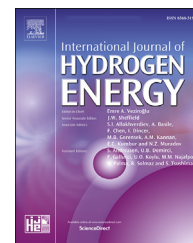


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Renewable hydrogen production: A techno-economic comparison of photoelectrochemical cells and photovoltaic-electrolysis

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HIGHLIGHTS

- Photoelectrochemical (PEC) cells.
- Techno-economic analysis.
- Comparison PEC system with conventional water electrolysis (PV-E).
- Potential techno-economic benefits of PEC over PV-E are uncertain and limited.

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ABSTRACT

The present paper reports a techno-economic analysis of two solar assisted hydrogen production technologies: a photoelectrochemical (PEC) system and its major competitor, a photovoltaic system connected to a conventional water electrolyzer (PV-E system). A comparison between these two types was performed to identify the more promising technology based on the levelized cost of hydrogen (LCOH). The technical evaluation was carried out by considering proven designs and materials for the PV-E system, and a conceptually design for the PEC system extrapolated to future, commercial scale.

The LCOH for the off-grid PV-E system was found to be 6.22 \$/kg_{H2}, with a solar to hydrogen efficiency of 10.9%. For the PEC system, with a similar efficiency of 10%, the LCOH was calculated to be much higher, namely 8.43 \$/kg_{H2}. A sensitivity analysis reveals a great uncertainty in the LCOH of the prospective PEC system. This implies that much effort would be needed for this technology to become competitive on the market.

Therefore we conclude that the potential techno-economic benefits that PEC systems offer over PV-E are uncertain, and even in the best case, limited. While research into photoelectrochemical cells remains of interest, it presents a poor case for dedicated investment in the technology's development and scale-up.

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Introduction

To meet the rising global energy demand and simultaneously reduce the greenhouse gas emissions as well as the dependence on fossil fuels, the development of sustainable energy sources is essential. Hydrogen is considered a future energy carrier since it has a high gravimetric energy density and good storage possibilities. However, at present most of the hydrogen is produced by steam reforming of natural gas or coal, which causes the emission of large amounts of carbon dioxide. Water electrolysis represents an alternative technology, which currently delivers 4% of the global hydrogen supply [1]. When coupled with a renewable energy source like solar or wind, this technology can be treated as a sustainable process. By doing so it is also able to meet the challenges related to the intermittent nature of e.g. sunlight, through decoupling energy generation and consumption.

An alternative that has attracted much interest over the last few years is photoelectrochemical (PEC) hydrogen production, which directly converts solar radiation to hydrogen. Through the absorption of solar photons in a semiconductor material and the use of electrocatalysts, water is split into hydrogen and oxygen, described by two half-reactions, namely $4\text{H}^+ + 4\text{e}^- \rightarrow 2\text{H}_2$ (Hydrogen evolution reaction, HER) and $2\text{H}_2\text{O} + 4\text{h}^+ \rightarrow \text{O}_2 + 4\text{H}^+$ (Oxygen evolution reaction, OER).

While the focus of our paper is on photoelectrochemical hydrogen production, we note that photoelectrochemistry has broader applications in CO_2 activation and solar fuels production [2]. This paper compares the economics as well as the performance of a PEC system and an off-grid solar-driven water electrolysis plant (PV-E). These standalone systems are designed for a production rate of $10 \text{ t}_{\text{H}_2}/\text{day}$ and are exposed to similar conditions. For the technical investigation, we analyzed different possible PEC designs to find a promising concept which can serve as a basis for our analysis. Photovoltaic (PV) systems and electrolyzers are already available on the market and therefore a selection of existing technologies is carried out. Having the same products while using the same input parameters, the economic comparison between the technologies is mainly influenced by their system costs. The overall results are expressed by the levelized cost of hydrogen (LCOH).

Since the pioneering work of Fujishima and Honda [3] using a TiO_2 photo-electrode coupled with a platinum cathode to describe the PEC water splitting process nearly five decades ago, extensive efforts have been made to construct efficient photocatalyst systems for solar energy utilization. Most literature focuses on the selection of a suitable material, since it strongly determines the system efficiency; especially the choice for the photoelectrode and for catalysts is of importance [4]. In addition, some laboratory-scale experiments have been carried out to improve the solar-to-hydrogen efficiency [5]. A summary of the latest developments within research on photoelectrochemical cells can be found in Ref. [6,7]. Most literature that focuses on economic evaluation does usually not compare different technologies and therefore concentrates either on PV-E or PEC systems [8–12]. For example, a

detailed techno-economic analysis by the US Department of Energy (DOE), which represents a key reference of the present analysis, gives a detailed overview over four different types of PEC systems [9].

Another key paper is by Shaner et al., who compared two different PEC systems and two types of PV-E systems regarding their technical and economic viability. The results show a lower LCOH for the PEC system than for the off-grid PV-electrolyzer. However, the cost calculation of some major components of the PEC system were based on commercial PV parts and commercially available electrolyzers, which can be quite different from a real PEC system in which both parts are integrated in one device. In addition, strong cost reduction has occurred since their publication, especially for the PV panels, which makes new research necessary.

Despite intense and promising research during the last years on PEC technology, no system is yet commercially available. The present paper will analyse if, and under what conditions, PEC devices can outcomplete solar hydrogen production through PV-electrolysis. It builds on the research of [9,13], taking into account new developments and details within these technologies.

