mV\,h^{-1}$	0.004	0.00204	[39,40]
Cell voltage EoL	V	2.12	1.904	Calculation
Mean cell voltage	V	1.96	1.802	Calculation
Current density	$A\,cm^{-2}$	2	5	[1]
Stack operating temperature	°C	65	65	
Stack operating pressure	bar	30	30	
Active cell area	cm^2	1500	10'000	[1]
Active stack area	m^2	69.45	59	Calculation
Cells per stack		463	59	Calculation
Stack lifetime	h	80'000	100'000	[1]
Pump efficiency	%	26.27	26.27	[41]
Energy demand product drying	$kWh\,(kg\,H_2)^{-1}$	0.05	0.05	[16]
Power electronics efficiency	%	98	98	[42]
Dry cooler energy demand	kW	82	82	[43]
System lifetime	a	20	20	[7]

Table 2. Construction KPIs of the proton exchange water electrolysis (PEMWE) stack/input data for the LCI of the PEMWE stack construction.

Parameter	Unit	State of the art	Future development plant	References
Active cell area	cm^2	1500	10,000	[1]
Membrane material		Nafion N117	Nafion N112	[44,45]
Cathode catalyst		Platinum supported on Vulcan XC72 carbon black (40 wt% Pt/C)		[46,47]
Cathode catalyst loading	$mg\,cm^{-2}$	0.2	0.05	[48,49]
Anode catalyst		Rutile iridium oxide (IrO_2) on titanium dioxide (TiO_2) support (weight ratio 3 IrO_2/TiO_2)		[50,51]
Anode catalyst loading	$mg\,cm^{-2}$	2	0.4	[50]/[1]
Porous transport layer material anode		Titanium, 30% porosity	Titanium, 50% porosity	[52]/[38]/[53]
Porous transport layer thickness anode	mm	1	0.7	[38]/[53]
Porous transport layer coating anode		0.1 $mg\,cm^{-2}$ iridium	None	[50]/[53]
Bipolar plate material		Titanium		[54]
Bipolar plate thickness	mm	2.5	0.1	[55]
Bipolar plate coating material anode side		Platinum		[48]
Bipolar plate coating amount	$mg\,cm^{-2}$	0.04	0.02	[48]

given in Supporting Information 1, Section S4. Note, that, e.g., the active cell area shows up in both datasets as it affects the operation of the stack as well as the resulting material demand for the construction. As can be seen in Table 2, the material demand for the construction of the PEMWE stack is expected to decrease dramatically in the future.

2.4. Modeling

Figure 2 depicts the data flow through the respective models and LCA phases in this study. In order to determine the environmental impact of the system, detailed input and output balances for each system component in every lifecycle phase are needed for the LCA model. These data are called LCI illustrated in the central box (3) in the data flow scheme. In order to produce these tables, a detailed set of system data is required that anon is derived from an electrochemical PEMWE system model (1). The design of each system component is based on modeling of the electrolyzer stack in combination with construction KPIs. To this end, the boundary conditions for the operation of the stack and the system have to be elaborated from operational KPIs. These boundary conditions are subsequently fed into the PEMWE model, yielding detailed mass and energy balances for the operation of every system component. The electrolyzer model (1) and LCI (3) thus require each a set of data input (Section 2.3).

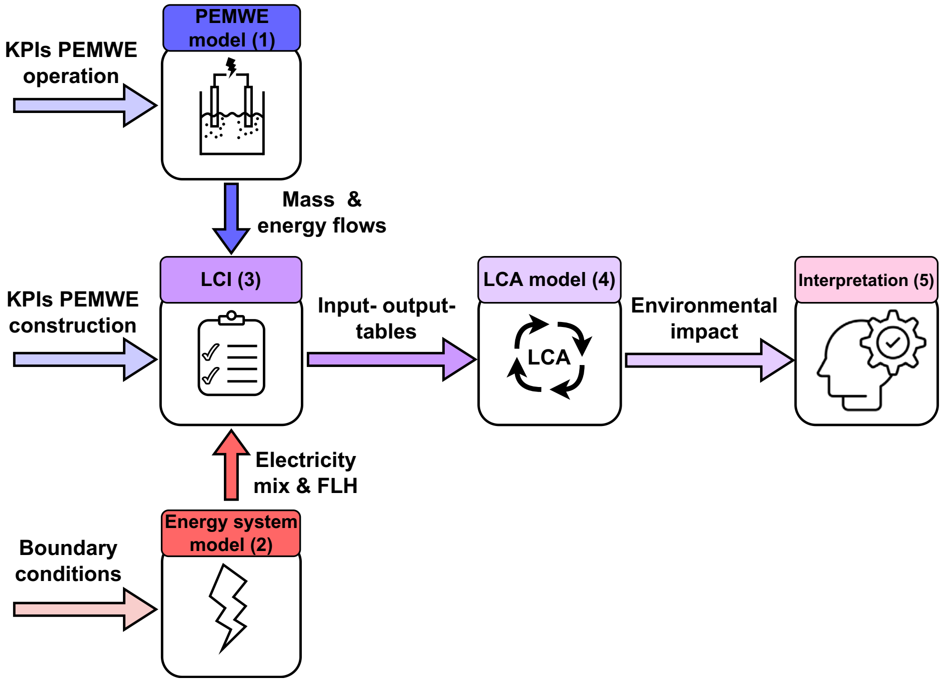

Figure 2. Data flow through the respective models and life cycle assessment (LCA) phases in the study.

Furthermore, the source of electricity for the plant operation affects the environmental impact significantly. Therefore, an estimation of the future electricity mix is required. The penetration of intermittent renewable electricity sources anon affects the full load operation hours (FLH) of the plant and hence the amount of produced hydrogen, which in turn affects the environmental impact per unit of produced hydrogen. For the estimation of the future electricity mix and the identification of the annual FLH, a separate model of the background energy system (2) is employed.

2.4.1. Energy System Model

For the energy system model, we use a model of the German energy system in 2045. It covers all energy demands, which are described in ref. [26]. It must not use any fossil fuels as energy carriers nor as base for petrochemical products. The spatial resolution is one node per federal state. The temporal resolution is one timestep per hour. A description of the model equations can be found in ref. [27]. For photovoltaic, we use a mix of 50% rooftop and 50% open field plants. In accordance with,[28] we assume the rooftop PV installations to be mono silicon wafers only. The electrolysis is modeled consistently with the values given in Table 4. From the results of the energy system model, we calculate a dedicated electricity mix for the electrolysis. It is the average energy mix of all timesteps, weighted with the power consumption of the electrolysis during each timestep. Using this dedicated energy mix in the LCA is equivalent to running the LCA with the energy mix in each timestep and averaging the results afterward. However, it greatly simplifies the procedure, as the LCA has to be conducted only once.

The results are shown in **Table 3**. The shares of biomass power plants and the hydrogen turbines are very low. This is because these energy sources are only used when energy is scarce in the system. The electrolysis, however, is usually run when there is an energy surplus (from wind and photovoltaic) in the system. For this reason, biomass power plants and hydrogen turbines are not considered in the LCA The results further show that the electrolysis operates at significantly lower full load hours in the decarbonized electricity mix as in the SoA scenario. This is because the electrolysis together with the hydrogen storage acts as the main seasonal energy storage in the energy system. In summer, it absorbs a lot of the infeed from photovoltaics, producing much more hydrogen than needed and fills the hydrogen storage. In winter, electricity demand is higher due to heating from heat pumps and supply from photovoltaics is lower. Then, the electrolysis runs only during the photovoltaic peak for a few hours per day, and the remaining hydrogen demand is covered by the hydrogen storage. This leads to 3235 full load hours for the electrolysis.

2.4.2. PEMWE Model

First of all, the stack is modeled according to its technical restrictions giving the mass and energy flows of all relevant species during operation. Subsequently, every system component is designed according to the respective mass and energy balance in order to determine the energy and auxiliaries demand in the operation and the material demand for construction. These data are then fed into the LCA model. The electrochemical model is set up according to Bensmann et al.[29] A detailed model description including all relevant mass and energy balances is given in Supporting Information 1, Section S3. The results of

Table 3. Results of the energy system model.

