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# Solar to sustainability (S2S): a comparative life cycle assessment of hydrogen production with a focus on a photoelectrochemical anion exchange membrane reactor

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This study employs a comparative life cycle assessment to provide data-driven insights into hydrogen production methods, uncovering the environmental impact of steam methane reforming (SMR), wind proton exchange membrane water electrolysis (PEMWE), solar PV PEMWE, photoelectrochemical (PEC) PEM reactors and PEC anion exchange membrane (AEM) reactors. The assessment employs a cradle-to-gate approach using SimaPro as the LCA software, with data from the ecoinvent database (*i.e.* v3.8) and published literature. Notably, 1 kg of hydrogen produced is considered a functional unit. Key environmental impacts, including global warming potential, ozone depletion, eutrophication, acidification and water use, are evaluated using the ReCiPe 2016 Midpoint method (H). The results demonstrate that hydrogen production through the PEC AEM reactor has the lowest environmental impact compared to other methods. The PEC AEM reactor shows the lowest global warming potential of 1.17 kg CO<sub>2</sub> eq per kg H<sub>2</sub> in the comparative LCA study. The highest human carcinogenic toxicity potential (HCTP) of 1.5 kg 1,4 DCB-eq per kg H<sub>2</sub> was obtained for the PEC PEM reactor. Wind PEMWE has the highest mineral resource scarcity (MRS) of 0.0839 kg Cu-eq per kg H<sub>2</sub> produced as the mining, processing and manufacturing of permanent magnets for wind turbines involve rare earth elements. SMR has the highest value of land use (0.189 m<sup>2</sup>a crop-eq per kg H<sub>2</sub>) due to the large scale facility and infrastructure required in the SMR process. Moreover, a sensitivity analysis is conducted to assess the effect of regional energy supply on the global warming potential (GWP) associated with various hydrogen production methods. This study offers valuable insights highlighting the significance of considering various environmental impacts to facilitate informed decision-making for sustainable design.

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## Sustainability spotlight

A comparative life cycle assessment of SMR, wind PEMWE, solar PV PEMWE, PEC PEM and PEC AEM reactors is conducted to understand the environmental impact caused by different hydrogen production methods. The study uses the ReCiPe midpoint (H) method to categorise environmental impacts into 18 standardised impact categories. Comparative LCA shows the environmental benefits of hydrogen production using a PEC AEM reactor for hydrogen production. The GWP of the PEC AEM reactor is the lowest at 1.17 kg CO<sub>2</sub>-eq per kg H<sub>2</sub>.

## Introduction

The excessive reliance on fossil fuels has resulted in various issues, such as air pollution, global warming and energy crisis.<sup>1</sup> Two primary strategies exist to address environmental concerns and energy issues. One feasible approach involves enhancing the efficiency of traditional energy sources, while the other involves substituting them with renewable energy sources.<sup>2</sup> Solar energy is a key renewable energy source for lowering

greenhouse gas emissions and creating a sustainable society.<sup>3</sup> Despite the ongoing expansion of its market size, the intermittency of solar energy must be addressed to facilitate its wider adoption beyond temporary electricity generation.<sup>4</sup> Electricity generation based on renewable energy systems offers a more environmentally and socioeconomically viable substitute for fossil fuel-based systems. Moreover, establishing a reliable energy source can expedite the shift to a low-carbon economy, aiming for a 45% decrease in emissions by 2030 to fulfil the objectives of the Paris Agreement.<sup>5</sup>

Solar electricity is used in electrochemical reactions to convert solar energy into fuels or valuable molecules, including hydrogen, hydrocarbons, and ammonia. Moreover, hydrogen is

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characterised by a high heating value of  $141.8 \text{ MJ kg}^{-1}$ , producing no carbon dioxide gas during pure hydrogen gas utilisation.<sup>6</sup> Currently, the most common and widely used approach for hydrogen production involves using steam methane reforming (SMR) with hydrocarbons and water, which generates high emissions and exhibits resource use throughout its life cycle.<sup>7</sup> Solar-driven hydrogen production technologies can be primarily classified into three groups: photocatalysis (PC), solar photovoltaic water electrolyzers (PV WEs) and photoelectrochemical (PEC) water splitting.<sup>8</sup> In PC, water-splitting semiconductor powders (such as  $\text{TiO}_2$  and  $\text{SrTiO}_3$ ) are scattered within the liquid phase. These powders capture sunlight to produce charge carriers and engage in either water reduction or oxidation reactions.<sup>9</sup> However, specific wide-bandgap semiconductor materials have a restricted absorption window for wavelength utilisation,<sup>10</sup> causing a reduction in solar-to-hydrogen (STH) efficiency. A further difficulty arises from the need for the reliable separation of the generated  $\text{H}_2$  and  $\text{O}_2$  gases.<sup>11</sup> Meanwhile, solar PV WE has greater STH efficiency. In solar PV WE, PV modules and electrolyzers can be linked to produce  $\text{H}_2$ .<sup>12</sup> Although solar PV WE can be scaled substantially, the economic viability and environmental consequences of hydrogen production using this method are doubtful.<sup>13</sup> This concept can be further integrated into a PEC reactor arrangement.<sup>14</sup> A PEC reactor consolidates many capabilities into a single device, encompassing light absorption in semiconductor photoelectrodes and electrochemical processes on the photoelectrode's surface.<sup>8</sup> With significant advances in solar-based water splitting, integrated devices with comparable STH efficiency and sustainability are essential.<sup>15</sup> A PEC reactor contains two photoelectrodes, a membrane, an electrolyte and a compartment. Membranes are crucial to PEC reactors because they enable selective ion transport. They maximise hydrogen production and minimise the recombination reaction, allowing the electrochemical processes to run effectively.<sup>16</sup> Membranes are generally classified into three main categories: alkaline membrane, proton exchange membrane (PEM) and anion exchange membrane (AEM). The constraints of PEM and alkaline exchange membranes have been successfully resolved by notable advancements in AEM.<sup>17</sup> AEM minimises fluctuations in the differential pressure of the electrodes and mitigates gas crossover.<sup>18</sup> Furthermore, owing to its reduced thickness, it exhibits a lower ohmic overvoltage. It is compatible with deionised water or electrolytes with lower alkalinity.<sup>19</sup> Utilising a less expensive metal catalyst is more beneficial than platinum owing to its lower alkalinity.<sup>20,21</sup> In addition, if 1% of the land-mass is covered with 10% efficient PEC reactors, 36 TW of energy will be produced to meet the world's anticipated energy needs by 2050.<sup>12</sup>

The existing body of literature focuses significantly on developing new and efficient PEC reactors. Karaca and Dincer<sup>22</sup> conducted an experimental investigation using new conic geometry electrodes with a PEM (Nafion) in the PEC PEM reactor for hydrogen production. The anode comprised  $\text{TiO}_2$ ; the cathode was  $\text{Cu}_2\text{O}$ , with both electrodes immersed in KOH solution (0.1 M). The maximum STH of 1.82% was obtained at  $1.81 \text{ mA cm}^{-2}$ , and the maximum hydrogen flow rate was  $4.5 \mu\text{g}$

$\text{s}^{-1}$  with an external voltage of 2.3 V under illumination. Qureshy and Dincer<sup>23</sup> used fluid flow simulation techniques and electrochemical modelling to study hydrogen generation in the PEC PEM reactor. The anode consisted of SS304 and was coated with  $\text{TiO}_2$ , while the photocathode featured a dome shape and was coated with  $\text{Cu}_2\text{O}$  on grade 2 titanium. A proton exchange membrane (Nafion 117) was used as a membrane sandwiched between the electrodes. The hydrogen production rate achieved was  $42 \mu\text{g s}^{-1}$ , resulting in an energy efficiency of 4.9%. Acar and Dincer<sup>24</sup> assessed the performance of a hybrid PEC chloralkali reactor. The reactor produced hydrogen and NaOH from industrial by-products. The hydrogen generation rate with solar irradiation of  $1200 \text{ W m}^{-2}$  was  $295 \text{ mL h}^{-1}$ .<sup>16</sup> A study on a tandem PEC reactor with a Mo-doped  $\text{BiVO}_4$  anode and  $\text{Cu}_2\text{O}$  cathode was carried out by Pan *et al.*<sup>24</sup> Their configuration achieved the highest performance among tandem oxide reactors, with an unassisted STH efficiency of 3%. Li *et al.*<sup>25</sup> examined a tandem PEC reactor with a nanotextured  $\text{CuBi}_2\text{O}_4$  photocathode and a  $\text{TiO}_2$  array (nanorod) as the photoanode for facilitating unbiased water splitting. The structured nanoarray design reduces the length of the electrode. This tandem PEC reactor achieved an STH efficiency of 1.23%. Jang *et al.*<sup>26</sup> examined the creation of a solution-based regrowth method in hematite photoanodes. They achieved an STH efficiency of 0.91% in a tandem reactor by combining a Si-photocathode with a  $\text{Fe}_2\text{O}_3$  photoanode. Bedoya *et al.*<sup>27</sup> evaluated a 2D Multi-physics model for a novel photoelectrochemical reactor to analyse the photoelectrode under concentrated irradiation. They studied factors such as thermal management, redox couple, hydrodynamic conditions, materials and surface properties. The investigation concluded that solar flux could enhance the kinetic rate and charge transfer. Modestino and Haussener<sup>15</sup> evaluated the comprehensive incorporation of the overall components of the PEC reactors. The study indicates that the PEC reactor for hydrogen generation requires modelling-based design guidelines, life cycle analysis and techno-economic assessments.