Methodology

The assessment of the hydrogen production technologies includes a technical and an economic evaluation. The latter is based on the results from the technical system analysis, which was carried out by performing a broad review considering relevant literature published from 2014 to the present time. The results are described in detail in section [Technical evaluation](#).

To compare the economic appeal of the two hydrogen production technologies, the levelized cost of hydrogen (LCOH) in \$ per kg was calculated. It reveals the price of hydrogen which the system needs to reach, in order to achieve a desired return on investment. The LCOH includes investment expenses as well as revenues and expenditures during the plant's lifetime, discounted to a reference date. It is calculated by dividing the present value of all expenses by the present value of hydrogen generation, resulting in

$$\text{LCOH} = I_0 + \frac{\sum_{t=0}^n \frac{OM_t + F_t}{(1+r)^t}}{\sum_{t=0}^n \frac{H_t}{(1+r)^t}}, \quad (1)$$

Where I_0 represents the initial investment in year t , OM_t the annual costs for operation and maintenance, F_t the annual fuel costs, H_t the hydrogen production (kg_{H_2}) and r the real discount rate [14].

The total system costs were calculated using a bottom-up costing method. First, a selection of the relevant components and cost parameters was carried out. Subsequently, the total project costs were calculated. For both technologies, the capital expenditures C_{CAPEX} are comprised of the module itself C_{module} and the balance of system (BoS) costs C_{BoS} in the form of

$$C_{\text{CAPEX}} = C_{\text{module}} + C_{\text{BoS}}. \quad (2)$$

BoS costs can then be divided into a hard- and soft-BoS share. The former includes wiring, mounting, the inverter and land

acquisition, while the latter is composed of non-material costs such as permits and installation. Due to economies of scale, the BoS costs vary with the size of the plant and are also dependent on the maturity of the observed technology.

Table 1 presents a summary of the baseline assumptions for the economic analysis. The production rate of the systems was set to 10 t_{H₂}/day, a scale similar to other techno-economic reports discussing photoelectrochemical water splitting [9,13] and typical of the today's project size, and a scale at which the benefits of scale-up have leveled off, beyond which point cost reductions should come from mass manufacturing of MW-sized units. The scope of the analysis is 20 years, which is a common period for techno-economic analyses [9,10,13,15,16]. A longer lifetime might be interesting, too, since some elements like PV panels are expected to have a longer lifespan (25 years [17]). However, this will increase uncertainties about costs of other system components. The geographical location has a great impact on the economic viability of the system and is adopted from Ref. [9], who assumed the location to be in the USA, in Daggett, California. The site is used for solar measurements and provides an average daily irradiance of 6.19 kW h/m²/day. The operating capacity factor takes into account planned and unplanned outages and represents the actual work performed in relation to the maximum work which can theoretically be performed. A factor of 90% is chosen, which is similar to the value in Ref. [9]. All economic conjectures are drawn upon values from the U.S market and refer to the year 2017, and it is assumed that the investment occurs within a one-year construction time period. The installation costs are assumed to be 20% of the capital costs, which is a value similar to Ref. [9,11]. It is assumed that these costs are the same for both systems. The installation of the PV-E systems requires more cabling and the installation of the electrolyzers. The PEC system on the other hand requires more piping and in addition the installation of the compressors. Again, for engineering and design, the same value is used for both systems, namely 5% of the capital costs which is in the same range as the assumptions made in Ref. [9,11]. In addition, the production of high purity oxygen by-product is vented to the atmosphere and no cost credit is taken into account.

Sensitivity analysis. Since PEC systems are not yet commercialized, the costs estimated in the economic analysis are subject to various assumptions and to a high degree of

uncertainty. Therefore, a sensitivity analysis is carried out by including the components and parameters with the greatest influence on the total costs. Generally, it can be assumed that costs for the technologies will decrease over time due to improvements in technology, new developments and a growing demand on hydrogen. In addition, for the analysis of the PV module, learning curves are used to estimate further potential.

Component-level technical analysis and cost assessment

This section provides the basis for our comparison, starting with an outline over the chosen system designs and the selected components. The second part covers the economic evaluation of the two technologies and this forms the starting point for the calculation of the LCOH.

Technical evaluation

To begin with, a technical analysis was carried out on the basis of a literature study and state of the art technology. For the PV-E system, approved designs and materials were studied. The PEC technology, on the other hand, needs to be examined more closely since a reliable system is not yet available on the market; for example, for some components a better and more stable material needs to be found.

To describe the performance of the technologies, the solar to hydrogen efficiency is used. This parameter is defined as the chemical energy of the produced hydrogen divided by the solar energy input in the form of

$$\eta_{\text{STH}} = \frac{m_{\text{H}_2} \Delta G}{P_s A_e} \quad (3)$$

where m_{H_2} represents the hydrogen production rate (kg/s), ΔG is the change in Gibbs free energy per mole of H₂ (at 25 °C $\Delta G = 237$ kJ/mol), P_s the solar energy input (kWh/m²) and A_e the illuminated photoelectrode area (cm²) [19].

The PV-E system

The components of the PV-E system were chosen by considering technical properties and examining current prices for photovoltaic modules and electrolyzers. Since a PV-E system consists of two separate parts, namely the photovoltaic module and the electrolyzer, they are outlined separately. Electrolyzers can produce pressurized H₂ at 30 bar and therefore no compressors need to be added to the overall system [20]. Using these results, an optimization of the PV-E system was performed, which reveals an ideal weighting between the two devices.