Energy source	Share in the energy mix
Photovoltaic roof	23.56%
Photovoltaic open field	23.56%
Wind onshore	29.14%
Wind offshore	23.62%
Biomass power plants	0.12%
Hydrogen turbines	0.01%
Plant case	**Annual FLH**
SoA plant	8000 h
Future development plant	3235 h

the PEMWE model for both plant cases are given in **Table 4**. Note that the specific energy demand of the electrolysis process includes the cell degradation and is therefore somewhat larger than relevant literature values (generally, the specific energy demand for the beginning of life is given). The total energy demand includes the efficiency of the PE and the energy demand for the BoP. For a detailed listing of all mass and enthalpy flows at every system state point of each component refer to Supporting Information 1, Section S3.

3. Life Cycle Assessment

In this section, the goal and scope of the study are defined (3.1). The LCI is presented (3.2), and the LCIA method is explained (3.3). Please note that the interpretation is given in Section 4.

3.1. Goal and Scope

The goal of the study is to quantify the potential environmental impacts of an SoA PEMWE plant and track their origin in order to identify hot spots in a fully transparent study. Furthermore, the prospective impact reductions for future technological developments of the plant, yielding a reduction in material and energy demand, in a completely decarbonized energy system shall be assessed. The plant is scaled to an electricity input of 5 MW to the electrolyzer stacks. The fU of the study is the construction, operation, and decommissioning of a 5 MW PEMWE plant with a reference flow of 1 kg of produced hydrogen at a pressure of 30 bar, temperature of 25 °C, and 5.0 quality (99.999% purity).

The technological system boundary comprises a cradle-to-grave analysis with modeling according to the cutoff approach including the BoP as given in **Figure 3**. The focus of the study is set on the construction and operation phases since the EoL handling of PEMWE systems is still in its infancy. An extended cradle-to-cradle approach in accordance with circular economy would be of great interest; however, due to the maturity of the technology combined with its long lifetime, the second life possibilities and recycling potentials to date are limited. In industrial PEMWE systems, no recycled material is employed for stack relevant components, and therefore, no assumptions regarding recycled materials are done.

The temporal system boundary is set in respect to an overall plant lifetime of 20 years. However, individual components of the plant are characterized by shorter life expectancy, and thus a replacement of the equipment is considered according to their respective lifetime (for a detailed discussion of every system component refer to Supporting Information 1, Section S4). The SoA system is constructed and goes into operation in 2020. As stated before, a future development plant electrolyzer with the according electricity mix is accounted for in this study. The future development system is assumed to be constructed in 2045. The construction, operation, and EoL are assumed to take place in Germany. Note that the origin of raw materials is considered globally. The construction phase of the hydrogen purification unit is not considered in this study due to a lack of available data. Furthermore, in order to avoid double counting, the operation and construction of the water purification system are not modeled separately, as they are included in the employed dataset. In this study, three separate scenarios as given in **Table 5** are analyzed.

3.2. Life Cycle Inventory

The LCA model is subdivided into several layers as given in **Figure 4**. Accordingly, the LCI data are designated to the respective system layers. The highest layer comprises the three life cycle phases construction, use, and EoL. Each of these phases is further subdivided into system descriptive layers. The construction phase comprises five layers, according to the system hierarchy. In

Table 4. Results of the proton exchange water electrolysis (PEMWE) model.

Parameter	Unit	State of the art	Future development plant
Lifetime hydrogen production	t	16,253	6979
Specific energy demand electrolysis	kWh (kg H_2)$^{-1}$	53.60	49.28
Dryer energy demand	kWh (kg H_2)$^{-1}$	0.05	0.05
Feed pump energy demand	kWh (kg H_2)$^{-1}$	0.03	0.03
Circulating pump energy demand	kWh (kg H_2)$^{-1}$	0.70	0.43
Cooling water circulating pump energy demand	kWh (kg H_2)$^{-1}$	0.05	0.04
Dry cooler energy demand	kWh (kg H_2)$^{-1}$	0.82	0.77
Total energy demand	kWh (kg H_2)$^{-1}$	56.33	51.61
Water demand (ultrapure)	kg (kg H_2)$^{-1}$	9.3	9.3

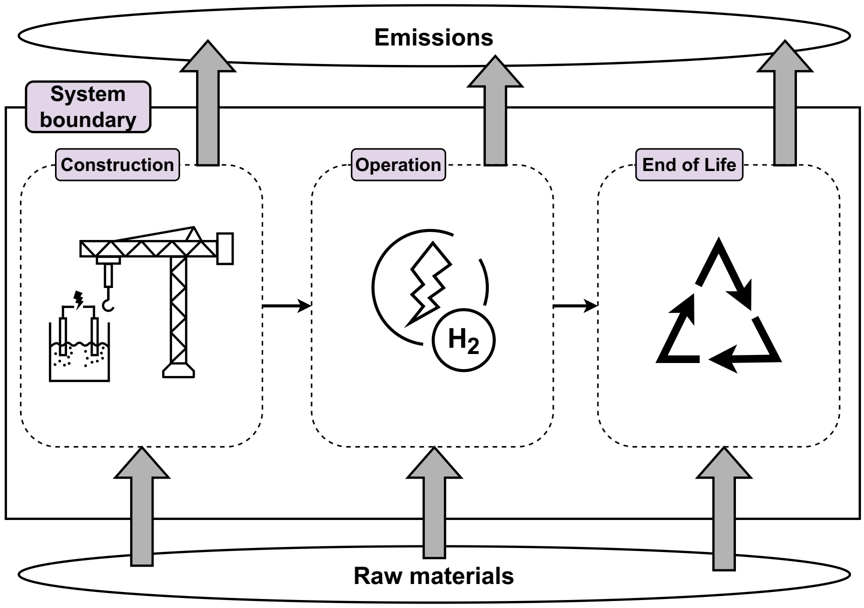

Figure 3. Technological system boundary for the life cycle assessment (LCA) of the proton exchange water electrolysis (PEMWE) plant at hand.

Table 5. Scenario definition for the study.

Scenario	Plant	Electricity mix	Annual FLH
Scenario 1	State of the art	German grid mix 2018–2023	8000 h
Scenario 2	State of the art	Decarbonized	3235 h
Scenario 3	Future development	Decarbonized	3235 h

the first construction layer, the overall system is assembled from the system components, e.g., stack, heat exchangers, pumps, etc. The next layer represents the manufacturing of each system component. This hierarchy is pursued to the lowest layer, where raw materials are processed to intermediate products, e.g., the manufacturing of the anode catalyst ink for the CCM from the catalyst material and solvent. The use phase comprises one single layer in which the desired product, hydrogen, is produced from water and electricity in the electrolysis process. Note that the produced oxygen is vented and not further used. Therefore, the system does not contain any multifunctionality. The EoL is an inversion of the construction phase. In the first EoL layer, the electrolysis plant is manually dismantled to the respective system components. In the next layer, each system component is treated according to the cutoff approach either leaving the system or pursuing the layer hierarchy until the embodied materials are disposed or cross the system boundary for recycling.

The LCI for the use phase can be directly derived from Table 4. As discussed earlier, the LCI for the construction phase is based on a component design based on the PEMWE model. An overview of the LCI of the construction phase on system level is given in **Table 6**. The LCI includes the anticipated lifetime of each component as well as the technical boundary conditions of the system along with the boundary conditions of the energy system, e.g., the future development case solely requires “half” a stack as the possible stack scaling is greater than the system scaling (Table 1) and no stack replacement is required due to the increased stack lifetime on one hand and the reduced FLH in scenario 3 on the other hand. The piping is not considered in this study, as its sizing depends on the specific application.