The life cycle assessment (LCA) methodology is an effective tool for evaluating the environmental impacts of a product and promoting a more sustainable strategy in product development.<sup>28</sup> Zhang *et al.*<sup>29</sup> conducted a cradle-to-gate life cycle net energy assessment of a photoelectrochemical reactor for sustainable hydrogen generation and chemical hydrogenation. The PEC device utilised a tandem arrangement, including a  $\text{BiVO}_4$  as the upper photoanode absorber and a silicon heterojunction (SHJ) photovoltaic cell as the lower absorber. The findings suggest that the efficiency of the PEC reactor can be enhanced by linking hydrogenation. Karaca *et al.*<sup>13</sup> developed a novel PEC reactor utilising a Nafion membrane to produce clean hydrogen, accompanied by a comparative environmental impact assessment study. The PEC reactor utilised a  $\text{Cu}_2\text{O}$  photocathode as the upper cell,  $\text{TiO}_2$  as the photoanode in the lower cell and a Nafion membrane with an area of  $254 \text{ m}^2$ . A comparison was conducted between the PEC PEM reactor, solar PV PEMWE, and wind PEMWE to produce 1 kg of hydrogen. Their findings indicated that the global warming potential was ( $1.1 \text{ kg CO}_2 \text{ eq}$ ) for the PEC PEM reactor, making it a clean and



environmentally sustainable solution compared to others. Sadeghi *et al.*<sup>30</sup> carried out an environmental impact assessment of standalone solar-driven four-step thermochemical (Cu–Cl) hydrogen production. A comparative study was carried out on SMR, solar PV PEMWE, biomass gasification, solar Cu–Cl, and electrolysis using wind energy. The results showed that their cycle had 11-fold less GWP than steam methane reforming without carbon capture and sequestration. Sadeghi *et al.*<sup>31</sup> conducted a comparative economic and life cycle assessment of solar-based hydrogen production systems. The product life cycle model was a cradle-to-gate LCA model that assessed the environmental impact of solar PV PEMWE, solar thermal electrolysis, coal gasification and SMR. Their studies suggested that SMR and coal gasification, although cheap, emit large emissions. In contrast, solar PV PEMWE and solar thermal electrolysis are more environmentally favourable but expensive systems. Bicer and Dincer<sup>14</sup> investigated the impact of ammonia production by applying a PEC PEM reactor under concentrated sunlight. The PEC PEM reactor was based on a Cu<sub>2</sub>O photocathode in a stainless-steel plate with membrane electrode assembly. The analysis showed that the electrochemical ammonia synthesis driven by hydrogen from the PEC reactor significantly reduced the total environmental impact by almost 50% with respect to steam methane reforming-based ammonia production. The comparison between emerging hydrogen production technologies and the conventional SMR process is essential to identify pathways with the most significant potential for reducing environmental impacts and supporting the transition towards more sustainable and low-carbon energy systems.

PEC AEM water splitting is considered one of the most promising technologies for hydrogen production because the process does not emit CO<sub>2</sub> during operation. They use AEM (less expensive and environmentally sustainable metal catalysts other than platinum) under alkaline conditions.<sup>20,21</sup> However, additional technological advancements are necessary for the complete industrial implementation of PEC AEM reactors. Environmental impact assessments should follow prospective studies to provide significant design solutions for developing truly sustainable PEC reactors.<sup>32</sup> However, to the best of our knowledge, no studies have been conducted to estimate the possible environmental advantages of PEC AEM reactors. In this context, the LCA technique provides a framework for quantifying the environmental impacts of hydrogen generation processes.<sup>33</sup> Furthermore, emphasising and quantifying the environmental effects resulting from the manufacture of PEC AEM reactors might aid in shifting toward sustainable development goals (SDG) 12 (“Responsible Production and Consumption”) and SDG 7 (“Affordable and Clean Energy”) through the development of an environmentally friendly hydrogen manufacturing process. Considering the established methodology of LCA, the acquired results might help additional follow-up activities and allow for an analysis of this technology in relation to mature hydrogen production technologies, such as SMR,<sup>34</sup> wind PEMWE,<sup>35</sup> solar PV PEMWE or PEC PEM reactor.<sup>13</sup> The information obtained from LCA can be used as a framework for designing PEC reactors utilising durable and

less toxic materials, thereby mitigating their adverse environmental impacts, particularly in relation to SDGs 14 and 15, which address “life below water” and “life on land,” respectively.

This study examines the cradle-to-gate product life cycle model to evaluate the environmental impacts of six hydrogen production methods: SMR, wind PEMWE, solar PV PEMWE, PEC PEM reactor, and PEC AEM reactor. These methods include several technologies, from the prevalent fossil fuel-based SMR process to cleaner alternatives utilising renewable energy such as solar PV and wind coupled to an electrolyser for electrolysis and advanced PEC integrated systems for solar-based electrochemical water splitting. The results reported in this study can open a new avenue in the area of sustainable PEC AEM reactors. Additionally, assessing their environmental implications can offer a broader understanding of how the environmental impact of PEC AEM reactors may be reduced.

## Methods

LCA is a vital tool for evaluating the potential environmental impacts of a product throughout its entire life cycle. This encompasses the raw material extraction, manufacture, usage, and post-use stages. Each stage of the life cycle has a different influence on the environment. ISO 14040-43 establishes the LCA framework in four distinct phases:<sup>36</sup>

- (a) Definition of goal and scope (ISO 14040)
- (b) Primary materials and energy analysis of all inputs and outputs (ISO 14041)
- (c) Impact assessment (ISO 14042), and
- (d) Results interpretation (ISO 14043)

### Goal and scope definition

This study aims to investigate and analyse the environmental impact of six hydrogen production methods, PEC AEM reactor, PEC PEM reactor, solar PEMWE, wind PEMWE and SMR, using LCA. Lab-scale LCA is a useful instrument for environmental advisory tools for new emerging technologies.<sup>37</sup> The purpose of this study is to offer useful data to direct future investigations on the PEC AEM reactor. The ReCiPe 2016 midpoint approach transforms the obtained life cycle inventory results into a limited number of indicator scores. This study relies on midpoint indicators to maintain transparency and minimize uncertainty. Life cycle impact assessment (LCIA) results are easier to read when midpoints are converted to endpoints. However, the level of uncertainty rises with each aggregate stage.<sup>5</sup> The impact indicators are categorised into 18 environmental impact categories: global warming, particulate matter, stratospheric ozone depletion, fossil resources, freshwater ecotoxicity, global warming, freshwater eutrophication, human toxicity (cancer), human toxicity (non-cancer), ionising radiation, land use, marine ecotoxicity, marine eutrophication, terrestrial acidification, terrestrial ecotoxicity, and water use.

The study model's hydrogen production in India for the year 2025 using SimaPro software (version 9.4.0.3) and the Ecoinvent v3.8 dataset (released in September 2021), which is valid



through 2024. The environmental impacts of hydrogen production methods are investigated from a cradle-to-gate perspective. The impact assessment method chosen for this study is ReCiPe 2016 Midpoint (H). The consensus model, also known as the Hierarchist model of ReCiPe, is used in this research because of its widespread applicability in various scientific models. This method is based on commonly accepted timeframes and other considerations.<sup>38</sup> The scant information concerning the end-of-life of photoelectrochemical reactors, coupled with their early-stage (non-mature) technological

development, poses challenges to carrying out LCA studies from a cradle-to-gate perspective.<sup>28</sup> In addition to the limited end-of-life data, the operation phase of the PEC systems was excluded owing to minimal direct emissions and the lack of standardised performance data at this early stage of technological development. Additionally, recycling has not been given much consideration. However, recycling impacts are essential for a comprehensive understanding of the environmental impacts resulting from PEC reactors.<sup>33</sup> A functional unit of one kilogram of hydrogen produced is employed, a standard

