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Perspectives for a sustainable implementation of super-green hydrogen production by photoelectrochemical technology in hard-to-abate sectors

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A B S T R A C T

The energy transition's success hinges on the effectiveness to curbing carbon emissions from hard-to-abate sectors. Hydrogen (H_2) has been proposed as the candidate vector that could be used to replace fossils in such energy-intensive industries. Despite green H_2 via solar-powered water electrolysis being a reality today, the overall defossilization of the hard-to-abate sectors by electrolytic H_2 would be unfeasible as it relies on the availability of renewable electricity. In this sense, the unbiassed photoelectrochemical water splitting (PEC), as inspired by natural photosynthesis, may be a promising alternative expected in the long term. PEC could be partly or even completely decoupled from renewable electricity and then, could produce H_2 autonomously. However, some remaining challenges still limit PEC water splitting to operate sustainably. These limitations need to be evaluated before the scaling up and implementation. A prospective life cycle assessment (LCA) has been used to elucidate a positive performance scenario in which the so-called super-green H_2, or photo-H_2, could be a sustainable alternative to electro-H_2. The study has defined future scenarios by conducting a set of sensitivity assessments, determining the figures of operating parameters such as i) the energy to produce the cell; ii) solar-to-hydrogen efficiency (STH); and iii) lifetime. These parameters have been evaluated based on two impact categories: i) Global Warming Potential (GWP); and ii) fossil Abiotic Depletion Potentials (f-ADP). The mature water electrolysis was used for benchmarking in order to elucidate the target performance in which PEC technology could be positively implemented at large-scale. Efficiencies over 10% (STH) and 7 years of lifetime are compulsory in the coming developments to achieve a positive scaling-up.

1. Introduction

Most of the hard-to-abate sectors belong to the backbones of our global economy and their sustainable ongoing energy transition will be critical to reaching a net zero world. The European economy has committed to net-zero carbon dioxide (CO_2) emissions by 2050 (European Commission, 2021). Together with the climate crisis, the EU transition to a resilient energy system has been set as a matter of urgency in the recent REPowerEU Plan (European Commission, 2022). According to the COP 27, fossil-free value chains need to be built in the coming years. If fossil-free electricity is a prerequisite in the coming transition, the production of bulk materials (e.g., cement, iron, steel, aluminium, etc.) needs to be fossil-free. These materials are basic components of any renewable infrastructure such as wind turbines, PV modules, and transmission & distribution power lines. Achieving a feasible decarbonization/defossilization synergy in the production of basic materials will certainly define the success of the global energy transition.

Hard-to-abate sectors are typically based on extremely high-temperature processes (often greater than 1000 °C) achieved by burning fossil fuels (Neuwirth et al., 2022). These processes require high-density energy sources so they cannot be simply electrified using renewables. In this sense, hydrogen (H_2) has been proposed as the preferred fuel within the European Commission's Long-term strategic vision (European Commission, 2018). H_2 can provide the high temperatures required in these energy-intensive manufacturing processes. Nevertheless, around 80% of the 90 Mton of H_2 used in 2020, came from fossil fuels and resulted in 900 Mton of CO_2 emissions (International Energy Agency, 2021). For the transition period, sustainable development and implementation of cutting-edge technologies may unfold new decarbonization pathways for the hard-to-abate sectors.

Low-carbon H_2 can currently be produced via mature water electrolysis (WE) powered by a decarbonized grid electricity, photovoltaic, wind, or hydropower. A recent environmental study has identified the material efficiency of the electrolyzers and the land use as the main hotspots of this mature technology, suggesting the necessity to consider complementary H_2 production systems soon (Terlouwa et al., 2022). If the PEC efficiency is higher than the overall WE efficiency, which includes the PV solar panel/wind turbine efficiency plus the electrolyzer efficiency, then PEC may have a lower land demand. Despite the spread of WE being clear in this decade, the feasibility of WE to defossilize hard-to-abate sectors would be only guaranteed if enough renewable electricity is available. In this sense, producing sustainable H_2 from

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abundant sunlight and water, called here "super-green H_2", could be a supporting alternative to defossilize energy-intensive sectors. It was estimated that only 0.6% of solar power from the overall 7650 TW of Earth's incident sunlight would be enough to meet the projected 43 TW energy demand for the year 2100 (Abbott, 2010; Lewis and Nocera, 2006). The main drawback of a large-scale deployment of any sunlight-based H_2 technology is the intermittent nature of solar energy. At its current stage, large-scale production of H_2 from sunlight (PEC) would involve also extensive areas, large conversion devices, and the necessity of storage systems. These facts make these technologies still unfeasible from both economic (e.g., high capital cost) and environmental perspectives (e.g., increasing the amount of materials and resources, energy to fabricate the device, etc.).