Table 7 shows the material demand for the construction of a single stack for both the SoA plant and the future development plant electrolyzer. Note that this depiction of the material demand is cumulative comprising the catalyst level to stack level (Figure 4). A detailed breakdown of the stack according to the respective system levels is given in Supporting Information 1, Section 4.1.

3.3. Life Cycle Impact Assessment

The life cycle of the analyzed system is modeled in the LCA software GaBi.[30] The data regarding the foreground system are obtained as described earlier with subsequent expert validation. The data of the foreground system are supplemented by generic data from the ecoinvent database version 3.8[31] for the background system. In accordance to the guidelines for LCAs of hydrogen applications[22,23] the CML2001, last updated 2016 LCIA methodology is employed. To relate to the concept of planetary boundaries, the impact categories GWP on a 100 years basis (GWP 100), ADP, acidification potential (AP), EP, and human toxicity potential (HTP) are considered in this study.

4. Results and Discussion

The discussion of the results is conducted by reference to the modeling approach according to the respective system layers illustrated in Figure 4. First, the environmental impact of the overall system is presented and discussed (4.1). Leading on,

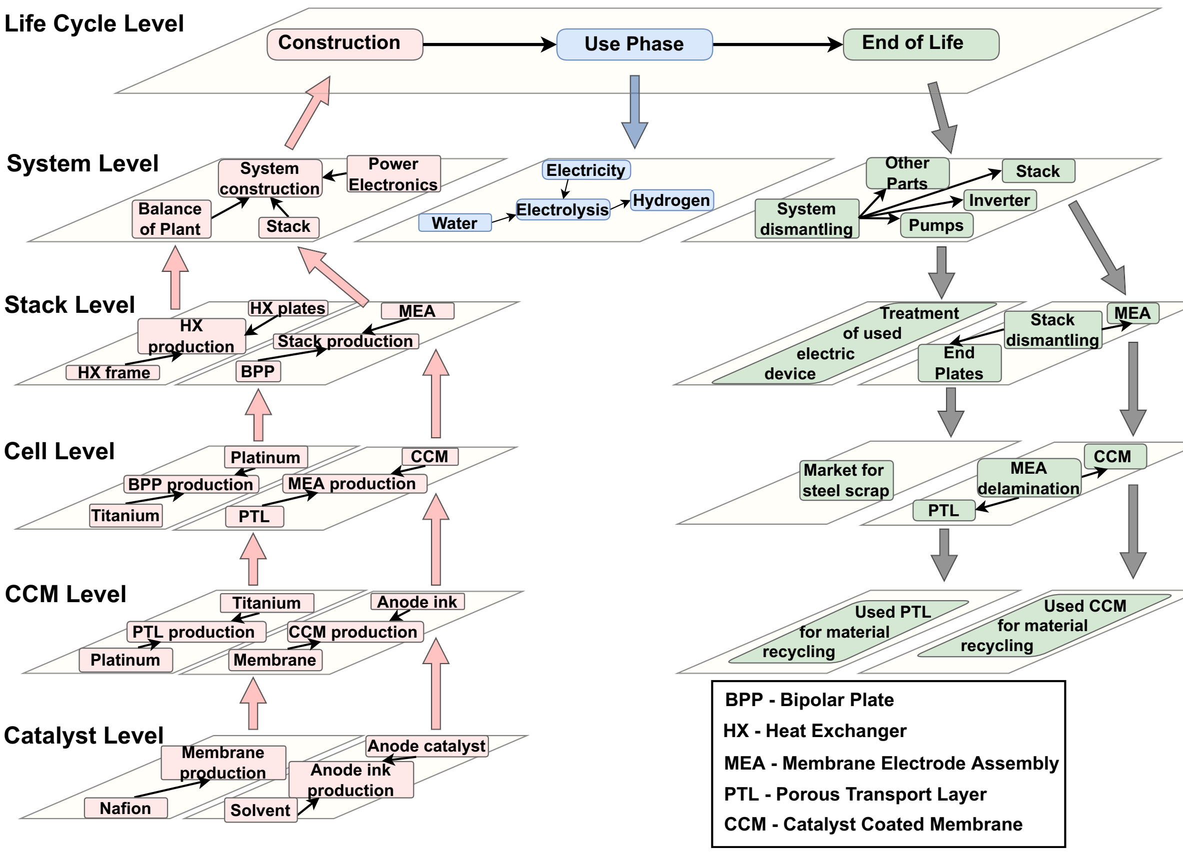

Figure 4. Life cycle assessment (LCA) model approach.

Table 6. Life cycle inventory (LCI) of the system construction.

Component	Unit	Value SoA	Value future development	Employed ecoinvent dataset
Stack	Pieces	4	1	Own model
Anode gas water separator	kg	660.3	628.3	Own model
Cathode gas water separator	kg	356.3	356.3	Own model
Feed pump	Pieces	2	2	Market for water pump, 22 kW—GLO
Circulating pump	Pieces	2	2	Market for water pump, 22 kW—GLO
Stack cooling heat exchanger	kg	1340.4	1306.1	Own model
Condenser	kg	1157.7	1159	Own model
Dry cooler	Pieces	1	1	Own model
Cooling water circulating pump	Pieces	2	2	Market for water pump, 22 kW—GLO
Power cables	m	50	50	Model according to[56]
Data cables	m	2000	2000	Market for cable, data cable in infrastructure—GLO
Control unit	Pieces	1	1	Market for control cabinet, heat and power co-generation unit, 160 kW electrical—GLO
Power electronics	Pieces	22	22	Market for inverter 500 kW—GLO
Foundation	m^3	4.5	4.5	Market for foundation plate—GLO
Housing	Pieces	2	2	Market for intermodal shipping container, 40-foot—GLO

Table 7. Material demand for one proton exchange water electrolysis (PEMWE) stack (state-of-the-art (SoA) stack 2.5 MW, future stack 5 MW).

Material	Amount SoA [kg]	Amount future development [kg]
Titanium	996.71	118.58
Carbon paper	8.75	7.43
Nafion	30.25	7.14
Platinum	0.188	0.079
Iridium	2.465	0.407
Activated carbon	0.24	0.102
FKM	80.56	38.16
Copper	17.06	107.93
Stainless steel	156.20	677.02

the impact of the system operation (4.2) and the construction (4.3) are presented. Finally, a sensitivity analysis is conducted (4.4).

4.1. Overall Environmental Impact

Figure 5 shows the overall environmental impacts according to the described scenarios. The absolute values on the right refer to scenario 1. This value is set as a benchmark of 100%. Potential impact reductions (or promotions) of the respective scenarios can be derived accordingly. It can be seen that the potential environmental impact of the system is reduced significantly when the same plant is operated in a completely decarbonized energy system (scenario 2). A further decrease can be observed due to the decreased energy and material demand of the system in scenario 3. This is, however, on a considerably lower scale than the effect of the energy system decarbonization. Interestingly, the ADP increases almost fivefold when operating the plant with completely decarbonized electricity. This can be traced back to two implications. First, the background system in the prospective scenarios still employs not defossilized datasets, e.g., in the datasets for the manufacturing of solar PV modules and wind turbines, electricity from fossil resources is employed. In a completely defossilized energy system, a further impact reduction can thus be expected. Furthermore, the construction of wind turbines, as well as photovoltaic modules, requires a significant amount of copper and further critical materials. Due to the comparatively small scaling of the wind turbines and PV modules, a similarly large amount of these materials is required per unit of produced electricity, which anon affects the ADP impact category. Lastly, renewable energy systems are intrinsically complex systems that are currently experiencing intense progresses. Consequently, further developments that are affecting especially the resource demand can be anticipated.