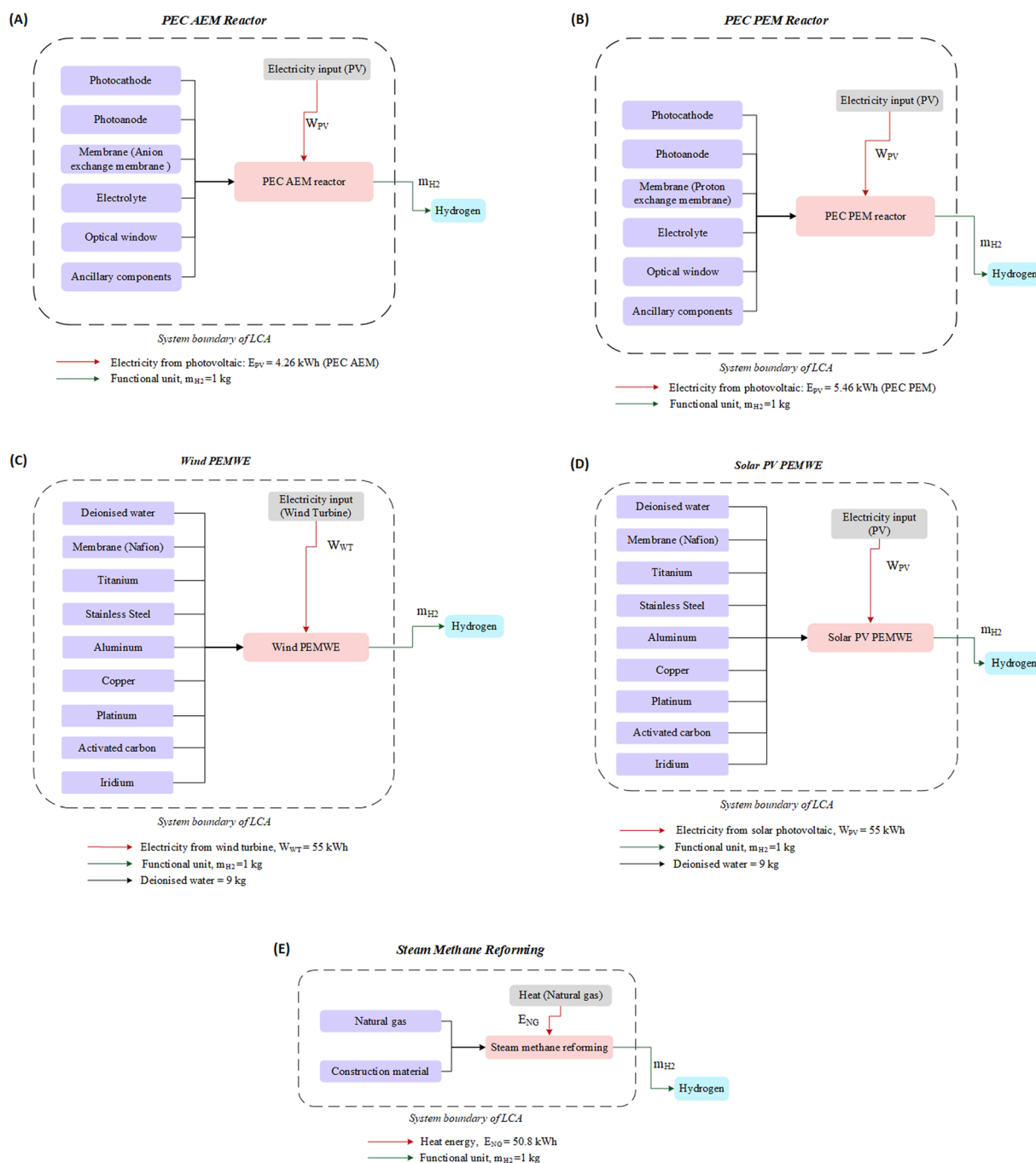


Fig. 1 System boundary for life cycle assessment of different hydrogen production methods: (A) PEC AEM reactor, (B) PEC PEM reactor, (C) solar PV PEMWE, (D) wind PEMWE and (E) steam methane reforming (SMR).



approach in life cycle assessment studies on hydrogen production methodologies.<sup>39</sup> This standardisation allows for a straightforward but accurate comparison with various hydrogen production processes.

### Inventory for material and energy input

The fabrication of hydrogen production processes is modelled utilising secondary data from published research articles. Material and energy inputs are necessary for the life cycle inventory phase. Here, the material resources, energy flows and emissions are quantified. The inventory for different hydrogen production techniques is described in this section.

### Photoelectrochemical AEM reactor

PEC water splitting is regarded as one of the most promising ways for hydrogen production because it utilises the renewable energy of solar light and does not produce direct CO<sub>2</sub> emissions.<sup>40</sup> PEC reactors consist of two photoelectrodes, a membrane, an electrolyte and a compartment in a single integrated system. Membranes enable the selective movement of ions, making them a crucial part of PEC reactors. They facilitate the effective operation of electrochemical processes, maximizing hydrogen production and minimizing recombination reactions.<sup>16</sup> The constraints of proton and alkaline exchange membranes have been successfully resolved by significant developments in AEM.<sup>17</sup> Anion exchange membranes can be used in low-alkaline electrolytes or even deionised water.<sup>19</sup> Moreover, a non-corrosive environment eliminates the necessity for expensive catalysts from platinum group metals and allows for the utilisation of more cost-effective intermediate metal group catalysts,<sup>20</sup> such as nickel. The membrane utilized in the PEC AEM reactor comprises a quaternary ammonium cation, which has high alkaline stability and is more economical.<sup>21</sup> Generally, AEM technology is characterized by low cost and high stability, making it an efficient option for hydrogen production<sup>41</sup> in photoelectrochemical reactors. The system boundary for the PEC AEM reactor is illustrated in Fig. 1A.

The energy efficiency of the PEC AEM reactor is denoted as follows:

$$\eta_{\text{PEC\_AEM}} = \frac{\dot{m}_{\text{H}_2} \times \text{LHV}_{\text{H}_2}}{\dot{W}_e + I_r A_i}, \quad (1)$$

where  $\dot{m}_{\text{H}_2}$  is the hydrogen mass flow rate,  $\dot{W}_e$  is the electrical energy harvested from a solar PV panel, LHV represents the lower heating value,  $I_r$  represents the input solar radiation and  $A_i$  is the incident area of the reactor.

The material inventory for building the PEC AEM reactor is presented in Table 2 and is obtained from a study by Karaca *et al.*<sup>13</sup> However, an external electrical input of 4.26 kWh is required to power the PEC for one kilogram of hydrogen production. The membrane surface area was 254 cm<sup>2</sup>. The operating specifications for the PEC AEM reactor described in Table 1 were calculated from the electrochemical mathematical modelling carried out in a previous study by Tarique *et al.*<sup>42</sup>

**Table 1** Operational parameters of the PEC AEM reactor in the LCA study<sup>a</sup>

| Parameter                                     | Amount                  |
|---|-------------------------|
| Input electricity (W)                         | 0.7                     |
| Solar power input (W)                         | 52.2                    |
| Hydrogen mass flow rate (kg s <sup>-1</sup> ) | 45.6 × 10 <sup>-9</sup> |
| Energy efficiency (%)                         | 11.23                   |

<sup>a</sup> Source: Tarique *et al.*<sup>42</sup>

**Table 2** Material requirements for 1 kg of hydrogen production for a PEC reactor<sup>a</sup>

| Component                      | Mass (kg) |
|--------------------------------|-----------|
| Flanges (PVC)                  | 6.58      |
| Optical window (acrylic glass) | 2.40      |
| Bolts                          | 2.05      |
| Nuts                           | 0.26      |
| Metal washers                  | 0.19      |
| Gaskets                        | 0.75      |
| Electrode (flat disc.)         | 2.94      |
| Electrode (conic disc.)        | 2.84      |
| Tubing (vinyl)                 | 0.27      |
| Connectors                     | 0.04      |

<sup>a</sup> Source: Karaca *et al.*<sup>13</sup>

The material needs for the production of 1 m<sup>2</sup> AEM were calculated based on an experimental study carried out by Zhang *et al.*<sup>43</sup> The requirements were obtained by thermodynamic heating and boil-off of the solvents and unreacted compounds in the experiment, and the power of stirring was not considered. The membrane weight was calculated to be 3.4 mg cm<sup>-2</sup> based on the area of the membrane, stoichiometry of the reactions and molecular weight of the membrane. Table 3 illustrates the inventory for membrane manufacturing.

### Photoelectrochemical PEM reactor

The material and energy inputs for the life cycle inventory analysis phase were obtained from the available literature. The novel geometry of the PEC PEM reactor was developed by the Clean Energy Research Laboratory (CERL), Ontario Tech.<sup>13</sup> The photoelectrochemical reactor developed uses a p-type Cu<sub>2</sub>O semiconductor coated in stainless steel mesh as a photocathode, and the photoanode is TiO<sub>2</sub> coated in stainless steel mesh. Moreover, the membrane in the reactor consisted of Nafion 117 (a proton exchange membrane) with a catalyst coating of PtB (3 mg cm<sup>-2</sup> at the cathode side) and IrRuO<sub>x</sub> (3 mg cm<sup>-2</sup> at the anode side). The material inventory for a photoelectrochemical reactor with PEM as a membrane is determined by Karaca and Dincer.<sup>13</sup> Additionally, for 1 kg of H<sub>2</sub> generation, the necessary external power to the PEC PEM reactor is computed as 5.46 kWh. The operational parameters of the PEC PEM reactor are presented in Table 4. Fig. 1B depicts a description of the system boundary using LCA analysis for H<sub>2</sub> generation using a PEC PEM reactor.