Several sunlight-based technologies are being developed, including photovoltaic-water splitting (PV-EC), photocatalytic water splitting (PC), photobiological H_2 production, and photoelectrochemical water (H_2O) splitting (PEC) (Song et al., 2022). Among them, photoelectrochemical (PEC) water splitting may operate directly and therefore, it could be a sustainable route in the future timeframe (Chen et al., 2018; Peerakiatkhajohn et al., 2016). In general, a feasible PEC performance must rely on a high efficiency of sunlight harvesting as well as the long durability of electrode materials. During unassisted PEC, photoelectrodes, which are fabricated by using the proper semiconductor and electrocatalysts materials, can absorb sunlight photons splitting water into H_2 and O_2. Despite the PEC technology could produce H_2 directly from solar radiation in future applications, at the current stage of development, this technology requires an electrical bias to overcome overpotentials and support solar energy conversion. Some lab-scale designs have been proposed to conduct unassisted PEC water splitting including a dual-absorber tandem cell system (Brillet et al., 2012) or photovoltaic tandem (PEC/PV) design (Haussener et al., 2013). Now, a research niche within PEC technology is to select the proper photoelectrode materials taking into account: (i) a wide light absorption spectrum; (ii) long-lasting materials; (iii) low-cost; (iv) great abundance; (v) appropriate positions of electronic band edges; and (v) low overpotential (Alqahtani et al., 2020; Kim et al., 2017; Pan et al., 2018; Prabhakar et al., 2020; Venkatesh et al., 2020; Yang and Wu, 2017). No doubt from the sustainable perspective, PEC components should be made of earth-abundant materials. Abundant materials such as light absorbers and co-catalysts may substitute the traditional platinum (Pt), bismuth vanadate ($BiVO_4$), or even the earliest explored titanium dioxide (TiO_2). In this sense, the application of hematite (Fe_2O_3) has been attracting attention given its numerous advantages (Najaf et al., 2021): i) a suitable energy band position and 2–2.2 eV of bandgap, which can theoretically absorb 40% of photons in the solar spectrum; ii) its earth-abundance and cost-effectiveness; iii) its stability under a wide pH range; and iv) its non-toxicity. Nevertheless, its relatively low photochemical conversion efficiency limits its scale-up.

The economics of the PEC technology has gained attention in recent years (Gaillard and Deangelis, 2016; James et al., 2009; Maljusch et al., 2018; Grimm et al., 2020), but its environmental sustainability remains unclear. Some studies envisage potential benefits (Dincer and Acar, 2015; Greenblatt, 2018; Sathre et al., 2016), but given the uncertainty bonded to the low Technology Readiness Level (TRL), more specific studies are needed. From previous studies, it can be concluded that the challenge is currently to enhance PEC water-splitting efficiency to achieve a large-scale implementation cost-effectively (Grimm et al., 2020). Solar-to-hydrogen (STH) efficiency should be increased while the energy to fabricate the PEC and equipment cost production should be minimized. PEC device durability is still far from the 25 years lifetime of commercial PV panels and electrolyzers. PEC electrodes last less than 1000 h due to corrosion (Segev et al., 2022). While energy efficiencies have been improved, the stability stays behind limiting the PEC scaling-up. Medium/long-term performance targets from the environmental perspective must be defined to guide the coming developments.

This work analyzes the technological enablers of PEC technology to produce H_2 sustainably when compared with the high TRL water electrolysis and explores the benefits of PEC H_2 application within hard-to-abate sectors. For this purpose, an *ex-ante* life cycle assessment (LCA) tool has been used to define the prospective scenarios. The tool has been previously applied by the authors to explore the windows of opportunity of other emerging technologies (Aldaco et al., 2019; Rumayor et al., 2018, 2019, 2022a) as well as to explore the possibilities to decarbonize hard-to-abate sectors such as cement (Rumayor et al., 2022a), soda ash (Rumayor et al., 2020) and fine chemicals (Rumayor et al., 2021). In a previous study carried out by the authors, the energy intensity to fabricate some components of the PEC device (e.g., catalysts) was found to be the main contributor to the Global Warming Potential (GWP) and the fossil Abiotic Depletion Potential (f-ADP) of H_2 production by PEC (Rumayor et al., 2022c). Indeed, the necessity of an optimal fabrication process (e.g. thin-film deposition) has been claimed in some studies (Peerakiatkhajohn et al., 2016; Sathre et al., 2016). The novelty of the present study is the prospective evaluation of several performance parameters, including the energy for cell fabrication, the Solar-to-Hydrogen efficiency (STH), and durability, so verifying the performance in which H_2 produced via the PEC route may lead to real environmental benefits. We could conclude that STH around 10% paired with a lifetime of 7 years may lead to a positive PEC performance from the environmental perspective when compared with other alternatives. The results obtained in this study could provide the future directions of PEC technology, encouraging clean and carbon-free H_2 production in the coming energy transition.