The global average for the GWP impact of the hydrogen production is in the order of 12 kg CO_2-eq. kg H_2^{-1}.[32] Note that the emissions are strongly governed by the production technology. In the following, the GWP results of this study are benchmarked against literature values for the current SoA hydrogen production technologies of gray and blue hydrogen, respectively. Gray hydrogen is produced by SMR, whereas for blue hydrogen the generated carbon dioxide is captured and stored upon emission. The specific emissions further heavily depend on the scope of the respective studies, the modeling approach, and the assumed technological boundary conditions such as the methane emission rate and the carbon capture rate in the case of blue hydrogen. For a methane emission rate of 0.2% Bauer et al. report, a GWP of 10.48 kg CO_2-eq kg H_2^{-1} and in combination with a carbon capture rate of 93%, 2.67 kg CO_2-eq kg H_2^{-1} for the production of gray and blue hydrogen, respectively.[33] Thus, the potential impact of gray hydrogen is considerably larger than the results for the production of green hydrogen as determined in scenarios 2 and 3 of this study. The potential impact of blue hydrogen for the reported best-case scenario is somewhat lower than the ones for green hydrogen from this study. However, with possible impacts as large as 12.33 kg CO_2-eq kg H_2^{-1} for higher methane emission rates and lower carbon capture rates, respectively,[33] it can be concluded that only with best-case assumptions can blue hydrogen outperform the production of green hydrogen. In order to give detailed assertions regarding the benchmarking of green hydrogen, a harmonization of the impacts regarding scope, methodology, and technological boundary conditions is required.

Table 8 shows a further subdivision of the environmental impact of all analyzed impact categories regarding the life cycle phases. It can be seen that the impact is driven by the use phase of the system in every scenario. The construction phase only has a minor effect on the overall impact and the EoL phase does almost not contribute at all, with shares no larger than 0.08%

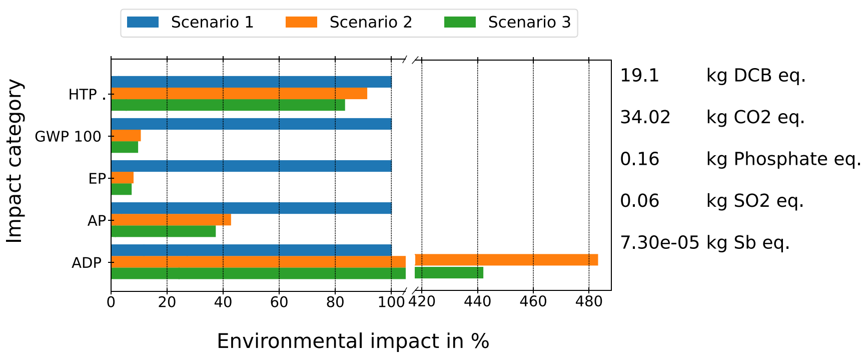

Figure 5. Overall impacts of the analyzed scenarios—the absolute values on the right refer to the impact per unit of reference flow of scenario 1 (scenario definition in Table 5). This value is set as a benchmark of 100%. Potential impact reductions of the respective scenarios can be derived accordingly.

Table 8. Impacts for all life cycle phases in every scenario for each analyzed impact category.

Impact category	Unit	Scenario 1						Scenario 2					
		Construction		Use phase		EoL		Construction		Use phase		EoL	
		Absolute impact	Relative share	Absolute impact	Relative share	Absolute impact	Relative share	Absolute impact	Relative share	Absolute impact	Relative share	Absolute impact	Relative share
GWP 100	kg SO_2 eq.	0.055	0.16%	33.97	99.83%	0.0012	0.003%	0.099	2.79%	3.45	97.13%	0.0028	0.08%
AP	kg SO2 eq.	0.0015	2.47%	0.06	97.53%	7.39E-07	0.001%	0.002	8.81%	0.0245	91.19%	1.73E-06	0.006%
EP	kg PO_4^{3-} eq.	0.0003	0.18%	0.15	99.82%	5.58E-07	0.0004%	0.0005	4.01%	0.0117	95.98%	1.29E-06	0.01%
HTP	kg DCB eq.	0.519	2.72%	18.58	97.25%	0.005	0.028%	1.171	6.72%	16.24	93.20%	0.013	0.07%
ADP	kg Sb eq.	8.58E-06	11,75%	6.44E-05	88.25%	1.17E-09	0.002%	1.98E-05	5.63%	0.0003	94.37%	2.64E-09	0.0007%

Impact category	Unit	Scenario 3					
		Construction		Use phase		EoL	
		Absolute impact	Relative share	Absolute impact	Relative share	Absolute impact	Relative share
GWP 100	kg SO_2 eq.	0.061	1.90%	3.17	98.02%	0.0026	0.081%
AP	kg PO_4^{3-} eq.	0.0009	4.20%	0.022	95.80%	1.56E-06	0.006%
EP	kg DCB eq.	0.0003	2.76%	0.012	97.23%	1.14E-06	0.010%
HTP	kg Sb eq.	1.023	6.43%	14.88	93.49%	0.012	0.077%
ADP	kg SO_2 eq.	1.77E-05	5.49%	0.0003	94.51%	2.29E-09	0.0007%

in every scenario. For this reason, the EoL is not separately shown in and not further analyzed in this study. It can be seen that the share of the construction phase increases in scenarios 2 and 3. However, the overall impact is still driven by the use phase of the system.

As the use phase shows such an outstanding share on the overall environmental impact in every scenario, a further analysis of the impact origins in the use phase follows. Even though the share of the construction phase seems of subsidiary importance for every scenario and impact category, a further investigation of the construction phase is suggestive due to the required critical materials.

4.2. Use Phase

Figure 6 shows the environmental impact of the system operation of every scenario with regard to the origin of the impact. The absolute values on the right refer to the environmental impact of the use phase in scenario 1. This value is set as a

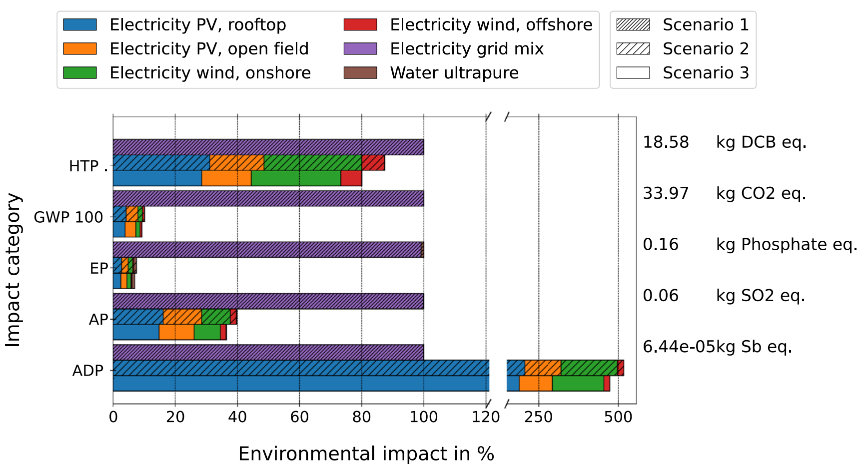

Figure 6. Environmental impact of the use phase—the absolute values refer to the impact per unit of reference flow of scenario 1 (scenario definition in Table 5). This value is set as a benchmark of 100%. Potential impact reductions of the respective scenarios can be derived accordingly.

benchmark of 100%. Potential impact reductions (or promotions) of the respective scenarios can be derived accordingly.

As anticipated, the generation of electricity dominates the environmental impact of the use phase for each scenario by far. In fact, solely in the EP impact category, the provision of the water for the chemical reaction shows a noticeable impact. Interestingly, the decarbonization of the energy system triggers an impact reduction potential several orders of magnitude larger than the technological development and thus the efficiency increase of the plant operation as can be seen from the impact reductions between scenarios 1 and 2 and scenarios 2 and 3, respectively. The further impact reduction potential of the operation due to the decreased energy demand of the plant in the future seems limited.