**Table 3** Detailed life cycle inventory of the anion exchange membrane<sup>a</sup>

| Materials requirements  | Value  |
|---|--------|
| Polysulfone (g)   | 21     |
| <i>N,N</i> -Dimethylacetamide (DMAc) (g)                      | 468    |
| Chloromethylmethylether (CMME) (g)                            | 35     |
| Imidazole (g)   | 7      |
| NaOH (g)  | 3      |
| Methanol (g)  | 16     |
| Water, cooling, unspecified (m <sup>3</sup> )                 | 0.0015 |
| Water, completely softened (g)                                | 171    |
| Energy and processing requirements                            |        |
| Heat, other than natural gas (kJ)                             | 7      |
| Steam in the chemical industry (g)                            | 2      |
| Electricity (Wh)  | 22     |
| Heat, natural gas (kJ)  | 20     |
| Heat, unspecified, at chemical plant (boil-off solvents) (kJ) | 0.305  |

<sup>a</sup> Source: Zhang *et al.*<sup>43</sup>**Table 4** Factors evaluated in the LCA study of the PEC PEM reactor for green hydrogen production<sup>a</sup>

| Parameter   | Value                   |
|---|-------------------------|
| Input electricity (W)                               | 0.9                     |
| Solar power input (W)                               | 52.2                    |
| Mass flow rate H <sub>2</sub> (kg s <sup>-1</sup> ) | 47.1 × 10 <sup>-9</sup> |
| Energy efficiency (%)                               | 6.3                     |

<sup>a</sup> Source: Karaca *et al.*<sup>13</sup>

### Solar PV PEMWE and wind PEMWE

Proton exchange membrane water electrolysis (PEMWE) is a promising technology for hydrogen production from renewable energy sources. Direct current (DC) power is derived from sustainable energy sources, such as solar, wind, and biomass.<sup>44</sup> Solid polysulfonated membranes, which are proton-conducting, such as Nafion, are used in PEMWE technology. The material required to construct 1 MW PEMWE is estimated from a study carried out by Bareiß *et al.*<sup>35</sup> Table 5 shows the life cycle inventory for constructing 1 MW PEMWE and is described in Fig. 1C as a construction material.

The power consumption of a PEMWE producing 1 kilogram of H<sub>2</sub> with a 60% energy efficiency is calculated using eqn (2):

$$\eta_{\text{PEMWE}} = \frac{\dot{m}_{\text{H}_2} \times \text{LHV}}{\dot{W}_{\text{elec}}} \quad (2)$$

where LHV represents the lower heating value of hydrogen (120.1 MJ kg<sup>-1</sup>).

The estimated electricity usage for producing 1 kilogram of hydrogen using PEMWE is calculated to be 55.6 kWh (200.17 MJ). The LCA considers the power input from “wind and solar PV independently” for the PEMWE. Fig. 1C and D depict the

**Table 5** Construction material requirements for 1 MW PEMWE<sup>a</sup>

| Material         | Mass (kg) |
|------------------|-----------|
| Titanium         | 528       |
| Stainless steel  | 100       |
| Aluminium        | 27        |
| Nafion           | 16        |
| Copper           | 4.5       |
| Activated carbon | 9         |
| Iridium          | 0.75      |
| Platinum         | 0.075     |

<sup>a</sup> Source: Bareiß *et al.*<sup>35</sup>

system boundary of a life cycle analysis for H<sub>2</sub> generation using wind PEMWE and solar PV PEMWE.

### Steam methane reforming

Steam methane reforming is the most widely used method for the production of hydrogen, contributing to about 50% of the world's hydrogen production.<sup>45</sup> Methane and steam react over a nickel-based catalyst at a high temperature (900 °C) and high pressure (3–25 bar) in the well-established commercial process of reforming natural gas to produce hydrogen.<sup>46</sup> Moreover, the resultant combination can be used to manufacture various products, including different organic chemicals. It is popularly known as synthesis gas (or syngas). The SMR hydrogen production facility is described by hydrogen production and petroleum refinery operation, and the dataset is readily available in the ecoinvent database v3.8. Building the plant in the software was, therefore, not necessary. Fig. 1E illustrates the system boundary of an LCA study of the SMR process. For the life-cycle analysis of the SMR-based hydrogen production process, the Ecoinvent v3.8 database is used. A petroleum refinery is incorporated into the production facility. The energy requirements are supplied on-site by burning natural gas in a gas engine. Table 6 outlines the operating parameters used in the study of SMR hydrogen generation.

## Results and discussion

A life cycle assessment was carried out using a cradle-to-gate system boundary to evaluate the environmental impacts of the

**Table 6** Operating parameters used in the study of steam methane reforming hydrogen generation<sup>a</sup>

| Parameter  | Value                  |
|--|------------------------|
| Energy consumption per kg of H <sub>2</sub> produced (kWh) | 50.8                   |
| Operating lifetime in years                                | 20                     |
| Load factor (%)  | 85                     |
| Annual H <sub>2</sub> yield (kg)                           | 3.18 × 10 <sup>8</sup> |
| Lifetime H <sub>2</sub> yield (kg)                         | 6.36 × 10 <sup>9</sup> |
| Hydrogen plant energy efficiency, based on LHV (%)         | 76                     |
| Hydrogen plant energy efficiency, based on HHV (%)         | 89                     |

<sup>a</sup> Source: Spath and Mann.<sup>34</sup>

PEC AEM reactor. Although the detailed methodology is presented in the methods section, it is important to note here that the life cycle inventories were developed from peer-reviewed literature. The results were later compared using four hydrogen production methods: SMR, wind PEMWE, solar PV PEMWE, and PEC PEM reactor. The insights gained from this LCA study could provide a baseline for a better understanding

of the environmental performance of hydrogen production methods and highlight the broader implications of adopting a PEC AEM reactor for hydrogen production methods. The system boundary is based on the cradle-to-gate reactor life cycle, and the functional unit is 1 kg of H<sub>2</sub> production. The environmental impact is based on 18 indicators, and the characterised LCA results are detailed in this section.

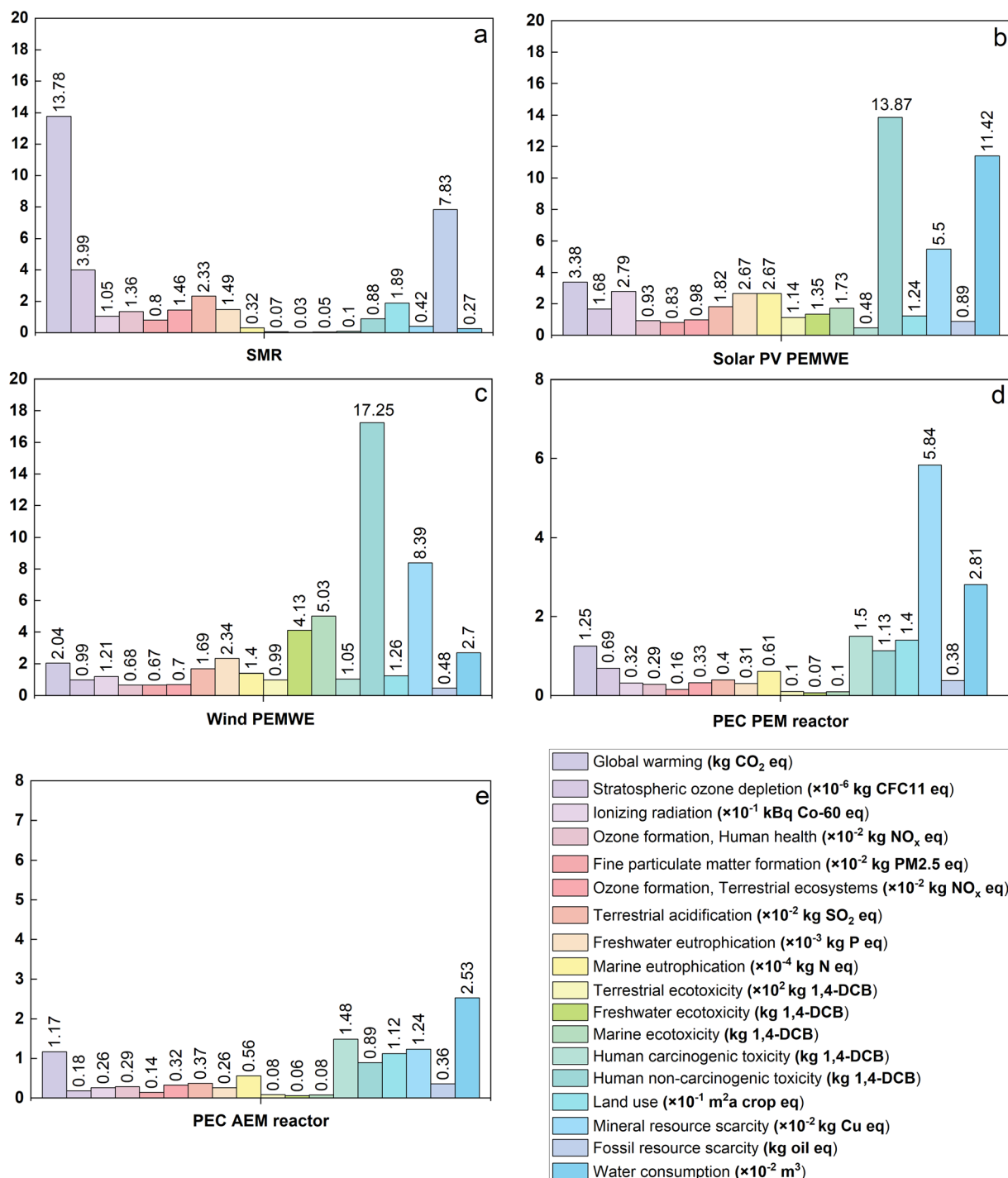


Fig. 2 Environmental impact categorised into 18 impact indicators for different hydrogen production methods: (a) SMR, (b) solar PV PEMWE, (c) wind PEMWE, (d) PEC PEM reactor, and (e) PEC AEM reactor.