Photovoltaic-system. The selection of the photovoltaic system is based on literature analysis and on analyzing the current PV market, which is currently dominated by crystalline silicon (c-Si) PV cells with commercial efficiencies of up to around 24% [21]. Silicon is the current standard material used in industry because of its relatively low cost as well as good efficiency, steadiness and durability. Since this type has some drawbacks, such as an energy intensive production and a relatively low theoretical efficiency [22], other types like

Table 1 – Summary of the assumptions required to carry out the economic analysis for the considered PEC and PV-E systems.

Parameter	Unit	Value	Source
Hydrogen production rate	t _{H₂} /d	10	[9,11,13]
Economic lifetime	Years	20	[9,10,13,15,16]
Construction period	Years	1	[9]
Operating capacity factor	%	90	[9]
Inflation rate	%	1.9	[9,13]
Real discount rate	%	12	[13]
Average labor rate for staff	\$/h	25	[18]
Land cost	\$/m ²	0.15	[9]
Average solar irradiance	kWh/m ² /d	6.19	[9,12]
Installation	% of hard BoS	20	[9,11]
Engineering and design	% of hard BoS	5	[9,11]

multi-junction solar cells or CdTe (Cadmium telluride) thin film panels were included in the analysis. However, most technologies are not yet commercially available or need a large scale-up. In addition, an increase in efficiency is often accompanied by higher costs, while cheaper technologies are frequently less efficient and lack durability [22]. Hence, in this research a crystalline silicon single-junction panel was chosen with an efficiency of 18%.

Electrolyzer. Compared to PV panels, the market for electrolyzers is relatively small and is developing more slowly. At present, the alkaline electrolyzer is the current standard technology on the market, and is considered to be technically mature [23]. With a moderate efficiency of 59–70% [23] and relatively low system costs in the range of 860–1240 \$/kW it is favoured in most industrial sectors [24]. Besides alkaline systems, the proton exchange membrane (PEM) electrolyzer represents another emerging technology with efficiencies up to 80–90% [25]. It is also commercially available but more expensive (around 1350–2200 \$/kW) and produced in lower quantities [24].

Alkaline electrolyzers have major issues with intermittent and fluctuating power sources, such as cross-diffusion of the product gases under low system loads, a slow start-up as well as a slow loading response [8,26,27]. Compared to alkaline systems, PEM water electrolysis is more suitable for the coupling with a PV system. Its flexibility to handle fluctuating input currents and the expectation of large cost reduction in the future will make it a good choice for a combined system [8,16,28,29].

Combined PV-E system. To match the output voltage of the PV system and the voltage of the electrolyzer at its design point, in general a DC-DC converter is needed. However, when using a PEM electrolyzer, a converter is not necessarily required [29], since the loss caused by non-optimal operation is expected to be the same as the loss due to the use of a DC-DC converter [13,28]. Therefore, a moderate efficiency for the electrolyzer of 61% is chosen, which is lower than the typical efficiencies of PEM electrolyzers in the range of 65–83% [30]. In addition, the electrolyzer does not require a transformer and rectifier, because the PV module delivers direct current.

Scaling the electrolyzer to the maximum power output of the PV plant results in a low capacity factor for the electrolyzer. Since the electrolyzer costs represent a considerable part of the overall costs, an optimization between the scale of the photovoltaic system and the electrolyzer unit was performed, to find an ideal balance between these two technologies. A detailed description of the optimization can be found in the Supporting Information.

Fig. 1 presents the resulting curve obtained by the optimization. It reveals an ideal operating point at which the area of the PV panels is designed for a maximal solar irradiance of $P_{S,design} = 800 \text{ W/m}^2$. This leads to an increase of the PV capacity by 4% and a reduction of the electrolyzer size by 11% compared to a design point at $P_{S,max} = 925 \text{ W/m}^2$. As a consequence, the capacity factor of the electrolyzer increases by 3 %-points, up to 31%.

The PEC system

There exist roughly 30 design alternatives for PEC water-splitting devices [11] with no clear favorite so far. This large amount of design possibilities makes it difficult to strictly

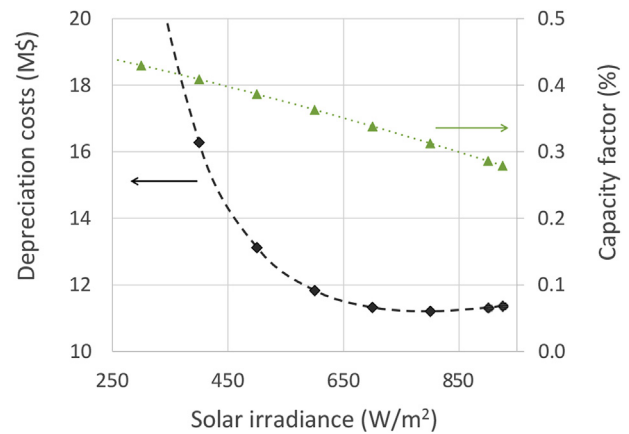


Fig. 1 – Resulting curves obtained by optimizing the ratio between the area of the PV panels and the electrolyzer units for the PV-E system. The upper bound of the solar irradiance was given by $P_{S,max} = 925 \text{ W/m}^2$. The dashed curve shows an optimal design point at around $P_{S,design} = 800 \text{ W/m}^2$, at which the total depreciation costs are lowest. The dotted curve shows the capacity factor of the electrolyzer.

separate the PEC system from PV-E systems, as it creates a seamless transition between these two technologies [5]. Therefore, a detailed technical analysis was carried out, starting with a selection of a specific PEC type, followed by a thorough assessment of the main components through analyzing essential properties, i. e. efficiency, lifetime and potential productivity. The selection of the components was mainly based on a detailed DOE-report by James et al., supplemented and adjusted by updated data amongst others found in Ref. [11,13].