2. Methods

2.1. Goal and scope

PEC technology offers the opportunity to operate in an unassisted way using sunlight energy and water. However, some remaining drawbacks need to be overcome to push this technology toward a higher stage of development. This paper is an early-on assessment of the PEC H_2 technology to evaluate the technology enablers to operate sustainably. We aim to define a better-performance scenario of PEC to produce H_2. This may serve to complement other green alternatives such as the water electrolysis (WE) within the context of the energy transition of hard-to-abate sectors (Fig. 1). We have focused on the environmental categories of GWP and f-ADP. As a result, these are the main chosen categories to maximize the decarbonization/defossilization synergy during the energy transition of hard-to-abate sectors. We have used the mature technology of WE as benchmarking. The benchmark scenarios were labelled as PV-WE and W-WE, depending on the electricity source. PV-WE and W-WE were powered by photovoltaics (PV) and wind (W), respectively. Specifically, the reference scenarios were based on proton exchange membrane (PEM) electrolysis given its high TRL value (TRL 8) (Pinsky et al., 2020). Through the comparison, we were able to define a

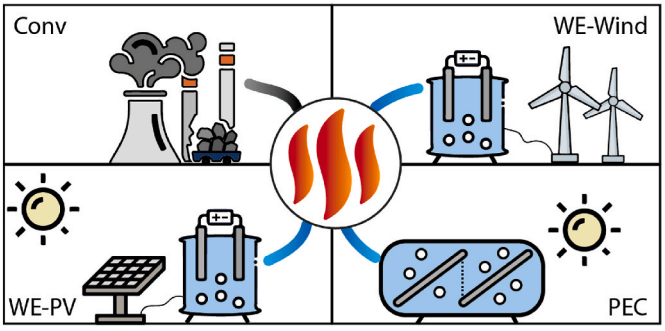

Fig. 1. Green heat production to push the energy transition of hard-to-abate sectors. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

window of opportunity in which PEC technology may operate sustainably from the environmental perspective. The objective was to elucidate a positive performance scenario in terms of energy intensity for cell fabrication, STH, and lifetime. This positive scenario can be of assistance to further analyze the decarbonization/defossilization synergy in any hard-to-abate sectors. In a final example, we display the environmental benefits of introducing H_2 from PEC technology in the European cement sector.

The system was analyzed from a cradle-to-gate perspective and therefore, the system boundary includes the extraction of raw materials, energy production, the operation step as well as the compression of H_2. According to our purpose, both H_2 distribution, transportation, utilization, and end-of-life are excluded from the scope of this study. As the objective of the technology is to replace fossil heat of hard-to-abate sectors, the functional unit (FU) was fixed as 1 MJ at 20 MPa of heat from H_2 (120 MJ/kg) following similar studies in the field (Osman et al., 2022).

The purpose of this study is to define the technology enablers of PEC technology to produce H_2 sustainably. Therefore, we have used the mature water electrolysis as benchmarking given its current TRL value (TRL 8–9). The system boundary of 1 MJ of H_2 produced by PEC as well as the reference electrolysis are shown in Fig. 2. We have considered the unassisted PEC scenario (Fig. 2 (a)) that produces 1 MJ of H_2 upon sunlight irradiation. This scenario was selected as it can border the complete window of opportunity of PEC technology to produce clean H_2. Notice that in practical applications, an external bias is still needed to split water by PEC technology.

Briefly, the PEC water splitting process occurs in two half-reactions, namely hydrogen evolution reaction (HER) ($2H^+ + 2e^- \rightarrow H_2$) and oxygen evolution reaction (OER) ($H_2O + 2h^+ \rightarrow 1/2O_2 + 2H^+$) (Chen et al., 2016). The PEC process is based on the production of electron-hole pairs in the selected photoanode and photocathode materials. Electrons reduce water driving the HER at the photoanode, while holes oxidize water driving the OER at the photoanode. We have used the performance parameters displayed in Table 1 to conduct the mass and energy balances. An amount of water of 0.075 kg/MJ is needed according to stoichiometry.

We have calculated the illuminated photoelectrode area (A_e) using the solar-to-hydrogen efficiency (STH) (Eq. (1)). The STH parameter is defined as the chemical energy of the produced H_2 divided by the solar energy consumed. Considering an average daily solar radiation (P_S), an average STH is defined as follows:

$$STH = \frac{m_{H2} \cdot \Delta G}{A_e \cdot P_s} \cdot 100 \quad \text{(Eq.1)}$$

STH can be determined by using the cell voltage and photocurrent density (j) considering a 100% selectivity towards H_2 (cathode) and O_2 (anode) (Kuang et al., 2017). This is equivalent to a faradaic efficiency of 100% for both compounds in their respective electrodes (Eq. (2)). While today's faradaic efficiency on the cathode is, at best, around 90% (Kalanur and Seo, 2022; Tan et al., 2023), we do neglect in this work as a preliminary assumption the formation of any by-product.

$$STH = \frac{j\left(\frac{A}{m^2}\right) \cdot 1.23\ V}{P_s\ \left(\frac{W}{m^2}\right)} \cdot 100 \quad \text{(Eq.2)}$$

In addition, we have estimated the environmental impacts in the practical operation of PEC when assisted by an applied bias. In this case, we have estimated the energy efficiency using the "applied bias photon-to-current efficiency" (ABPE) parameter which considered the external bias voltage that is applicated (V_{bias}) (Eq. (3)) (Chen et al., 2010):

$$\text{ABPE} = \frac{j\left(\frac{A}{m^2}\right) \cdot (1.23 - V_{bias})(V)}{P_s\ \left(\frac{W}{m^2}\right)} \cdot 100 \quad \text{(Eq.3)}$$

The scenario labelled as biased-PEC is used as an intermediate reference. To calculate the electricity requirements, we have used a bias voltage of 0.5 V and a photocurrent density of 10 mA/cm^2 as an average performance (Chatterjee et al., 2022).