## Environmental impact assessment across 18 indicators

Fig. 2 shows the cradle-to-gate environmental impact of the 18 indicators provided by ReCiPe 2016. The lowest impacts are obtained for the PEC AEM reactor (Fig. 2e), while the SMR, solar PV PEMWE, wind PEMWE and PEC PEM reactors bear the more significant impacts.

## Climate and atmospheric impacts

Global warming potential (GWP) is a crucial environmental impact category for assessing renewable energy systems and represents a quantified measure for weighting the climatic impacts of different greenhouse gas (GHG) emissions.<sup>47,48</sup> GWP is expressed in kg CO<sub>2</sub> equivalents and is the amount of energy the emission of 1 ton of gas is absorbed by the emission of 1 ton of CO<sub>2</sub> over a specified period.<sup>49</sup> The current study uses LCA methodology to evaluate the global warming potential of the five hydrogen production methods. Hydrogen production methods include SMR, wind PEMWE, solar PEMWE, PEC PEM, and PEC AEM. The results indicate that the hydrogen production by the PEC AEM reactor has the lowest GWP (1.17 kg CO<sub>2</sub> eq per kg H<sub>2</sub>). For the PEC AEM reactor, the production of acrylic glass shields is the major contributor to GWP and has a relative contribution of 39.53%, while 20.85% comes from PVC manufacturing of the frame. For every kg of polyvinyl chloride (PVC) produced, approximately 2 kg of CO<sub>2</sub> is emitted<sup>50</sup> and relies on ethylene derived from oil.<sup>51</sup> The PEC PEM reactor has the second lowest GWP (1.25 kg CO<sub>2</sub> eq per kg H<sub>2</sub>), followed by wind PEMWE and solar PV PEMWE. The GWP of SMR is highest at 13.78 kg CO<sub>2</sub> eq per kg H<sub>2</sub>. Hydrogen production by steam methane reforming relies on fossil fuels for energy and feedstock, resulting in CO<sub>2</sub> production.<sup>13</sup> The GWP of hydrogen production *via* SMR has been widely reported in the literature in the range of 10–14 kg CO<sub>2</sub> eq per kg H<sub>2</sub>, depending on the methodological approach and system boundary description.<sup>52</sup>

Stratospheric ozone depletion (SODP) is the thinning of the stratospheric ozone layer and is caused by emissions of chlorofluorocarbons (CFCs), halons and NO<sub>x</sub>.<sup>53</sup> This depletion allows increased levels of UV-B radiation to reach the earth's surface and damages human and animal health.<sup>54</sup> The ODP is expressed in kg CFC-11 equivalents. Based on the findings of the study, it is estimated that SMR has the highest SODP ( $3.99 \times 10^{-6}$  kg CFC-11 eq per kg H<sub>2</sub>). The largest contributor is halon 1301, which is used as a fire suppressant in mobile and stationary fire extinguishers in industrial facilities. The hydrogen produced by solar PV PEMWE ( $1.68 \times 10^{-6}$  kg CFC-11 eq per kg H<sub>2</sub>) is followed by wind PEMWE ( $0.99 \times 10^{-6}$  kg CFC-11 eq per kg H<sub>2</sub>) and PEC PEM ( $0.69 \times 10^{-6}$  kg CFC-11 eq per kg H<sub>2</sub>). The manufacturing of solar-grade silicon for the production of solar PVs is the main cause of high SODP. The lowest SODP impact is from the PEC AEM reactor, which is estimated at  $0.18 \times 10^{-6}$  kg CFC-11 eq per kg H<sub>2</sub>. Regarding the PEC AEM reactor, the manufacturing of steel electrodes (54.61%) and gasket production (34.97%) are the major relative contributors to this impact category. The iron and steel industry has noted unintended CFCs, hydrochlorofluorocarbon (HCFCs), and halon emissions.<sup>55</sup>

## Human health impacts

Ionising radiation (IR) is an environmental impact category associated with the harm to human health and ecosystems resulting from radionuclide emissions during a product's life-cycle. This is reported in kBq Co-60 equivalents. According to the LCA study, Solar PV PEMWE ( $2.78 \times 10^{-1}$  kBq Co-60 eq per kg of H<sub>2</sub>) has the highest ionising radiation potential, followed by wind PEMWE ( $1.21 \times 10^{-1}$  kBq Co-60 eq per kg of H<sub>2</sub>) and SMR ( $1.05 \times 10^{-1}$  kBq Co-60 eq per kg of H<sub>2</sub>). It has been determined that the primary source of ionising radiation during the PV panel production process is the aluminium processing step.<sup>56</sup> However, the ionising radiation potential of the PEC PEM and PEC AEM reactors is similar.

The environmental impacts of ozone formation on human health (OFHH) and terrestrial ecosystems (OFTE) are due to the photoelectrochemical reaction of non-methane volatile organic compounds (NMVOCs) or nitrogen oxides (NO<sub>x</sub>) emitted into the atmosphere. Although ozone can negatively affect human health and cause respiratory problems when inhaled, it can also prevent vegetative development and resilience, thereby compromising ecosystems. Ozone formation for terrestrial ecosystems and human health is expressed in kg NO<sub>x</sub>-equivalents.<sup>57</sup> SMR has the highest environmental impact in this category, amounting to  $1.36 \times 10^{-2}$  kg NO<sub>x</sub>-eq per kg of H<sub>2</sub> for human health and  $1.46 \times 10^{-2}$  kg NO<sub>x</sub>-eq per kg of H<sub>2</sub> for terrestrial ecosystems, which is followed by solar PV PEMWE. At the same time, the PEC PEM and PEC AEM reactors have a similar impact on human health due to ozone formation ( $0.29 \times 10^{-2}$  kg NO<sub>x</sub>-eq per kg of H<sub>2</sub>).

Fine particulate matter formation (FPMF) comprises tiny airborne particles less than 2.5 µm in diameter. Human health is at risk of these airborne particles, especially for people who have respiratory conditions. In addition to water and biogenic organic species, particulate matter can contain chemical species, such as SO<sub>2</sub>, NO<sub>x</sub>, or volatile organic compounds (VOCs).<sup>57</sup> This is indicated in kg PM 2.5 equivalents. According to the LCA study, hydrogen production by solar PV PEMWE has the highest FPMF and a value of  $0.83 \times 10^{-2}$  kg PM 2.5 eq per kg of H<sub>2</sub>. Nickel processing for PV panel production is a major contributor to FPMF.<sup>56,58</sup> The lowest impact is from the PEC AEM reactor in this category ( $0.14 \times 10^{-2}$  kg PM 2.5 eq per kg of H<sub>2</sub>). The fine particulate matter emissions are mostly from upstream processes, such as material extraction and solar panel manufacture, not the operational phase of solar energy production. These emissions were included for methodological consistency although they are not regarded as a major social problem in the context of renewable energy systems.

## Ecosystem and land impacts

Terrestrial acidification (TA) is caused by the deposition of acidifying compounds in the atmosphere and is expressed in kg SO<sub>2</sub>-equivalents.<sup>59</sup> According to the comparative LCA study findings, solar PV PEMWE has the highest environmental impact owing to terrestrial acidification and has a value of  $1.82 \times 10^{-2}$  kg SO<sub>2</sub> eq per kg H<sub>2</sub>. It is succeeded by hydrogen production using SMR ( $2.33 \times 10^{-2}$  kg SO<sub>2</sub> eq per kg H<sub>2</sub>). The



primary cause of the terrestrial acidification impact category is nickel processing in PV manufacturing.<sup>56</sup> The lowest terrestrial acidification is of the PEC AEM reactor ( $0.37 \times 10^{-2}$  kg SO<sub>2</sub> eq per kg H<sub>2</sub>).