The relative share of each electricity source from the remaining environmental impact in scenarios 2 and 3 for each electricity source remains the same, as the electricity mix in both scenarios is the same (Table 3). Solely the absolute impact in scenario 3 is reduced due to the decreased energy demand of the plant. Therefore, the origin of the environmental impact for scenarios 2 and 3 is discussed collectively. The discussion is made exemplarily by reference to the GWP 100 and ADP. The impact from the electricity generation from PV (rooftop and open field combined) is significantly larger than the impact from wind (onshore and offshore combined). Electricity generation from PV rooftop almost causes half of the remaining impact in scenarios 2 and 3 followed by PV open field, wind onshore, and least impact from wind offshore. Anon, a significant increase in the ADP can be observed underlying the same coherences as discussed earlier. From Figure 6, one might conclude that the electricity generation from PV rooftop causes by far the largest amount on the impact. Note that the left-hand side and the right-hand side of the figure underlie different scales.

The cause for the dominating share of the electricity generation from PV is polydimensional. At the assumed plant location, the electricity generation from PV is less efficient than the one from wind. Hence, a large number of PV modules are required to meet the energy demand of the plant. Furthermore, the assembly of solar PV cells is primarily taking place in China. This gives rise to emissions due to the transport chain. Furthermore, the Chinese electricity grid heavily depends on fossil fuels causing a heavy ecological backpack for the PV modules.[34] Wind turbines on the other hand are primarily fabricated locally and therefore require less transportation and benefit from the advancing defossilization of the German electricity mix.

In order to assess further impact reduction potentials of especially the future development scenarios, the prospective LCA aspect needs to be incorporated more comprehensively for the background system such as a more detailed model of the electricity producing datasets in a completely defossilized energy system.

With the share of each electricity source from the electricity mix in scenarios 2 and 3 being approximately the same, it can be concluded that the operation of the plant at locations with large shares of offshore wind electricity would be most beneficial regarding the GWP 100.

4.3. Construction Phase

Figure 7 shows the potential environmental impacts of the construction phase for the SoA plant and the technological development on the system level. Anon, the SoA case is taken as benchmark, with the given respective absolute impact values of the system construction. As can be observed, for all impact categories, the construction of the electrolyzer stack and the PE dominate the environmental impact.

The reason for the dominating share of the two components is the requirement of precious and critical metals for both components. The stack comprises a large amount of titanium, platinum, and iridium as base material for the BPPs, the PTLs, and the catalysts (Table 7). The PE require a large amount of copper. The main reduction potentials for the future development scenario originate from the stack for all analyzed impact categories.

The share of the PE even increases in every category. This is due to the fact that the amount of required PE remains the same for both cases (22 units required for a 5 MW plant) while

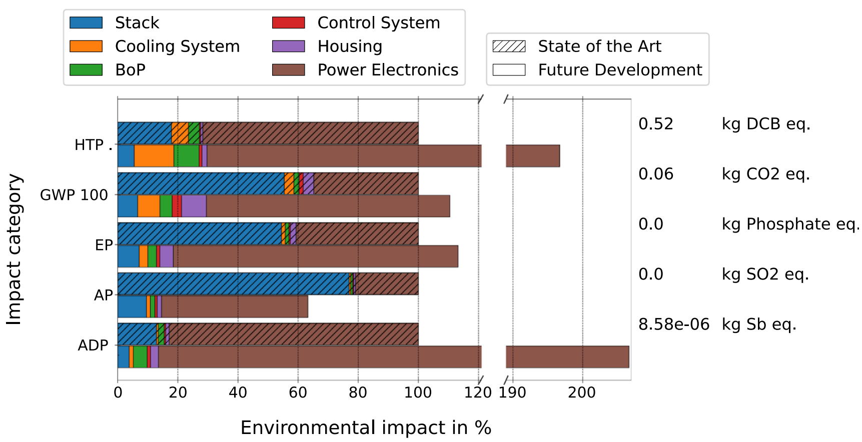

Figure 7. Environmental impacts of the construction phase on system level—The absolute values refer to the impact of the construction per unit of reference flow of the state-of-the-art (SoA) plant. This value is set as a benchmark of 100%. Potential impact reductions (or promotions) of the respective scenarios can be derived accordingly.

the material demand for the other components decreases. Strikingly, the impact in the categories EP, GWP ADP, and HTP increases for the future development case. This originates from the significantly lower load factor of the future case (compare 8000 FLH for SoA and 3235 FLH for future development) yielding a lower amount of produced hydrogen. Furthermore, no reductions in the material demand for the PE are assumed for their future construction. Consequently, this causes a larger impact per unit of reference flow for those categories, where the PE dominates the impact. It can be concluded that this is a serious data gap in the environmental assessment. In ecoinvent 3.8, only one single dataset of an inverter is considered. For LCA practitioners assessing a multi MW PEMWE plant, a considerate number of separate units of this 500 kW PE datasets would be required. This would severely overestimate the potential environmental impacts of the plant. Therefore, datasets representing units in the order of several 10 MW would be of great benefit not only for the environmental assessment of water electrolysis but also of other large-scale electricity-based processes, especially in the context of the electrification of industrial sectors.

The stack on the other hand dominates the impacts for three of the four analyzed impact categories in the SoA case. Therefore, a further analysis on the origins of these impacts is conducted. **Figure 8** shows the impacts of the stack construction per unit of reference flow. Once more, the SoA case is defined as benchmark at 100% with the given values for stack construction for the respective impact categories. It is evident that the CCM, the Bipolar Plate (BPP), and the porous transport layer (PTL) on the anode side dominate the impact of the stack by far for all analyzed impact categories. This is due to the requirement of platinum and iridium for the CCM as catalyst materials, the platinum coating and titanium as base material for the BPPs, and the iridium coating and titanium as base material for the PTLs on the anode side. Hence, these three components show the largest potential for impact reductions. For the BPPs, the thickness is drastically reduced (Table 2) yielding a dramatic reduction of the titanium demand per stack in the future development case. Similarly, the catalyst loadings on the CCM of platinum and iridium are reduced significantly (Table 2). As for the PTLs on the anode side, it is expected that the iridium coating will no longer be necessary along with a reduction of their thickness (Table 2). The share of the current collectors especially on the ADP and HTP increases significantly in the future development case. This is due to the increased active cell area in the future development case (the current collectors cover the complete active area at both ends of the stack, Figure S1 and S2, Supporting Information), while the thickness of the component remains the same. For this reason, the copper demand for the current collector increases significantly, yielding a larger impact of the component. Due to the fact that the CCM dominates the impacts of the stack for all categories, a closer investigation of the origins seems suggestive.

Figure 9 gives the environmental impacts of the CCM production. Once more, the SoA impacts are taken as benchmark with the given values for the impacts of the CCM production. As can be seen, the anode ink dominates the environmental impact for every impact category with shares in the order of 83%. The remaining impacts are caused by the cathode ink, whereas the membrane is negligible with shares no larger than 0.55%. Interestingly, the shares of each component are extremely similar for every analyzed impact category. This is due to the fact that the bulk of the impacts originate from the catalyst materials iridium and platinum. The ecoinvent database does not provide a separate dataset for iridium. However, iridium is a side product of platinum mining, and the supply is closely related to the platinum production. For these reasons, iridium is approximated by the ecoinvent platinum dataset, resulting in the observed phenomenon.

In the future development case, the overall impact of the CCM can be reduced by about 88% for every analyzed impact category. The anode ink still remains dominant with a share in the order of 66% is, however, slightly reduced. The membrane is also negligible in this case, with shares no larger than 0.61% for the analyzed impact categories. In the future development case, the total catalyst requirement can be reduced dramatically (Table 2). Anon, the same phenomenon of extremely similar shares for the respective components can be observed.