Panel based design. Among the different design possibilities for PEC systems, a non-concentrated panel based layout was selected (similar to type 3 mentioned in the DOE report). A panel design is a more mature design choice compared to solar concentrator systems, which can increase the light intensity. It is similar to a PV panel and absorbs photons to generate electrons for the electrolysis. The electrodes are in direct contact with the electrolyte, generating oxygen gas at the anode and hydrogen at the cathode. The panels are most likely composed of a multi-junction photon absorber to provide sufficient voltage for the reactions. Another design possibility, frequently mentioned in literature, is a PEC system based on nano particles, which tends to be much cheaper [9]. However, an explosive gas mixture is created, which should be avoided due to safety issues and system complexity in terms of additional product separation. In addition, not much research has been done on this type and therefore the existing data is subject to high uncertainties. By comparison, the development in terms of technology readiness level (TRL) and efficiency as well as durability is more advanced for the panel based design [11,31]. Furthermore, more possible design configurations exist for this type and a broader material portfolio is available.

One liquid-solid-junction. In general, there exist three possible design configurations within the panel based type [4]. First, a zero liquid-solid-junction design, within which the photoactive part is not exposed to the corrosive environment caused by the electrolyte. Since this type of setup has more similarities with a PV-E system instead of an integrated PEC device, it is not further considered in this analysis. Second, a one liquid-solid-junction design, where one side of the photoelectrode is immersed into the electrolyte. Finally, a system with two-liquid-solid-junctions, where the photoactive material as well as an additional anode and cathode are submerged into the electrolyte.

In our work the second alternative was chosen, which is schematically shown in Fig. 2. One part of the solar panel must withstand electrochemical reactions and corrosion, while the other side is in contact with ambient air. To the best of our knowledge, so far a solar to hydrogen (STH) efficiency of 16.2% has been achieved by using this layout [31]. Compared to the two liquid-solid-junctions, the lifetime can be extended and the material selection is simplified, which makes it more likely for this configuration to become a stable low-cost system [4,11].

No external bias. Furthermore it was assumed that the system operates spontaneously and does therefore not require an external electrical bias.

Material selection. The choice of the photoactive material has a significant impact on the efficiency and the lifetime as well as the costs of the PEC system. The photoactive layer consists of a doped semiconductor which absorbs photons and therefore generates a charge separation. Most of the materials in literature are based on thin film technology [4,9–12,31]. For the production of hydrogen a voltage of approximately 1.65 V needs to be provided by the cell, to run the HER, OER and make up for additional losses (overpotential) [32]. Since a high output voltage is often accompanied by the ability to use only a small part of the solar spectrum, multi-junction cells are preferred. Triple-junction amorphous Si is one of the promising photoactive materials for PEC cells [4,10,12,33] and was chosen in this work. Other possible materials, e.g. GaAs/GaInP with efficiencies of more than 16.2%

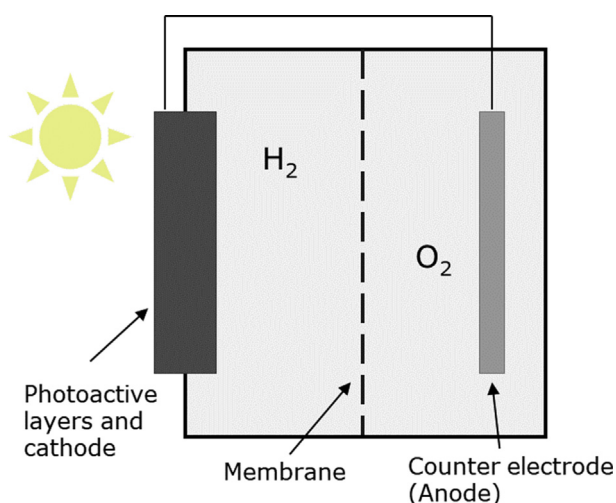


Fig. 2 – Schematic illustration of the selected PEC cell.

STH [34], were not considered any further since their costs are still too high. The assumed efficiencies for a-Si cell found in literature varied a lot depending on their source, with a resulting range of close to zero to 15% STH [11,35,36]. In this work we chose an efficiency of 10% which is assumed to represent a realistic value compared to the majority of the considered literature [4,9,10,12]. This is also in line with data found in Ref. [12], where the STH efficiency for PEC cells is assumed to be limited to 75–80% of efficiencies for PV cells. For the anode/counter electrode, which promotes the oxygen formation and can be directly attached to the housing of the PEC cell, there are various possible materials like stainless steel, RuO_x with Pt gauze or Nickel [11,12,31]. Most relevant literature is based on the latter, which is also chosen in this work. For the membrane we chose the same as in Ref. [11], which is an anion exchange membrane with the commercial name Nosepta[®], [11,37]. The area of the membrane is assumed to be 10% of the PV panel area [32].

Economic evaluation

Based on the results of the technical analysis, the following section summarizes the economic evaluation needed to calculate the levelized cost of hydrogen.