Freshwater eutrophication (FE) exhibits alterations in species probability density functions (PDFs), which correlate with total phosphorus concentration and are influenced by the type of freshwater (rivers or lakes), the group of species (heterotrophs and autotrophs), and climatic conditions.<sup>60</sup> It is expressed in kg P equivalents. Among the evaluated hydrogen production processes, it can be observed from Fig. 2b that solar PV PEMWE appears to have the highest freshwater eutrophication environmental impact of  $2.67 \times 10^{-3}$  kg P-eq per kg of H<sub>2</sub> and is also evident by the findings of the study by Celik.<sup>61</sup> The second highest freshwater eutrophication is obtained from wind PEMWE  $2.34 \times 10^{-3}$  kg P eq per kg of H<sub>2</sub>. PEC AEM reactor has the lowest freshwater eutrophication of  $0.26 \times 10^{-3}$  kg P-eq per kg of H<sub>2</sub>. Acrylic glass shield production has a relative environmental impact of 70.84% in this category.

Marine eutrophication (ME) is an ecological reaction in coastal waterways that introduces nutrients, mainly nitrogen (N), which can have severe effects. Nitrogen enrichment promotes planktonic growth, promotes organic carbon cycles and could cause oxygen depletion.<sup>62</sup> Solar PV PEMWE has a marine eutrophication value of  $2.67 \times 10^{-4}$  N-eq per kg of H<sub>2</sub>, followed by wind PEMWE  $1.4 \times 10^{-4}$  N-eq per kg of H<sub>2</sub>, PEC PEM reactor ( $0.61 \times 10^{-4}$  N-eq per kg of H<sub>2</sub>) and PEC AEM reactor ( $0.56 \times 10^{-4}$  N-eq per kg of H<sub>2</sub>).

The toxicity potential (TP) of a chemical emission is described in kg 1,4-dichlorobenzene-equivalents (1,4 DCB-equivalents). It is used as a characterisation factor at the midpoint level for freshwater ecotoxicity, human toxicity, terrestrial ecotoxicity and marine ecotoxicity. The ecotoxicological factor indicates a shift in the PDF of species resulting from variations in the concentration of a chemical in the environment. The factors for toxicological effects in humans are calculated separately for carcinogenic and non-carcinogenic impacts, indicating the variation in lifetime disease occurrence resulting from changes in substance intake. According to the LCA results, the PEC PEM reactor has the highest human carcinogenic toxicity potential (HCTP) of 1.5 kg 1,4 DCB-eq per kg H<sub>2</sub>. Similarly, the second-highest HCTP obtained from the PEC AEM reactor is 1.48 kg 1,4 DCB-eq per kg H<sub>2</sub>. PVC used in the reactor frame of the PEC system accounts for a relative contribution of 99.06% in terms of HCTP. PVC manufacturing uses elemental chlorine, which is a strong oxidant. The manufacturing creates an additional burden with a range of chlorinated compounds, organochlorine waste and byproducts. Most of these chemicals accumulate in the ecosystem, affecting fish, wildlife, and humans, and are dangerous at low doses. Chlorinated dioxins and furans pose significant health risks, even at modest levels of exposure.<sup>63</sup> The environmental impact of Solar PV PEMWE is the most significant among HNCTP, as indicated by its value of 13.86 kg 1,4 DCB-eq per kg H<sub>2</sub>. The second highest HNCTP is obtained from PEMWE coupled to the wind (17.25 kg 1,4 DCB-eq per kg H<sub>2</sub>), followed by PEC PEM (1.13 kg 1,4 DCB-eq per kg H<sub>2</sub>), PEC AEM (0.89 kg 1,4 DCB-eq

per kg H<sub>2</sub>) and SMR (0.88 kg 1,4 DCB-eq per kg H<sub>2</sub>). Metallising and the metal used behind the PV solar panel are key contributors in this environmental impact category and are used in solar PEMWE and partial-assisted electricity production in the cases of PEC PEM and PEC AEM reactors.<sup>64</sup> Furthermore, the primary source of the HNCTP is the sulfidic tailings from copper mining operations used to build wind turbines.<sup>13</sup> Additionally, in this study, terrestrial ecotoxicity, freshwater ecotoxicity and marine ecotoxicity are highest in the case of wind PEMWE and solar PV PEMWE. Wind PEMWE has a terrestrial ecotoxicity value of  $0.99 \times 10^2$  kg 1,4 DCB-eq per kg H<sub>2</sub>; the freshwater ecotoxicity and marine ecotoxicity were investigated to be 4.13 kg 1,4 DCB-eq per kg H<sub>2</sub> and 5.03 kg 1,4 DCB-eq per kg H<sub>2</sub>, respectively. The environmental impact of solar PEMWE reveals a terrestrial ecotoxicity of  $1.14 \times 10^2$  kg 1,4 DCB-eq per kg H<sub>2</sub>. In contrast, freshwater ecotoxicity has a notably higher burden of 1.35 kg 1,4 DCB-eq per kg H<sub>2</sub>. Similarly, marine ecosystems are subjected to a marine ecotoxicity value of 1.73 kg 1,4 DCB-eq per kg H<sub>2</sub>.

Land use (LU) describes the environmental impact of occupying, managing and reshaping land for human purposes. Two significant environmental impacts of land use are declining habitat availability and species variety.<sup>65</sup> Land use is expressed in m<sup>2</sup>a crop-equivalents. This study evaluated the SMR method of hydrogen production as having the highest value in land use (0.189 m<sup>2</sup>a crop-eq per kg H<sub>2</sub>). This is due to the large scale of the facility and infrastructure required in the SMR process. Meanwhile, hydrogen production by applying the PEC AEM reactor has the least impact on land use, with a value of 0.112 m<sup>2</sup>a crop-eq per kg H<sub>2</sub>.

### Resource depletion impacts

Mineral resource scarcity (MRS) is characterised by surplus ore potential (SOP), represented in kg Cu-equivalents. The primary process of mineral resource extraction decreases the ore concentration, ultimately increasing the quantity of ore generated per kg of extracted mineral resource.<sup>66</sup> Regarding MRS, the hydrogen generated by wind PEMWE has the greatest environmental impact, with a value of 0.0839 kg Cu-eq per kg H<sub>2</sub> produced. The mining, processing and manufacturing of permanent magnets for wind turbines involve rare earth elements. Four rare earth elements—neodymium, praseodymium, dysprosium, and terbium—are used to make permanent magnets.<sup>67</sup> The MRS value is followed by solar PV PEMWE (0.055 kg Cu-eq per kg H<sub>2</sub>), PEC PEM reactor (0.0584 kg Cu-eq per kg H<sub>2</sub>), PEC AEM reactor (0.0124 kg Cu-eq per kg H<sub>2</sub>) and SMR (0.0042 kg Cu-eq per kg H<sub>2</sub>). Solar PV PEMWE uses materials such as silver, cadmium, tellurium and indium, which are rare and extracted in only a few regions of the world.<sup>68</sup> Simultaneously, platinum group materials are employed as catalysts in PEC PEM for hydrogen production and are extremely scarce.<sup>69</sup>

The environmental impact associated with mining and the use of non-renewable resources is described by fossil resource scarcity (FRS). It is measured in kilograms of oil equivalents and is evaluated by dividing the higher heating value of the crude oil



by the used fossil fuels. According to the study, the FRS of SMR is the highest and has a value of 7.83 kg oil-eq per kg of H<sub>2</sub> produced. Natural gas is used as a raw material, and heat source is the major contributor to this category,<sup>70</sup> followed by solar PV PEMWE, wind PEMWE and PEC PEM reactor. The lowest FRS is from PEC AEM (0.36 kg oil-eq per kg H<sub>2</sub>). The relative contribution of PVC frame (31.81%), acrylic glass (37%) and steel production (21.13%) are among the highest contributors in this category. The manufacturing of PVC utilises petroleum as a fossil feedstock.<sup>50</sup> Additionally, steel production relies on a traditional blast furnace, which uses high-grade coking coal and is a finite fossil resource.<sup>71</sup>

The key factor in water usage is the amount of freshwater consumption (WC), measured in m<sup>3</sup> of water consumed. Fig. 2b shows that hydrogen produced by solar PV PEMWE contributes the most significant value of water consumption ( $11.42 \times 10^{-2}$  m<sup>3</sup> kg<sup>-1</sup> H<sub>2</sub>). Water usage in the manufacturing processes of solar PV significantly exceeds operational consumption. Water usage in the production of silicon is around 180 kg kg<sup>-1</sup>, while its conversion to multi-crystalline requires about 470 kg kg<sup>-1</sup>; hence, each kWp requires between 3.7 and 5.2 tons of water.<sup>72</sup> Moreover, the consumption of silver paste used in solar cell production involves a large amount of wastewater containing heavy metals and toxic chemicals.<sup>73</sup> If inadequately handled, this wastewater may be discharged into water bodies, contaminating water supplies and adversely affecting aquatic organisms and ecosystems. The water consumption in the PEC AEM reactor is  $2.53 \times 10^{-2}$  m<sup>3</sup> kg<sup>-1</sup> H<sub>2</sub>. The reactor frame of PVC is the major relative contributor (43.10%) in this impact category. The average water usage necessary for polymer production is 3 m<sup>3</sup>/t PVC, as per BREF.<sup>74</sup> The SMR has the lowest water consumption among the evaluated hydrogen production methods.