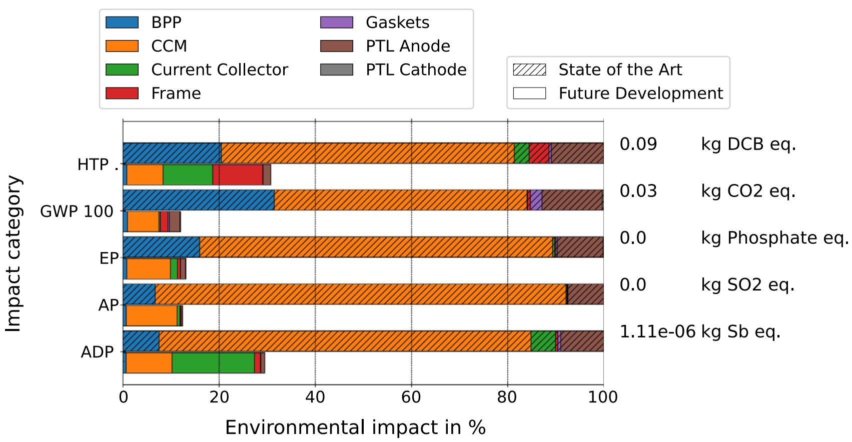

Figure 8. Environmental impacts of the construction phase on stack level—The absolute values refer to the impact of the construction per unit of reference flow of the state-of-the-art (SoA) plant. This value is set as a benchmark of 100%. Potential impact reductions of the respective scenarios can be derived accordingly.

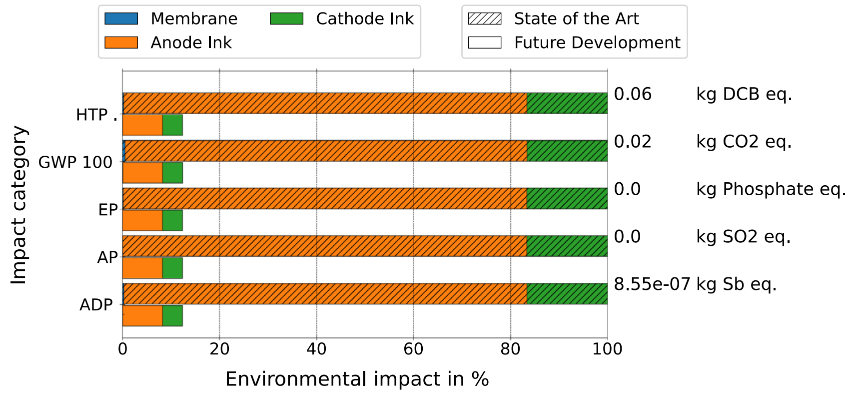

Figure 9. Environmental impacts of the construction phase on CCM level—The absolute values refer to the impact of the construction per unit of reference flow of the state-of-the-art (SoA) plant. This value is set as a benchmark of 100%. Potential impact reductions of the respective scenarios can be derived accordingly.

4.4. Sensitivity Analysis

As previously stated, the environmental impacts of the future development scenario, especially the ones of the construction phase, depend on the load factor of the plant. For this reason, an senstitivity analysis (SA) regarding the FLH operation of the plant is conducted. With an increasing load factor, more hydrogen can be produced in the plant lifetime, which affects the environmental impact per functional unit positively. Simultaneously, due to the increased operating hours, the stack reaches its EoL sooner, giving rise to additional component replacement. For the future development plant electrolyzer, the stack does not require any replacement below 6000 FLH. **Figure 10**a shows the environmental impacts of the overall plant operation depending on the FLH. Several scenarios were implemented with subsequently increasing FLH starting from 2000 h of full load operation, including the future development case at 3235 h of full load operation (Table 3).

As can be seen, the potential impacts in every analyzed impact category decrease with increasing FLH. An exemplary discussion of the results is given on the basis of the GWP. An overall reduction of the GWP of about 2.3% can be observed from the 2000 FLH case to the 8000 FLH case. Furthermore, it can be deduced that the impact does not decrease linearly with increasing FLH. The largest reduction of 1.21% occurs from 2000 FLH to 3235 FLH. The following FLH increases generate significantly lower reductions in the order of 0.5%. As anticipated, the absolute impact of the operational phase does not change with varying FLH. The absolute impact as well as the share of the construction phase, however, decrease with increasing FLH. A similar observation can be made for the EoL, however, on a significantly lower scale. The same reasoning can be deduced for the other analyzed impact categories, however, each on their respective scale.

Figure 10b gives the results of the SA regarding the FLH of the construction phase for the 2000 FLH and 8000 FLH cases. Anon, the results of the 2000 FLH case are taken as benchmark. The results for the construction phase confirm the previously observed impact reductions with increasing FLH. As can be seen, the PE dominate the impacts for all analyzed impact categories for both scenarios by far. The impacts of the other system components are reduced accordingly with increasing FLH.

As the PEMWE technology is comparatively young, and long-term operation data of large-scale plants is scarce, the lifetime of the electrolyzer stacks cannot be thoroughly established. Thus, assertions whether several stack replacements during the plant lifetime, one replacement or no replacement at all, are required cannot be cleared conclusively. Simultaneously, as observed earlier, the stack causes a significant share on the environmental impact for the plant construction yielding possibly not insignificant contributions to the impact. For this reason, a separate SA with a reduction of the stack lifetime to 20 000 h is conducted. **Figure 11** shows the results of the SA regarding the reduced stack lifetime for every scenario. Figure 11a shows the relative change of the impact for every analyzed impact category of scenario 1 when the stack lifetime is reduced to 20 000 h. It can be observed that the impact of the overall system solely shows a considerable sensitivity toward the stack lifetime in the impact categories AP, ADP, and HTP. Due to the decreased lifetime, the electrolyzer stacks need to be replaced 7 times during the plant lifetime yielding a total of 16 stacks over the complete system lifetime. This affects the resource demand for the plant construction and hence the respective impact categories. When exclusively assessing the plant construction, the sensitivity toward the stack lifetime is more prominent (Figure 11b) and can be observed for every impact category.

The SA for the overall impact and the one for system construction of scenario 2 are given in Figure 11c,d, respectively. Anon the relative change of the impact on life cycle level when the stack lifetime is reduced to 20 000 h is given in Figure 11c. As scenario 1 and scenario 2 both employ the SoA electrolyzer plant, the sensitivity toward the stack lifetime is similar. Due to the reduced full load operation in the completely decarbonized energy system, the stack solely needs to be replaced twice, yielding a total of 6 stacks over the complete system lifetime. Interestingly, the sensitivity of the ADP decreases and is essentially not existing in scenario 2. As the ADP in scenario 2 is significantly larger (Figure 5) along with the lower total amount of stacks, the additional resource demand for the stack replacement does not predominate in scenario 2. Anon, the sensitivity for the system