Regarding the benchmark WE technology, we have considered PEM water electrolysis (WE) powered by photovoltaic/wind electricity (PV/W). Wind electricity was displayed in the comparison since it has lower GWP and f-ADP than the current PV impacts (Table S5). We have selected PEM technology as it exhibits several advantages compared to alkaline water electrolysis (AEL) and solid oxide electrolysis cells

Table 1
Assumptions of PEC parameters used in the mass and energy balances.

Parameter	Value	Units	Information	Ref
P_s	4.8	kW·h/m^2·d	Average daily solar radiation	("JRC Photovoltaic Geographical Information System (PVGIS)," 2023)
ΔG	237	kJ/mol	Change in Gibbs free energy per mole of H_2	(National Institute of Standards and Technology)
STH	Variable	%	Solar-to-hydrogen ratio	
m_{H2}	10	ton/d	H_2 production rate	James et al. (2009)
E_{cell}	Variable	MJ/m^2	Energy required to produce the E_{cell}	
LT_{cell}	Variable	yr	Durability of the PEC cell[b]	

[a] Average value over Europe (Kaspar et al., 2019).
[b] The durability is assumed equal for each component of the PEC cell.

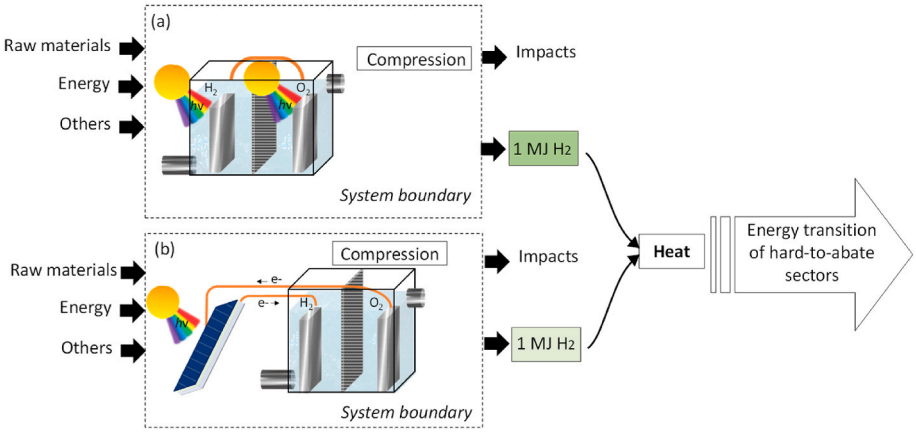

Fig. 2. System boundary of H_2 production to provide heat in the energy transition (1 MJ) by: a) unbiased-PEC; and b) PV-WE.

(SOEC) highlighting the higher H_2 purity and compact design (Burton et al., 2021).

In brief, H_2 PEM technology splits water molecule into H_2 and O_2 under the application of an electric current (Eq. (4)) (Kumar and Himabindu, 2019). The reference scenario (WE) was modelled in a previous study carried out by the authors (Rumayor et al., 2022b). According to the stoichiometric 1 kg of H_2 requires 9 kg of water, which is 0.075 kg/MJ as input. Note that PEM requires demineralization of water that involves a consumption between 18 kg and 24 kg of water (0.15–0.2 kq/MJ). However, as we are conducting a prospective LCA, we have considered the stoichiometric amount of water assuming a certain degree of energy efficiency in the demineralization process.

$$2\ H_2O(l) \rightarrow 2\ H_2(g) + O_2(g) \quad \text{(Eq. 4)}$$

We have disregarded downstream H_2 purification, but the energy required for compression was considered in the bivariate assessments. As an initial approach, the energy for compressing 1 MJ of H_2 up 20 MPa is assumed as 0.0098 kWh (Valente et al., 2017). On the other hand, the energy for pumping was neglected since the impact of this energy consumption is below 1% according to our previous results (Rumayor et al., 2022c).

2.2. Prospective life cycle assessment tool

An *ex-ante* life cycle assessment (LCA) tool has been applied in this study (Cucurachi et al., 2018) to evaluate the environmental performance of PEC H_2 production following the ISO standards 14040 (International Organization for Standardization, 2006a) and 14044 (International Organization for Standardization, 2006b). This procedure quantifies the raw material and energy requirements as well as emissions and wastes produced under a life cycle thinking perspective. The software GaBi Professional v9.5 (Sphera, 2022) and the Ecoinvent v3.8 database (Swiss Centre for Life Cycle Inventories, 2022) have been used to calculate the environmental categories and to model the background processes, respectively. We have used Europe geography (RER) as long as it is available. Since the European mix of renewable electricity (solar PV and wind) is not available, they were estimated using GaBi Software by using the latest statistics figures for EU-27 (International Renewable Energy Agency, 2020) found in Table S4 (Supporting Information). The two selected environmental categories were determined using the CML 2001 method (Guinée et al., 2001).