PV-E system

In Table 2 the specific parameters for the analyzed PV-E system are shown along with its capital expenses. A more detailed distribution of the cost components can be found in the Supporting Information in Table S1. The costs for the PV module, based on a crystalline silicon panel with an efficiency of 18%, were estimated to be $0.30 \text{ \$W}^{-1}$ [38]. The solar collection area was calculated by using Eq. (3) together with the efficiency of the overall PV-E system. The area of the whole PV-E plant is 4.07 times the PV surface area, including e.g. the electrolyzer and the control system. This factor was taken from Ref. [9], since we assumed the additional area to increase similar to the total plant area of the PEC system. In this analysis no inverter is included, which is already mentioned earlier while describing the technical analysis. For the PEM electrolyzer no transformer and rectifier is required since the

Table 2 – Summary of technical parameters and respective costs for the main components of the considered PV-E system.

	Value	Source
Photovoltaic system		
Efficiency	18%	[38]
Photovoltaic area	$4.8 \cdot 10^5 \text{ m}^2$	[38]
PV module	0.30 $\text{\$/W}$	
Mounting material	0.08 $\text{\$/W}$	[17]
Wiring	0.09 $\text{\$/W}$	[17]
Electrolysis system		
Efficiency	61%	[39]
Stack cost	0.40 $\text{\$/W}$	[39]
Hard BoS	0.375 $\text{\$/W}$	[39]
Combined PV-E system		
Efficiency	10.9%	
Process contingency	20% of direct costs	[9,11]
Other soft-BoS	5 $\text{\$/m}^2$	[17]

PV panels deliver direct current. The costs for the stack were estimated to be $0.40 \text{ \$/W}^{-1}$ with an efficiency of 61% [39]. The lifetime of the electrolyzer stack is estimated to be 7 years [13] and the replacement costs for the stack decrease every period, based on learning curves, and were assumed to be 75% of the initial costs after 7 years and 60% after 14 years, respectively. The PV module was assumed to last the whole lifetime of 20 years of the plant. Additional costs e.g. for permit and side preparation, are added with a factor of $5 \text{ \$/m}^2$ to the calculation which is in line with recent data from Ref. [17].

PEC system

Table 3 shows the technical parameters and capital expenses for the main components of a PEC system at commercial scale. In Table S2 a more detailed cost overview can be found. For the costs of the photoactive component $45 \text{ \$/m}^2$ was estimated. Although some previous reports worked with a more optimistic value of $15 \text{ \$/m}^2$ [9,11], a more pessimistic and, in our opinion, more realistic value was used for the calculation. More details can be found in the Supplementary Information. The costs for glass were estimated to be $10 \text{ \$/m}^2$. We assumed this value to be higher compared to PV systems ($5 \text{ \$/m}^2$ [13]), since the surface is not fully connected to the back side of the housing and therefore needs to be more rigid to give structure to the cell.

The membrane was included with a cost factor of $50 \text{ \$/m}^2$ [13] which is expected to decrease significantly when produced in large scale [9]. For the housing costs of $20 \text{ \$/m}^2$ were assumed to be realistic. Compared to PV systems ($\approx 5 \text{ \$/m}^2$) these costs are higher, since PEC cells set higher demands like a better resistance to the electrolyte as well as a greater stability for the membrane. This value resembles other assumptions in literature [9,11]. For the whole PEC module the resulting costs are $153.7 \text{ \$/m}^2$ which corresponds to approximately $1.01 \text{ \$/W}$. In addition to the module costs, a gas processing system comprising two-stage gas compressors [9,13], piping, condensers and intercooling, as well as water management and system controlling are included by using data published in the DOE analysis [9]. For the contingency a percentage of 30% of the uninstalled costs was estimated, since PEC systems represent a less mature technology compared to the PV-E system. It should be noted that this study does not take a costs credit for the by-product O_2 into account, which is generated during the reaction. Finally, the replacement of the PEC cell was expected to be performed every 7 years and the costs for a PEC cell were assumed to decrease alike the electrolyzer by applying learning curve theory.

Table 3 – Summary of technical parameters and respective costs for the considered PEC system.

	Value	Source
Efficiency	10%	[4,9,10,12]
PEC area	$5.3 * 10^5 \text{ m}^2$	
Module	$153.7 \text{ \$/m}^2$	
Hard-BoS	$46.0 \text{ \$/m}^2$	
Soft-BoS	$115.2 \text{ \$/m}^2$	
Process contingency	30% of direct costs	

Results and discussion

PV-E system

The techno-economic analysis of the photovoltaic-electrolysis system results in a LCOH of $6.22 \text{ \$/kg}_{\text{H}_2}$. Fig. 3 shows the breakdown of the overall costs; more details can be found in Table S1. The first 3 bars reveal the distribution of the costs for the PV-E system in $\text{\$/kg}_{\text{H}_2}$. For the first and second bar, the costs are broken down into the PV and electrolyzer part respectively, to show the ratio between these two parts. The costs for the electrolyzer are higher than the costs for the PV system, namely $3.92 \text{ \$/kg}_{\text{H}_2}$ compared to $2.30 \text{ \$/kg}_{\text{H}_2}$, respectively. This gap is even larger without optimizing the scale of these two plant components. Through optimization, more PV panels were added to decrease the number of electrolyzer units, which led to an increase in the capacity factor from 28% to 31%. Consequently, the area of the photovoltaic panel increased by 4% while the size of the electrolyzer section was reduced by 11%. It is likely that the BoS costs of the electrolyzer will experience a significant decline within the next few years since there is room for economies of scale and therefore the production volume can still be increased largely. The third bar reveals the overall system costs, showing that the module costs make up a large part of the costs.