Among the 18 impact categories, climate and atmospheric impact indicators (GWP and SODP) show the most substantial reduction for solar-based methods compared to SMR. Ecosystem, human health and resource depletion impact indicators show mixed trends depending on the technology. SMR, although currently the most used method for hydrogen production, depends on fossil fuels, making it unsustainable in the long run. Solar PV PEMWE and wind PEMWE use grid electricity and offer cleaner production at the point, but their overall environmental benefits depend significantly on the carbon intensity of the grid. PEC water splitting enables direct solar-to-hydrogen with minimal environmental impact although it remains an emerging technology.

### Characterised LCA results of a PEC AEM reactor

A careful investigation of the distribution of environmental impacts for each photoelectrochemical anion exchange membrane reactor component can offer suggestions for future improvement. Fig. 3 illustrates the comparative contribution of the photoanode, the photocathode, the anion exchange membrane, frame PVC, gaskets, acrylic glass shield, nuts, metal washers, vinyl tubing and connectors. The units corresponding to each impact category are depicted in Fig. 2.

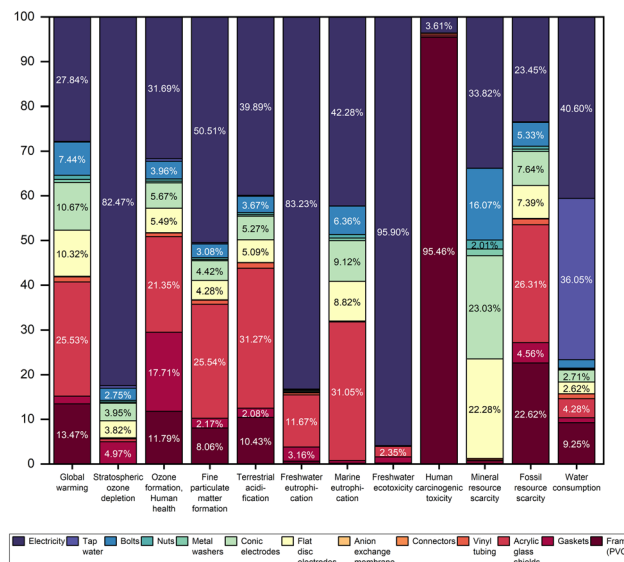


Fig. 3 Environmental impact of PEC AEM reactor components is categorised into 10 important environmental indicators.

The PEC AEM reactor frame is made up of PVC and has a significant environmental influence on human carcinogenic toxicity potential (95.46%), fossil resource scarcity (22.62%) and global warming potential (13.47%). Manufacturing PVC creates an additional burden with a range of chlorinated compounds, organochlorine waste and byproducts. Most of these chemicals accumulate in the ecosystem, affecting fish, wildlife, and humans, and are dangerous at low doses. Moreover, chlorinated dioxins and furan pose significant health risks, even at modest levels of exposure.<sup>63</sup> For every kg of PVC produced, approximately 2 kg of CO<sub>2</sub> is emitted<sup>50</sup> and relies on ethylene derived from oil.<sup>51</sup>

Flat disc electrodes have an environmental impact on categories like mineral resource scarcity (22.28%), global warming (10.32%) and fossil resource scarcity (7.39%). Similarly, the conic electrodes have impacts on mineral resource scarcity (23.03%), global warming (10.67%), marine eutrophication (9.12%), and fossil resource scarcity (7.64%). The manufacturing of steel used for the production of electrodes depends on minerals and is a major contributor to the environmental impact of mineral resource scarcity. Producing steel requires a significant amount of energy based on fossil resources<sup>75</sup> for intensive mining, refining and manufacturing activities responsible for global warming and fossil resource scarcity.

The partial electricity generated by solar PV panels has an environmental impact on freshwater ecotoxicity (95.90%), freshwater eutrophication (83.23%), stratospheric ozone depletion (82.47%), and fine matter particulate formation (50.51%). PV manufacturing produces emissions of toxic substances, such as nitrogen dioxide, sulfur hexafluoride, sulfur dioxide and silicon tetrachloride,<sup>76</sup> which affect the ecosystem. The silicon manufactured is purified using a chemical purification process to remove oxides<sup>77</sup> and produce hyper-pure polysilicon. Mining activities can lead to habitat disruption



and erosion, leading to fine particulate matter formation and nutrient runoffs into freshwater. Acrylic glass shields used as a window to allow solar radiation to fall on the photoelectrode surface have an environmental impact on terrestrial acidification (31.27%), marine eutrophication (31.05%), fossil resource scarcity (26.31%), fine particulate matter formation (25.54%) and global warming (25.53%). The primary environmental problems with PMMA manufacturing are high energy consumption and the need to handle enormous amounts of very dangerous and deadly hydrogen cyanide, which produces ammonium sulphate waste. Consequently, the chemical industry is interested in finding a substitute method. Crude oil and condensate gas are the primary fuels utilized to supply the majority of the energy required to make PMMA,<sup>78</sup> which is responsible for emissions of SO<sub>x</sub> and NO<sub>x</sub>, causing terrestrial acidification. The acetone cyanohydrin (ACH) pathway for producing methyl methacrylate (MMA), the monomer for poly (methyl methacrylate) (PMMA), poses the most significant hazardous risk to aquatic, terrestrial, and atmospheric ecosystems. The ACH route entails toxic substances, including ammonia, hydrogen cyanide, and acetone cyanohydrin, significantly contributing to marine eutrophication.<sup>79</sup>

The gaskets are used in the PEC AEM reactor to prevent leakages and mainly impact ozone formation, human health (17.71%) and stratospheric ozone depletion (4.97%). Vulcanisation, mixing and shaping during rubber manufacturing contribute to VOC species, such as aromatics, *m/p* xylene, naphthalene, *o*-xylene and carbon disulfide and are responsible for ozone formation, impacting human health.<sup>80</sup> Tap water used for electrolysis accounts for 36.05% environmental impact of water consumption. Anion exchange membrane, vinyl tubing, metal washers, connectors, bolts and nuts have the least environmental impact among all the categories.

### Comparison of environmental impacts between PEC PEM and PEC AEM reactors

Fig. 4 shows the relative contributions of the PEC AEM and PEC PEM reactors. A relative comparison is carried out to better understand the environmental impact of PEC AEM and PEC PEM reactors. In this study, eighteen impact indicators were obtained during the life cycle assessment by applying the ReCiPe method, and the ten most influential indicators are illustrated in Fig. 4. The impact category units are not depicted in Fig. 4; however, they are clearly illustrated in Fig. 2. As evident from the figure, PEC AEM has a lower impact in all categories than PEC PEM. Stratospheric ozone depletion, global warming potential, mineral resource scarcity, freshwater ecotoxicity and freshwater eutrophication are among the least.

The relatively higher contribution of the mineral resource scarcity in the PEC PEM reactor (100% vs. 21.18% in the case of the PEC AEM reactor) could be explained using rare earth metals, such as platinum black and IrRuO<sub>x</sub>, as a catalyst<sup>13</sup> in PEC PEM reactors. Stratospheric ozone depletion is caused by chlorofluorocarbons (CFCs), halons and NO<sub>x</sub> emissions. Nafion membrane in this impact category has a relative contribution of 69.24% among the components used, increasing the overall

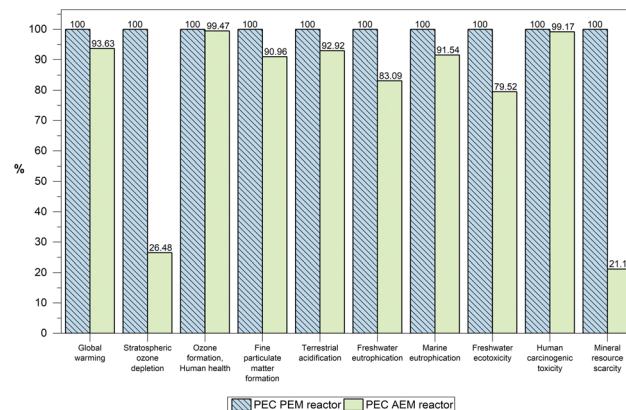


Fig. 4 Comparison between PEC PEM and PEC AEM reactor assembly for the 10 most important impact categories.

stratospheric ozone depletion. In the PEC AEM reactor, the greatest impact is due to PV electricity (82.47%). The synthesis of tetrafluoroethylene, a compound utilised in manufacturing Nafion and several fluoropolymers,<sup>81</sup> dramatically influences the SODP environmental impact category. The amount of electricity from solar PV is the major cause of the impact on freshwater ecotoxicity, freshwater eutrophication and fine particulate matter formation. Electricity from solar panels has a relative contribution of 96.58% and 95.90% for freshwater ecotoxicity in the case of the PEC PEM and PEC AEM reactors, respectively. Similarly, freshwater eutrophication is also influenced by electricity solar panels, with 86.18% relative contribution for PEC PEM and 83.23% for the PEC AEM reactor. PV manufacturing produces emissions of toxic substances, such as nitrogen dioxide, sulfur hexafluoride, sulfur dioxide and silicon tetrachloride,<sup>76</sup> impacting the ecosystem. The silicon manufactured is purified using a chemical purification process to remove oxides<sup>77</sup> and produce hyper-pure polysilicon.