A set of bivariate sensitivity analyses was conducted to evaluate the influence of the selected performance parameters on the chosen environmental categories. Despite STH and lifetime are important metrics for benchmarking, they do not indicate the whole energy efficiency of the system. Indeed, it should be considered every energetic input to the PEC technology (Sathre et al., 2016). Note that a PV-WE system operates at >1 A/cm^2 whereas PEC system generally operates at 10–100 mA/cm^2. This difference involves more photoelectrode area, more materials and therefore, more energy to fabricate the PEC components by thin-film deposition processes. In this context, if the impacts of the energy inputs as renewable energy consumed by the system fabrication go beyond the positive impact of the energy provided by the H_2 produced by PEC, the implementation of this technology becomes unfeasible. Accordingly, the first key figure of merit that we have evaluated is the influence of the PEC cell fabrication electricity requirement ($E_{fabrication}$) as well as the compression (E_{comp}) in comparison with the energy provided by PEC H_2 which was called here as the "net energy performance". On one hand, the $E_{fabrication}$ encompasses the energy needed to fabricate the active cell, for example using thin-film deposition processes, as well as the energy needed to assembly the cell and module. On the other hand, we define the net energy performance as the ratio between the energy produced by PEC, which is given as MJ of H_2, and the energy input to fabricate the electrode area (A_e) and to compress H_2 (E_{comp}) (Eq. (5)):

$$Net\ energy\ performance = \frac{LHV_{H2}\left(\frac{MJ}{kg}\right)}{\frac{E_{fabrication}\left(\frac{MJ}{m^2}\right)\cdot A_e(m^2)}{Lt_{cell}\ (yr)\cdot m_{H2}\left(\frac{kg}{yr}\right)} + E_{comp}\left(\frac{MJ}{kg}\right)} \quad \text{(Eq. 5)}$$

where A_e is the geometric cell area (m^2) and LHV_{H2} is the lower heating value of H_2 (120.0 MJ/kg)

After the definition of a target value for the energy requirement during cell fabrication and operation, we have analyzed the influence of the technological parameters: i) STH; and ii) durability in the key performance indicators (KPIs): i) GWP; and ii) f-ADP. The comparison with WE reference values allowed us to define the margin of opportunity to improve the PEC technology.

2.3. Exploring the environmental benefits in an energy-intensive sector: a case study

As a case study, cement manufacture has been chosen to demonstrate the benefits of future H_2 PEC implementation in an energy-intensive industry. According to the Ecoinvent, cement production requires 3.1 GJ of heat and 90 kWh of electricity per ton of cement whereas cement production involves an amount of CO_2 direct emissions of 672 kg of CO_2 per ton of cement. In this study the synergy that fossil fuel switching to H_2 may provide to the cement industry has been estimated as an example that could guide future analyses in other hard-to-abate sectors.

3. Results and discussion

3.1. Evaluation of the technological enablers

Fig. 3 shows the net energy performance results that were calculated as a bivariate analysis and considering the unbiased PEC system. We have ranged the energy requirements to fabricate the PEC module ($E_{fabrication}$) between 100 MJ/m^2 and 2000 MJ/m^2 and the PEC cell lifetime between 0.5 yr and 20 yr. In this analysis, we have fixed STH to 10%, which is the common benchmark found in the literature (Song et al., 2022), and it is used as reference when analyzing H_2 production by type-3 PEC cells (James et al., 2009; Shaner et al., 2016). As previously mentioned, the net energy performance is the ratio between the energy produced by PEC, which is given as MJ of H_2, and the energy input to fabricate the electrode area (A_e) and compress the H_2. Note that this area comes from Eq. (1) using PEC performance parameters as previously mentioned (STH, m_{H2}, etc.). Ratios above 1.0 (red line) are required for

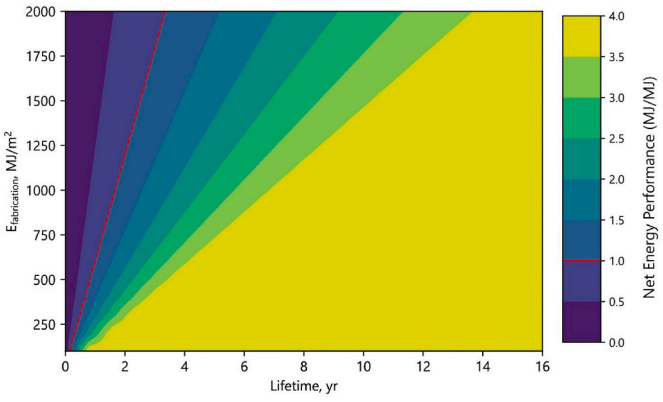

Fig. 3. Sensitivity analysis of the energy input for PEC cell fabrication and lifetime at 10% STH. The red line represents the case when the amount of H_2 energy produced is the same as the one used or embodied in the system for its production. NREL target is adapted from James et al., (2009). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