To identify the potential of the PV-E system, a closer look is taken at future costs for the PV module and the electrolyzer unit. A possible decline of the PV module and hard-BoS costs of approximately 50% in 10 years is assumed by the ITRPV report [17]. For the future costs of the electrolyzer stack a reduction to $148 \text{ \$/kW}$ can be expected, adopted from Ref. [16]. When including these optimistic assumptions into the cost calculation, a possible LCOH of $3.76 \text{ \$/kg}_{\text{H}_2}$ can be achieved.

PEC system

The LCOH for the PEC system is calculated by $8.43 \text{ \$/kg}_{\text{H}_2}$. The results are summarized in Fig. 3, in the two bars on the right, and more detailed in Table S2. The first bar reveals the PEC module to be the main cost contributor, accounting for nearly half of the entire costs. This is followed by the soft-BoS costs, where the contingency costs have the biggest influence since the uncertainties are still quite high within this new technology. The bar on the right in Fig. 3 shows a cost breakdown for the PEC module by oneself. The membrane and the photoactive material have by far the biggest influence on the costs, with $1.50 \text{ \$/kg}_{\text{H}_2}$ and $1.35 \text{ \$/kg}_{\text{H}_2}$ respectively.

Therefore, these two components were included in a sensitivity analysis to show their impact on the overall costs. However, many of the remaining costs are also marked by uncertainty, since PEC cells are not yet commercially build. Therefore, the allocation within this cost block can vary to a certain extent and some module components can even have more impact than expected in this research. The results of the sensitivity analysis are presented in Fig. 4. For the membrane an optimistic value of $15 \text{ \$/m}^2$ is estimated which is similar to a value provided by Ref. [11,40]. The pessimistic value is assumed to be $300 \text{ \$/m}^2$ for a mass-produced membrane. The membrane represents a large factor of uncertainty, even

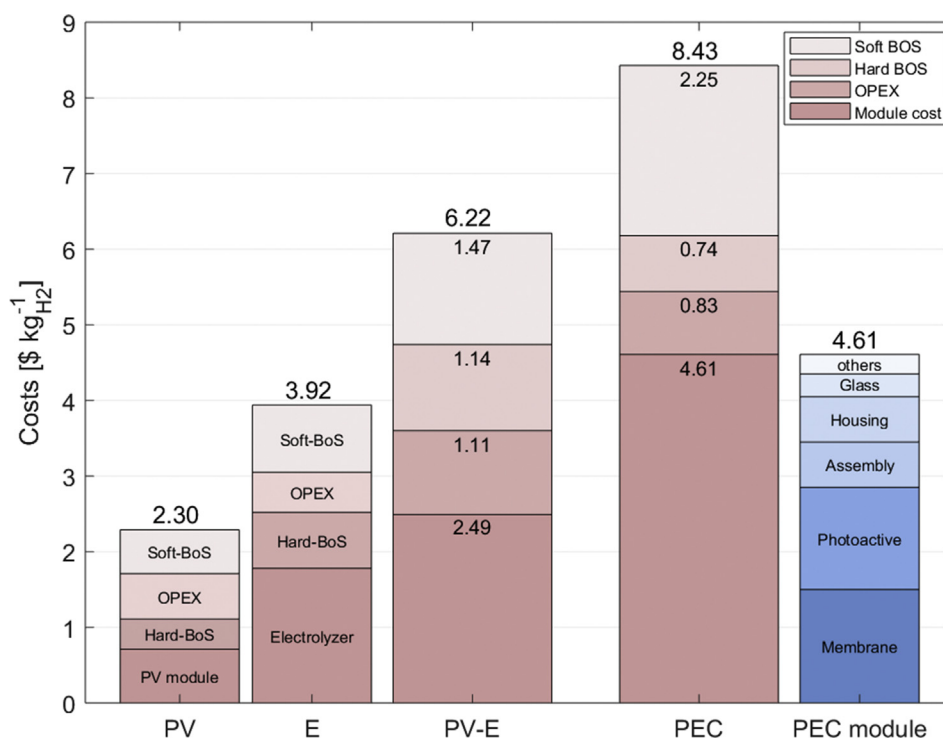


Fig. 3 – Breakdown of the costs for the photovoltaic system and the electrolyzer unit as well as the overall costs for the combined PV-E system and the integrated PEC system (brown bars), divided into the module costs, the OPEX as well as the hard- and soft-BoS costs, respectively. In addition, a detailed cost breakdown of the PEC module costs (blue bars). (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

though a strong decrease is possible through mass production [16]. It should be noted that it is still an ongoing challenge to find a suitable and stable membrane. In our PEC design, which is based on the work by Ref. [11], the selected membrane requires an acidic environment. Some earth-abundant catalysts, like in our case Nickel, are only stable in a neutral or alkaline environment. There are still challenges for the commercial implementation of the presented PEC design and there is a lot of ongoing research focusing on the development of stable membranes. For our techno-economic analysis, the choice of the parameters gives a good depiction of the still uncertain profitability of a PEC system.

Starting with an initial value of 45 \$/m² for the photoanode layer a high performance material, namely GaAs/GaNp, was

selected for the highest costs. Assuming mass production, the costs were calculated to be 393 \$/m² by using a simplified estimate with data found in Ref. [34,41]. For the optimistic scenario, 15 \$/m² were chosen, which was found in Ref. [11]. From today's view it is a major challenge to find high performance materials which can be competitive on the market.