### Sensitivity analysis

A sensitivity analysis was conducted to assess the effect of regional energy supply on the global warming potential associated with hydrogen production methods. The objective was to quantify variations in GWP resulting from regional differences in energy inputs while keeping all other model parameters constant. For steam methane reforming (SMR), the analysis involved varying the natural gas input sourced from combined heat and power (CHP) systems representative of three distinct regions: Europe (EU), India (IN), and the Rest of the World (ROW). This method effectively represents the regional differences in GWP linked to natural gas extraction, processing, and supply chains. However, for electrolysis-based systems (wind PEMWE and solar PV PEMWE) and photoelectrochemical (PEC) systems (PEC PEM and PEC AEM reactors), the sensitivity analysis focused on electricity input. The systems were modelled utilising grid-connected building-integrated photovoltaic (PV) electricity, with scenarios reflecting EU, IN, and ROW circumstances. These scenarios employed SimaPro and ecoinvent information to examine regional solar resources, PV



system performance, and upstream PV manufacturing emissions.

Fig. 5 shows the findings of the sensitivity analysis. The resulting GWP values for SMR were approximately 12.63 kg CO<sub>2</sub> eq per kg H<sub>2</sub> produced for EU, 13.78 kg CO<sub>2</sub> eq per kg H<sub>2</sub> produced for IN and 13.1 kg CO<sub>2</sub> eq per kg H<sub>2</sub> produced for ROW. The results show that the SMR scenario in India (IN) has the greatest effect on GWP. This outcome is expected because of the higher carbon content in India (0.82 kg CO<sub>2</sub> eq per kWh electricity).<sup>82</sup> However, both the electrolysis and PEC pathways were quite sensitive to the availability of electricity in the area. The effect of GWP on solar PV PEMWE ranged from about 5.29 kg CO<sub>2</sub> eq per kg of H<sub>2</sub> in the EU to 3.38 kg CO<sub>2</sub> eq per kg of H<sub>2</sub> in India and 4.24 kg CO<sub>2</sub> eq per kg of H<sub>2</sub> in the ROW (Rest of the World). The PEC PEM reactor produced 1.4 kg CO<sub>2</sub> eq per kg of H<sub>2</sub> in the EU, 1.25 kg CO<sub>2</sub> eq per kg of H<sub>2</sub> in IN, and 1.44 kg CO<sub>2</sub> eq per kg of H<sub>2</sub> in ROW. The PEC AEM reactor produced 1.27 kg CO<sub>2</sub> eq per kg hydrogen in the EU, 1.17 kg CO<sub>2</sub> eq in India, and 1.2 kg CO<sub>2</sub> eq in ROW. The sensitivity analysis shows that the location where the PV system is manufactured and the installation location significantly affect the GWP. This is mostly because of differences in the energy mix, varying solar irradiation and upstream emissions in different regions. The Indian grid relies largely on coal, which makes it carbon-intensive. However, the increased energy yield at high-irradiance installation sites in India counterbalances the higher GWP from PV module production, thereby reducing the GWP.<sup>83</sup> Wind PEMWE showed only small differences between regions, with emissions of about 1.82 kg CO<sub>2</sub> eq per kg of H<sub>2</sub> in the EU and 2.04 kg CO<sub>2</sub> eq per kg of H<sub>2</sub> in India and ROW. Because of cleaner electrical inputs during turbine production and the lower carbon intensity of the grid during operation, wind energy systems in the EU have a lower GWP than those in India.<sup>82</sup> The sensitivity analysis highlights the importance of producing hydrogen using renewable electricity. Implementing renewable hydrogen systems in regions with high solar insolation and integrating

solar PV with low embedded carbon intensity are key strategies for minimising environmental impact.

## Conclusions

Our study describes the cradle-to-gate life cycle assessment to understand the environmental impacts of different hydrogen production methods, such as SMR, wind PEMWE, solar PV PEMWE, PEC PEM reactor and PEC AEM reactor. Inventories describing the material, energy, and input required to extract raw materials, component manufacturing, and reactor assembly are reported for future follow-up studies. ReCiPe 2016 midpoint (H) is used in the study to categorise the environmental impact into 18 standardised impact indicators. The use of 18 midpoint indicators ensures a broad and balanced coverage of environmental impacts, such as fine particulate matter, freshwater ecotoxicity, global warming, ionising radiation, stratospheric ozone depletion, ozone formation (human health, terrestrial ecosystem), human toxicity (carcinogenic and noncarcinogenic), terrestrial acidification, freshwater eutrophication, marine eutrophication, ecotoxicity (freshwater, marine, terrestrial), water consumption, land use and resource scarcity (fossil, mineral). The key findings of this study can be outlined as follows.

- According to the LCA study results, PEC PEM has the highest human carcinogenic toxicity potential (HCTP) and has a value of 1.5 kg 1,4 DCB-eq per kg H<sub>2</sub>. This category is mainly influenced by the PVC production for the reactor frame, which involves vinyl chloride, a known human carcinogen. The HCTP for SMR is the lowest among the compared cases, with a value of 0.1 kg 1,4 DCB-eq per kg H<sub>2</sub>.

- The relatively higher contribution of the MRS in the photoelectrochemical proton exchange membrane reactor (100% vs. 21.18% in the case of the PEC AEM reactor) could be explained using rare earth metals, such as platinum black and IrRuO<sub>x</sub>, as a catalyst.

- The hydrogen produced by wind PEMWE has the most significant environmental burden according to the scarcity of mineral resources, representing a value of 0.0839 kg Cu-eq per kg H<sub>2</sub>.

- In this comparative LCA study, the hydrogen production by solar PEMWE has the highest fine particulate matter formation and has a value of  $0.83 \times 10^{-2}$  kg PM 2.5 eq per kg of H<sub>2</sub>.

- The GWP of SMR is the highest at 13.78 kg CO<sub>2</sub> eq per kg H<sub>2</sub> and is mainly due to the use of fossil fuels. This highlights the urgent need to move towards renewable energy-based hydrogen production pathways.

- The findings suggest that hydrogen production by the photoelectrochemical anion exchange membrane reactor contributes the least to GWP (1.17 kg CO<sub>2</sub> eq per kg of H<sub>2</sub>).

- The sensitivity analysis highlights the importance of producing hydrogen using renewable electricity. Implementing renewable hydrogen systems in regions with high solar irradiation and integrating solar PV with low embedded carbon intensity are key strategies for minimising environmental impact.

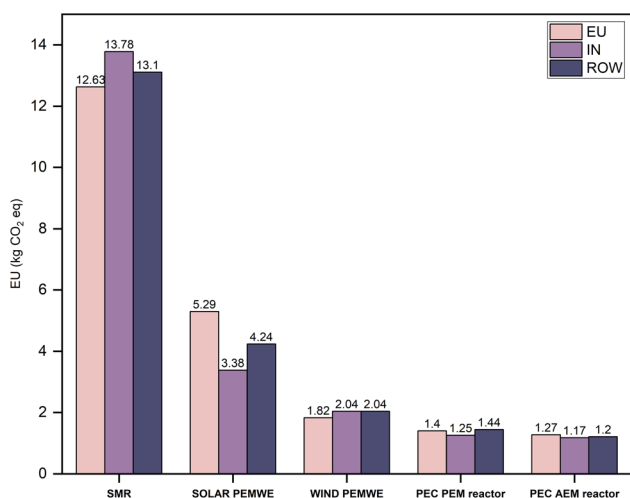


Fig. 5 Global warming impacts for 1 kg H<sub>2</sub> production using various hydrogen production methods and different energy and electricity sources.



This study serves as an initial attempt to assess the environmental implications of the PEC AEM reactor for hydrogen production. The combined LCA results may guide the transition from laboratory-scale research to the practical application of PEC hydrogen reactors. The results presented here highlight the environmental suitability of the PEC hydrogen reactor, offering valuable insights into the future eco-design of sustainable hydrogen production methods. PEC reactors adhere to SDG 7 (Affordable and Clean Energy) and SDG 12 (Responsible Consumption and Production), with a lower environmental impact than other hydrogen production technologies. As mentioned above, the impact may diminish in the near future owing to increased PEC manufacture, the possible replacement of membranes and the recycling of components.

## Author contributions

V. P.: writing—original draft, visualisation, literature review, and data collection and analysis. F. K.: conceptualisation, supervision, writing, review, and critical editing.

## Conflicts of interest

The authors declare no competing interests.

## Data availability

The authors confirm that the data supporting the findings of this study are available within the article. The data will also be shared on request.

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