a positive implementation at the industrial scale. It should be mentioned that the current lifetimes of photoelectrodes are found in the order of hours (Gao et al., 2023). To operate positively under such poor lifetimes fabrication energies below 250 MJ/m^2 would be needed. This may be only possible by improving the fabrication procedures of both the active materials and inactive materials (Sathre et al., 2016). A review of various LCAs regarding PV technology fabrication, which may be used as an estimation of PEC photoelectrodes fabrication, reports energies for the thin-film process between 300 MJ/m^2 and 1150 MJ/m^2 depending on the materials (Bracquene et al., 2018a; Peng et al., 2013; Sathre et al., 2014). Being the energy input for the second-generation PV solar cells as low as 59 MJ/m^2 according to Ecoinvent dataset. Since PV module fabrication is currently commercial, we can consider that a PEC energy fabrication value below 250 MJ/m^2 could be achievable in long-term developments. In order to keep the net energy ratio above 2.0, we can define a combination of a lifetime higher than 5 yr with energy requirements for PEC components fabrication below 500 MJ/m^2 as figures of merits for the next two decades (mid-term horizon). The energy for the cell fabrication value is near those values estimated by Sathre *et al* who conducted a prospective life-cycle energy assessment to investigate the possibilities of scaling up a PEC design. Specifically, they defined a value of 373 MJ/m^2 to produce the PEC cell in a "low energy input" scenario (without considering BOS). These authors appointed the necessity of efficient thin-film deposition processes as the key factor for future developments (Sathre et al., 2016).

Fig. 4 shows the influence of the STH efficiency and E_{cell} lifetime in the GWP and f-ADP categories related to 1 MJ of H_2 produced by PEC. The inventory of materials and energy per functional unit is calculated according Eq.S1 and Eq.S2 (Supporting Information). As mentioned in the methodology section, the results are calculated using the current impacts of EU-PV-solar mix (Fig. 4 (a and c)) as well as EU-wind mix (Fig. 4 (b and d)) that are relatively lower and representative of a long timeframe situation. Additional details regarding the EU-PV solar mix and EU-wind mix are given in the Supporting Information (Tables S4–S5). Fig. 4 includes the comparison with the GWP and f-ADP categories of 1 MJ of H_2 produced by WE. From the carbon footprint perspective, in terms of GWP, lifetimes over 7 years and 10% of STH efficiencies are required to compete with the WE as long as efficient thin-film deposition processes are used to fabricate the PEC cells (<500 MJ/m^2). However, the window of opportunity is quite narrower from the resource depletion perspective, in terms of f-ADP. Compared with the impacts of WE, increasing the STH near 15% is required to compete with W-WE. As mentioned before, PEC lifetimes are found in the order of hours whereas STH can be around 10% (Song et al., 2022; Li et al., 2023). This combination of lifetime/STH corresponds with the dark blue region in Fig. 4. However, 10% STH and a 7-year lifetime have been proposed as target values for future developments according to the projections by the National Renewable Energy Laboratory (NREL) (James et al., 2009). It must be beard in mind that the displayed bivariate results were calculated considering an unbiased PEC with a relatively efficient cell fabrication process and the energy needed for compression. For this reason, the energy intake of the system is minimum. H_2 can be produced by PEC with GWP and f-ADP near zero under proper technology development. Notice that in practical applications, an electrical bias is applied to prevent charge recombination between electron-hole pairs. Therefore, the impact of the scenario called biased PEC was calculated. An additional energy requirement value of 0.123 kWh/MJ has to be considered and then, the ABPE is 7.3% instead of 10% of STH (without the bias voltage). This increases the energy consumption intake by the system by around 27%. If an electrical bias is applied,