The preceding analysis of the PEC cell was carried out by using a STH efficiency of 10%. The optimistic case was conducted with an increase of the efficiency to 16.2%, which is, to the best of our knowledge, to date the highest efficiency reached for a PEC cell and is achieved by Ref. [31] on laboratory scale. The pessimistic value was adopted by 5%. The resulting Fig. 4 shows a strong and non-linear correlation of the efficiency and the LCOH of the system. An increase of the cell

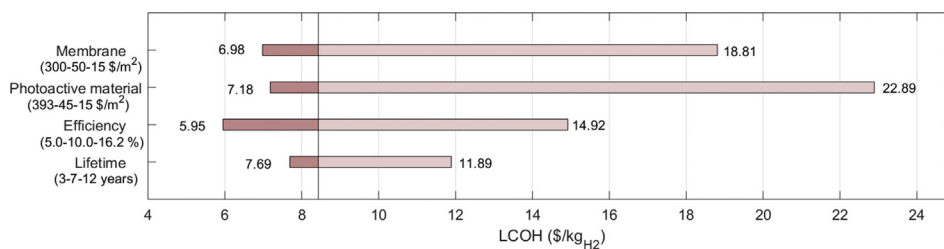


Fig. 4 – Sensitivity analysis for the PEC system on the basis of the costs for the membrane and the photoactive material as well as the efficiency and the lifetime of the whole plant. Each analysis represents the variation of a single parameter from the initial LCOH of 8.43 \$/kg_{H2} to a higher and lower value.

efficiency by 6%-points results in a decrease of approximately 25% of the overall costs. This indicates that high efficiencies are crucial for competitive PEC systems.

Another influential parameter is the lifetime of the PEC cell. The initial value is set to 7 years, which is similar to the stack of a PEM electrolyzer. This assumption is quite low compared to other components, since the degradation of the cell is high due to the presence of a corrosive electrolyte, even with the integration of a protective layer on top of the photoactive material. In addition, this value entails great uncertainty as there is no literature found which documents a duration of a PEC cell exceeding a few weeks. Nevertheless, other literature even suggest higher values for the lifetime [9,11,12]. The optimistic value was therefore chosen to be 12 years whereas for the pessimistic case 3 years was selected. Lifetime is important in order to achieve commercial success, but has a relatively small effect on the overall system costs, since it concerns mainly the cell component.

Comparison between PV-E and PEC

As shown in Fig. 3, the estimated LCOH is significantly higher for the PEC system compared to the PV-E system with 8.43 $\$/\text{kg}_{\text{H}_2}$ and 6.22 $\$/\text{kg}_{\text{H}_2}$ respectively. The PV-E module costs account only for 40% of the overall system costs compared to the PEC module which constitutes more than half of the overall costs. This can be explained mainly by additional components in the PEC device and more stringent requirements for the photoactive material. Another reason for the large influence of the PEC module on the overall costs is the relatively short lifetime of 7 years and complementarily the replacement costs, which applies also to the electrolyzer. The difference between the soft-BoS costs for both systems are, among others, the higher costs for contingency for the PEC system, which is due to greater uncertainties within this technology. The difference of the hard-BoS costs for the PEC and PV-E plant is because the PV-E system comprises two hard-BoS blocks, for the photovoltaic part and the electrolyzer. In addition, representing an integrated unit, less wiring material is needed for the PEC system.

In the present study we considered an off-grid PV-E system for the production of solar hydrogen. An advantage of this

system is, that it has the possibility of connecting to the grid, resulting in a significant increase in the capacity factor of the electrolyzer. An approximate calculation by using data provided in Ref. [13] reveals a LCOH of 4.17 $\$/\text{kg}_{\text{H}_2}$ for the grid connected device. It is important to stress that the produced hydrogen is then no more a solar hydrogen and not comparable to the PEC device, but shows the flexibility of the PV-E system.

The graph in Fig. 5 shows the resulting LCOH and its uncertainty for the PEC system. The latter was calculated by combining the results of the sensitivity analysis outlined in the previous sections. Since the different parameters influence each other, the resulting range for the hydrogen costs takes on a huge value. The figure elucidates the high uncertainty of the considered parameters and highlights the great range of the LCOH for the overall PEC system. For an optimistic case the LCOH of the PEC-system can go down to 2.51 $\$/\text{kg}_{\text{H}_2}$. A PV-E system, on the other hand, can reach a hydrogen cost of 3.76 $\$/\text{kg}_{\text{H}_2}$. However, for a pessimistic view the costs of the PEC system can be more than ten times higher than the considered LCOH of 8.43 $\$/\text{kg}_{\text{H}_2}$. The probability that such high costs will incur is, as shown by the graph, almost zero. Still, the results reveal a huge range for the LCOH and since the PEC system is not yet mass produced, many assumptions are afflicted with high uncertainty.

For the calculation of the land cost we included the same proportional increase of the solar collection area to get the overall plant area. For simplicity reasons, this proportional factor was assumed to be the same for both technologies. The land costs are a minor contributor to the overall costs, to be more accurate, a detailed analysis of the auxiliary devices needs to be carried out.

Since there is not much data available on long term degradation of especially the PEC module, we assumed that both systems run with maximal efficiency over the whole lifetime. Therefore we assumed that the cell performance does not degrade over time and also for the other components no degradation occurs over the lifetime.