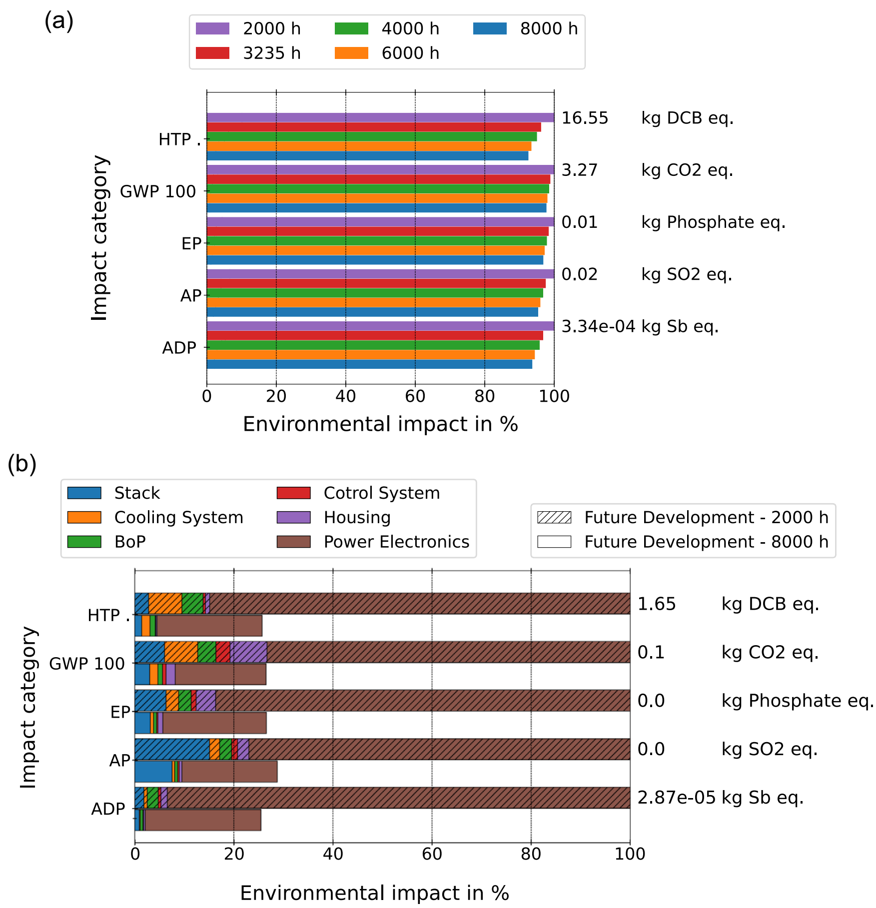

Figure 10. Results of the sensitivity analysis regarding the annual full load hours. a) Environmental impact on life cycle level. The absolute values refer to the impact per unit of reference flow for the case of 2000 h full load operation. This value is set as a benchmark of 100%. Potential impact reductions of the respective scenarios can be derived accordingly; b) environmental impact of the construction phase on system level. The absolute values refer to the impact of the construction per unit of reference flow case of 2000 h full load operation. This value is set as a benchmark of 100%. Potential impact reductions of the respective scenarios can be derived accordingly.

construction is more dominant, however, to a lesser extent than in scenario 1 due to the lower total amount of required stacks. The SA for the overall impact on life cycle level and the one for the system construction of scenario 3 are given in Figure 11e,f, respectively. As can be observed, the sensitivity in scenario 3 is significantly lower than for scenarios 1 and 2. This is due to the reduced material demand for the stack construction in the future along with the increased stack scaling. With the reduced stack lifetime, the stack needs to be replaced twice in scenario 3 yielding a total of 3 stacks over the complete system lifetime. Due to the lower number of required stacks along with the reduced material demand for the stack construction, the resource demand for the stack replacement decreases. When solely assessing the system construction, the sensitivity anon becomes more evident, however, to a lower extent as in scenarios 1 and 2. It can be concluded that the sensitivity of the overall impact per unit of reference flow regarding the stack lifetime is marginal and diminishes further in the future. In absolute terms, however, the stack lifetime and thereby the required stack replacements during the system lifetime does influence especially the resource demand as the material demand increases significantly with increasing stack replacements. In the future, this might eminently influence the availability of critical materials such as iridium.

5. Conclusion and Outlook

This study presented a detailed bottom-up cradle-to-grave LCA of a 5 MW PEMWE plant based on comprehensive electrochemical modeling of the system in consideration of crucial boundary conditions such as the cell degradation and the transformation of the underlying energy system.

Since the climate change boundary has been identified as core boundary, the results were discussed in detail in regard to the GWP 100. Consequently, a 5 MW SoA PEMWE plant causes a GWP 100 impact of 34 kg CO_2 eq. kg H_2^{-1}, while a shift to a fully decarbonized operation reduces the impact by 89%. A technological development of the plant reduces the potential impact by another 9%. Thus, the operation phase causes the largest share on the environmental impact while simultaneously posing the greatest reduction potential. The remaining environmental

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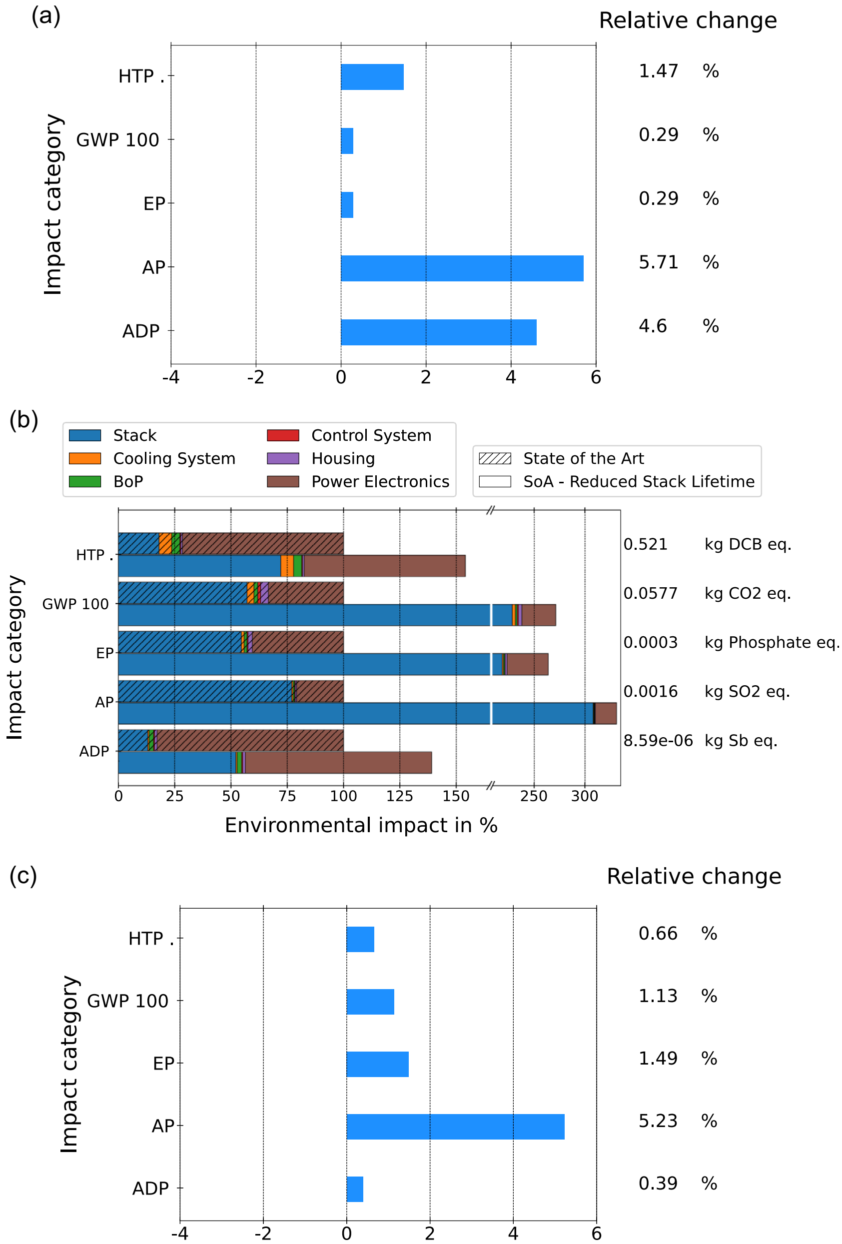

Figure 11. Results of the sensitivity analysis regarding the stack lifetime. a) Relative change of the environmental impact on life cycle level for scenario 1 when the stack lifetime is reduced from 80 000 to 20 000 h; b) Environmental impact of the construction phase on system level for scenario 1. The absolute values refer to the impact per unit of reference flow for the case of 80 000 h stack lifetime. This value is set as a benchmark of 100%. Potential impact promotions of the sensitivity analysis can be derived accordingly; c) relative change of the environmental impact on life cycle level for scenario 2 when the stack lifetime is reduced from 80 000 to 20 000 h; d) environmental impact of the construction phase on system level for scenario 2. The absolute values refer to the impact per unit of reference flow for the case of 80 000 h stack lifetime. This value is set as a benchmark of 100%. Potential impact promotions of the sensitivity analysis can be derived accordingly; e) relative change of the environmental impact on life cycle level for scenario 1 when the stack lifetime is reduced from 100 000 to 20 000 h; f) environmental impact of the construction phase on system level for scenario 3. The absolute values refer to the impact per unit of reference flow for the case of 80 000 h stack lifetime. This value is set as a benchmark of 100%. Potential impact reductions of the sensitivity analysis can be derived accordingly.

impacts still originate from the electricity generation, whereas solar PV has been identified as key driver of the impact. Thus, operation at locations with a large share of wind-based electricity can reduce the impact even further. Further impact reductions can be anticipated in a completely defossilized energy system. This further impact reduction potential stems from the defossilization of the prospective background system. In order to pinpoint the further reduction potentials in a detailed manner, the prospective transformation of the underlying background system needs to be included in the LCA model.