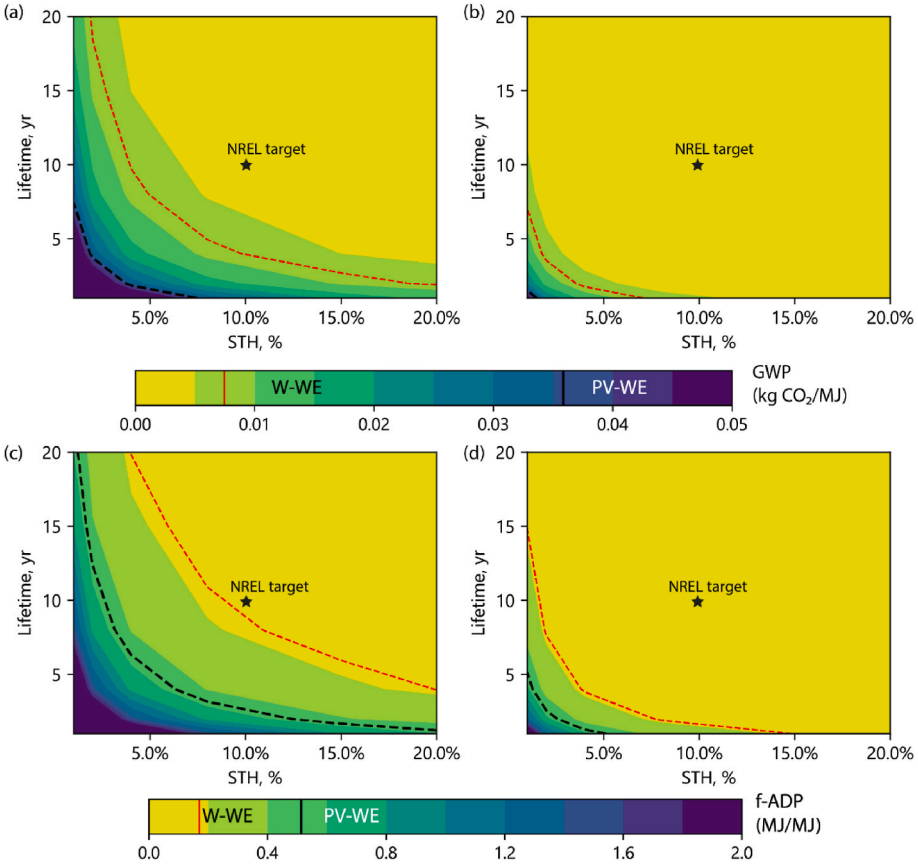

Fig. 4. Results of the bivariate sensitivity assessment in the GWP (a and b) and f-ADP (c and d). The effect of using EU-PV solar is shown in (a) and (c). The effect of using EU-wind electricity is shown in (b) and (d). Reference W-WE and PV-WE are adapted from Rumayor et al. (2022b) and detailed in the Supporting Information. NREL target is adapted from James et al., (2009).

we proposed to increase STH and durability targets near 15% and 10 yr, respectively.

3.2. Environmental synergies in the cement manufacture

Exploring the environmental benefits of the future implementation of any emerging technology within the industry is crucial to encourage its further development. We have conducted a first assessment approach to evaluate the environmental benefits of PEC implementation in the European cement sector in terms of GWP and f-ADP estimating the net energy for a large-scale PEC H_2 implementation. Note that this is an early-on approach given the low TRL of PEC. We have neglected the dynamic nature of the energy system, which would require further research. Because the electricity consumption by the cement plant is not the main hotspot (90 kWh/ton of cement), it was assumed to come from the grid mix. It should be mentioned that when assuming PV solar in the cement plant, the electricity contribution to the overall GWP and f-ADP could decrease to 7.3 kg of CO_2 eq and 117 MJ, respectively. Other factors such as avoiding material loss during fabrication, and even recycling, will reduce energy consumption and should be further analyzed. Fig. 5 shows the prospects of fossil demand reduction after the PEC H_2 integration in the cement sector. The values displayed in the diagram correspond to the NREL-conditions at 10% STH efficiency and 7 years lifetime using 500 MJ/m^2 of energy intake by the fabrication of the PEC system. On one hand, a reduction of around 55% in the f-ADP can be achieved by the proposed technology. On the other hand, the overall carbon savings obtained by the proposed technology are around 31%. This reduction was expected since 70% of CO_2 emissions come from the process reaction (Swiss Centre for Life Cycle Inventories, 2022). In order to reduce direct CO_2 emissions, carbon sequestration or even carbon

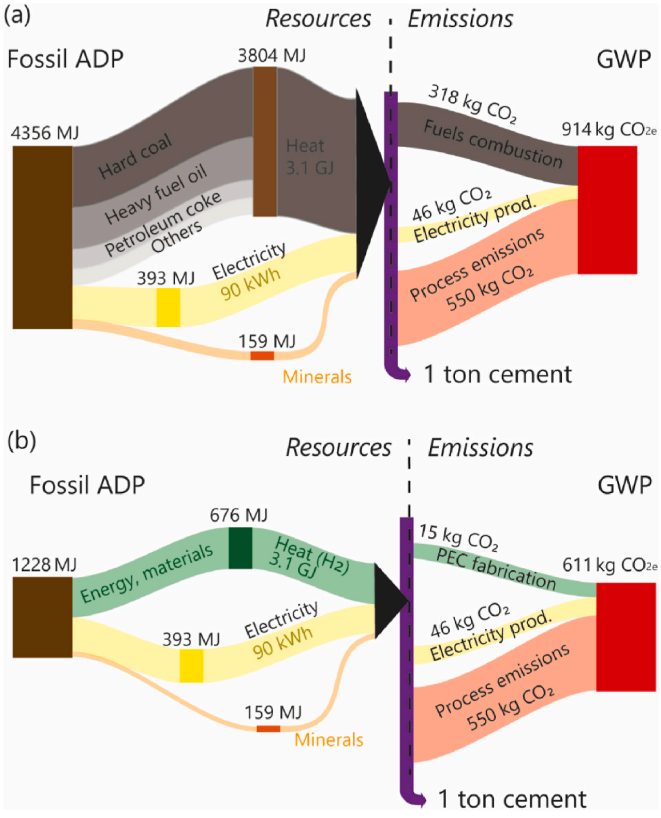

Fig. 5. Example of decarbonization/defossilization synergy of a) conventional cement production; and b) cement production using fuel switching to super-H_2 at the NREL-conditions (10% STH, 7 years lifetime) when cell operation and fabrication is powered with PV energy. Electricity for cement production is assumed to come from today's European grid mix.

recycling are the preferred solutions as demonstrated in a previous study carried out by the authors (Rumayor et al., 2022a). The overall GWP and f-ADP values when using PV-WE to provide 3.1 GJ of heat to cement would be 711 kg CO_{2e} and 2221 MJ, respectively. These values were calculated using the GWP and f-ADP figures of H_2 produced by WE (Supporting Fig. S1). The overall carbon savings by PV-WE are around 22% while f-ADP can be reduced by around 50%. If WE are considered to be coupled to wind electricity, the reduction in GWP and f-ADP could reach 32% and 74%, respectively. Accordingly, H_2 production by PEC technology may help in the transition of electricity-intensive industries.