It should be noted that the precise location of the plants has a significant influence on the LCOH when looking at the solar energy input. For our analysis we chosen a location with an average daily irradiation of 6.19 $\text{kWh}/\text{m}^2/\text{day}$. When carrying out this analysis for e.g. northern Europe with a much

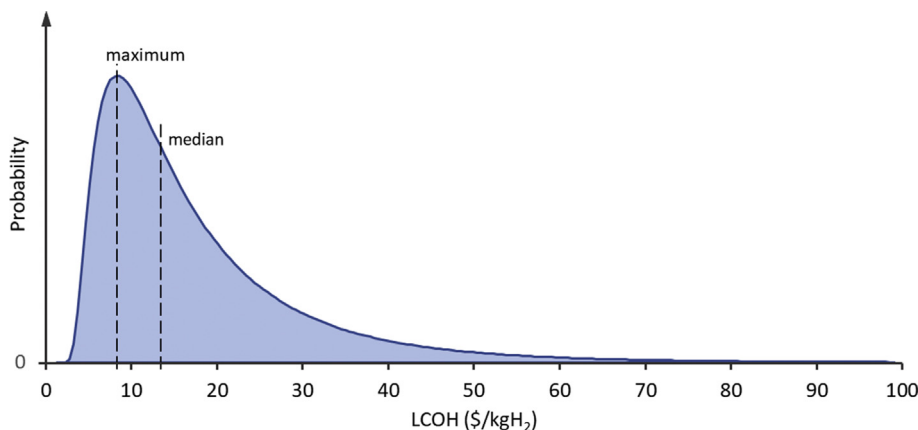


Fig. 5 – Schematic diagram illustrating the probability distribution of the LCOH for a PEC system using the results of the sensitivity analysis.

lower sun irradiation ($\approx 3.0 \text{ kWh/m}^2/\text{day}$) the LCOH would increase by more than 70%.

Comparison with previous literature

The results found during this techno-economic analysis were compared with previous studies. In Ref. [13] a similar comparison between two different PEC and two PV-E systems was performed. However, the resulting LCOH were higher, especially for the PV-E system (base-case $12.1 \text{ \$/kg}_{\text{H}_2}$). The difference between the values stems from the fact that our analysis includes updated prices for the PV panels and a higher efficiency, since a significant development occurred within this technology in the last few years. Another factor is that we include an optimization between the PV system and the electrolyzer, which lead to an increase in the capacity factor of the electrolyzer. The normalized costs for the PEC module published in Ref. [13] are in a similar range with a value of $11.4 \text{ \$/kg}_{\text{H}_2}$ for the base-case. The main difference is that we are considering a different PEC design and we consider a different panel area, similar to Ref. [9,11]. In addition, our estimated hard-BoS costs are lower since we considered lower costs for the mounting material. On the other hand, our calculation is based on higher soft-BoS share, as we expect higher values for the installation and contingency costs.

In the DOE report a LCOH of $10.36 \text{ \$/kg}_{\text{H}_2}$ was calculated, which is slightly higher compared to our results. The main difference lies in the different material costs for the PEC module and slightly lower soft-BoS costs, since we expect the installation costs to be lower which is mainly due to a higher production rate of our considered systems.

In [42] and [15] a similar range for the LCOH of PEC systems was published, showing a value of approximately $8 \text{ \$/kg}_{\text{H}_2}$ and $10.40 \text{ \$/kg}_{\text{H}_2}$, respectively. However, their sensitivity analysis reveals a much lower error bar for the cost of hydrogen compared to our results. This is mainly due to the higher material costs for the membrane and photoactive layer which were assumed in this analysis. Both studies do not show a detailed cost breakdown for the different material components.

Conclusion

This study concerns a comparative techno-economic analysis between a photoelectrochemical system (PEC) and an already commercially available system comprising a photovoltaic device connected to an electrolyzer (PV-E). The evaluated conceptual PEC system was based on a non-concentrated panel design with an efficiency of 10%.

For a benchmark system a crystalline silicon PV cell combined with an off-grid PEM electrolyzer with an overall efficiency of 10.9% was chosen. The calculated levelized production cost of hydrogen (LCOH) resulted in $6.22 \text{ \$/kg}_{\text{H}_2}$ for the PV-E system and $8.43 \text{ \$/kg}_{\text{H}_2}$ for the PEC system, respectively. The sensitivity analysis for the PEC device revealed a significant level of uncertainty with regards to the LCOH. It was carried out by varying the costs for the membrane as well as the semiconductor material and by changing the efficiency and lifetime of the overall system. The best-case scenario shows that there is a possibility to

quarter the LCOH, resulting in $2.51 \text{ \$/kg}_{\text{H}_2}$. However, according to our findings this cost is more likely to be higher than the initial LCOH; for the median scenario it is expected to nearly double.

This work demonstrates that it is unlikely for the PEC system to achieve lower hydrogen production costs compared to photovoltaic-electrolysis systems. Even under generous assumptions, PEC devices are costlier and less flexible in their application. As to the cost, we have shown that at present, the main obstacles are the stability of catalysts and an unfavorable trade-off between cost and lifetime of the semiconductor materials. With regard to flexibility of utilization, a PV-E system can be more efficiently embedded into the future energy system than a PEC device, because “PV” and “E” can be separately size-optimized to fit the needs of the future energy system and electricity grid. This leads us to conclude that while PEC, as a research field, remains of interest for the science, the prospects for successful commercialization are effectively absent. Therefore, a dedicated technology development effort is unwarranted.

Declaration of competing interest

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

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.ijhydene.2020.06.092>.

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