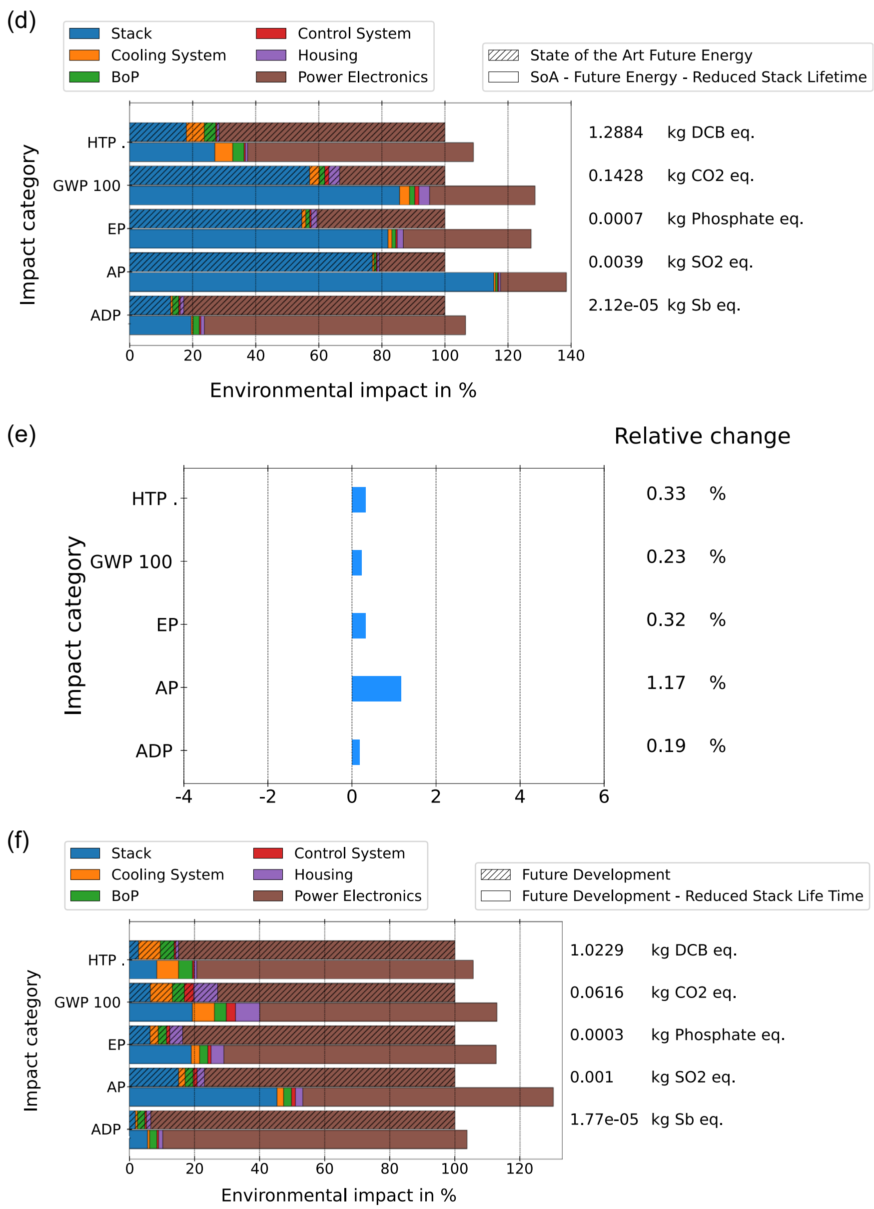

Figure 11. Continued.

When benchmarking the results for the production of green hydrogen against literature values for the production of gray and blue hydrogen from SMR, the green hydrogen production from completely decarbonized electricity outperforms gray hydrogen by several orders of magnitude. The comparison of green hydrogen with blue hydrogen shows that the latter can only outperform green hydrogen with best-case assumptions for the methane emission and carbon capture rates, respectively. For accurate assertions, however, a harmonization of the results regarding the scope, methodology, and technological boundary conditions is required, which is out of the scope of this study.

The detailed LCA model from a process engineering perspective allowed deep insights into the environmental impacts of the construction of the plant. The tracking of the environmental impact over the descriptive system layers facilitated the identification of the electrolyzer stack and especially the anode side catalyst material iridium as a hotspot. The impact assessment category ADP, however, lacks characterization for iridium and other rare earth elements. Thus, in order to further pinpoint the hotspots more accurately, alternative methods for the quantification of the resource demand, such as the cumulative exergy consumption (CExC), need to be implemented.

The technological development of the plant is regarded as central measure in order to implement a low impact hydrogen economy, as it provides not only a means for significant reduction of the energy demand during operation but also a dramatic reduction of the material demand for the construction of the plant, especially of critical and expensive materials such as platinum, iridium, and titanium.

Furthermore, the analyses have shown that the load factor of the plant affects the potential environmental impact. The larger the load factor, the more hydrogen can be produced during the system lifetime, which decreases the environmental impact per functional unit. The lifetime of the electrolyzer stacks and thus the required number of stack replacements in the complete lifetime of the system affect the overall impact per unit of reference flow only marginally and diminishes further in the future. Note, that the absolute impact, especially for the resource demand for the plant construction, does increase with the stack replacement.

Additionally, the study reveals that further investigations of large-scale PE are crucial in order to make valid assertions on the environmental impact of hydrogen systems and other electricity-based energy systems. This becomes even more evident for the scale-up of plants. Therefore, datasets representing units in the order of several 10 MW would be of great benefit not only for the environmental assessment of water electrolysis but also of other large-scale electricity-based processes, especially in the context of the electrification of industrial sectors.

In order to assess the environmental impact of the hydrogen supply in a complete hydrogen economy, in which the total hydrogen demand is supplied completely by water electrolysis, the LCA model at hand has to be scaled-up to several 100 MW and comprehended by models for the hydrogen supply via alkaline water electrolysis and high-temperature electrolysis at similar scale.

Furthermore, the scaled-up models for the respective hydrogen production technologies can then be combined with LCA models for the conversion of hydrogen to, e.g., methanol, ammonia, or e-fuels in order to assess the potential impacts of complete PtX process chains to depict a fully implemented hydrogen economy. Likewise, in order to distinctively relate the potential environmental impacts of a hydrogen economy to the concept of planetary boundaries, an absolute LCA can be conducted.[35–37] For an even more detailed identification of irreversibilities in the life cycle of hydrogen applications, exergy-based LCAs are recommended.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors declare no conflict of interest.

Author Contributions

J.G.M.: Conduct of the study, elaboration and implementation of the LCA model, processing of the results, conduct of the results' interpretation, preparation of the manuscript, preparation of the supporting information, and approval of the final manuscript; F.P.: implementation of the energy system model, preparation of the manuscript, and approval of the final manuscript; P.B.: processing of the results and approval of the final manuscript; M.B.: LCI of the catalyst ink production and approval of the final manuscript; B.B.: validation of the electrochemical PEMWE model, validation of the technical system data, validation of the supporting information, and approval of the final manuscript; R.H.R.: validation of the electrochemical PEMWE model, validation of the technical system data, preparation of the manuscript, and approval of the final manuscript; and C.M.: supervision of the study, preparation of the manuscript, validation of the LCA model, and approval of the final manuscript.

Data Availability Statement

The data that support the findings of this study are available in the supplementary material of this article.

Keywords

environmental impacts, hydrogen, life cycle assessment, polymer exchange membrane, water electrolysis

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