3.3. Future directions

To provide useable energy through emerging technologies such as PEC must ensure a net energy performance. To operate sustainably, the energy yielded by PEC has to be higher than the energy required to fabricate and operate the technology. In this study, we have evaluated prospectively the potential of H_2 PEC technology to produce net energy in an unassisted way. The key performance parameters include the STH efficiency, the PEC lifetime as well as the energy needs to fabricate the cell and operate the process (e.g. compression). Despite other powerful technologies that are currently available at a mature scale, such as WE, most of them depend on the availability of renewable electricity. We consider that the implementation of electricity-unassisted technologies will be crucial in the coming decade. In fact, one of the major advantages of PEC compared to PV-WE is the possibility to low land demand since PEC system is integrated in one single component (Frowijn and van Sark, 2021). Even though PEC requires more electrode area than the area of a WE device, WE technology is restricted to the availability of renewable fields (PV/W). Furthermore, PEC area could be reduced using a solar concentrator that can easily optimize the energy uptake, increasing the photoresponse of semiconductor materials (Kim et al., 2016). These devices could concentrate up to 10 times the solar energy input with no influence on the PEC performance (Haussener et al., 2013). Notwithstanding, as the PEC is an integrated system, the stability is poorer compared to WE as photoabsorbers and electrolyte are in contact (Ottone et al., 2019). Now, it is necessary not only to improve the stability but also to reduce the energy spent during the cell fabrication. As shown in this study the lifetime of the PEC cells may affect the net energetic yield, because of the energy intensity of cell production. Many advances can be currently found regarding photoelectrode production including semiconductors, substrates, etc. Traditional catalyst coating methods include hydrothermal, solvothermal, low-temperature sintering and electron bombardment processes while recent loading of photocatalyst materials onto conductive textiles such as carbon paper is being investigated (He et al., 2022). Recent advances are promising, thin film corrosion protection is a significant technical challenge to overcome. When designed properly, PEC systems not only can be used to produce green H_2, but also, wastewater treatment can be conducted (Pitchaimuthu et al., 2022) and even to reduce CO_2 synthesizing add-value chemicals (Li et al., 2022).

The operational challenges of PEC technology identified in the present study include STH, durability and energy intensity of the PEC fabrication. Those have been analyzed by a prospective LCA tool defining the performance in which PEC may operate positively from the point of view of the selected categories. However, it should be mentioned that these results have been obtained under certain assumptions and they are intended to give an outlook that supports further development, rather than a definitive demonstration of the complete environmental performance of PEC large-scale operation. Since the maturity level of H_2 production through bias free-PEC technology (TRL <4) is considerably different from the mature PEM-WE technology, the results are restricted to the data availability of PEC in comparison with PEM. Some assumptions have been made, such as the long durability of inactive components of the PEC cell (e.g. glass window, titanium, etc) or the neglection of the H_2 purification. At the current stage of

development of PEC technology, we did not consider the selection of inactive materials as well as the H_2 purification as major challenges. We aimed to identify the best performance scenario in terms of STH, durability and energy needs for the PEC cell fabrication process. Of course, detailed scenarios including infrastructure, downstream purification, etc. would be required prior the large-scale implementation. Additionally, consequential and dynamic LCAs that allow for exploring other technological and economic issues (e.g. the penetration of H_2 and renewables, the expected development of each technology, etc.) should be carried out when this technology overcomes the operating challenges.

4. Conclusions

Producing storable fuels from direct sunlight is a powerful alternative to achieve the energy transition, especially in those sectors considered energy-intensive. Photoelectrochemical water splitting (PEC) is a promising route to produce a storable fuel such as H_2, which may defossilize hard-to-abate sectors. Because PEC is expected to be scaled up in the coming decade, this study has been focused on defining those target parameters that would ensure a positive scaling-up from the environmental perspective. We have conducted a prospective life cycle assessment (LCA) to elucidate the target values of the key performance parameters including the STH efficiency and the lifetime and highlighting the importance of the energy intensity to produce the PEC cell. Water electrolysis (WE) technology was used as benchmarking since it is a mature renewable route to produce green H_2 at a commercial scale. PEC offer the opportunity to be partly or even completely decoupled from renewable electricity compared to WE. We have estimated a target value of 500 MJ/m^2 to fabricate the PEC cell. Energy values below this target would ensure that the impacts of the energy harvested by the system fabrication go beyond the positive impact of the energy provided by the H_2 produced by PEC. We have defined a positive scenario to compete from the environmental perspective with the mature alternative WE. The sensitivity analysis results suggest that research efforts should target STH efficiency and lifetime near 10% and 7 years, respectively. The target values found in this study could provide the future directions of PEC development encouraging clean and carbon-free H_2 production in the coming energy transition.

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.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.clpl.2023.100041.

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