

# Uncovering the true cost of hydrogen production routes using life cycle monetisation

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## HIGHLIGHTS

- Environmental externalities are crucial to sustainability assessments.
- Economical plus monetised LCA impacts provides an estimate of true cost of hydrogen.
- Ten hydrogen production technologies were assessed and compared on monetary basis.
- At present, steam methane reforming with CCS emerged as the most promising option.

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## ABSTRACT

Hydrogen has been identified as a potential energy vector to decarbonise the transport and chemical sectors and achieve global greenhouse gas reduction targets. Despite ongoing efforts, hydrogen technologies are often assessed focusing on their global warming potential while overlooking other impacts, or at most including additional metrics that are not easily interpretable. Herein, a wide range of alternative technologies have been assessed to determine the total cost of hydrogen production by coupling life-cycle assessments with an economic evaluation of the environmental externalities of production. By including monetised values of environmental impacts on human health, ecosystem quality, and resources on top of the levelised cost of hydrogen production, an estimation of the “real” total cost of hydrogen was obtained to transparently rank the alternative technologies. The study herein covers steam methane reforming (SMR), coal and biomass gasification, methane pyrolysis, and electrolysis from renewable and nuclear technologies. Monetised externalities are found to represent a significant percentage of the total cost, ultimately altering the standard ranking of technologies. SMR coupled with carbon capture and storage emerges as the cheapest option, followed by methane pyrolysis, and water electrolysis from wind and nuclear. The obtained results identify the “real” ranges for the cost of hydrogen compared to SMR (business as usual) by including environmental externalities, thereby helping to pinpoint critical barriers for emerging and competing technologies to SMR.

## 1. Introduction

Global decarbonisation of energy services is required to minimise the potentially catastrophic risks of anthropogenic climate change [1]. Given its suitability across a range of energy applications and carbon-neutrality at the point-of-use, hydrogen as a ‘green’ energy vector offers a unique cross-system opportunity for fundamental change in the energy landscape.

Of the 60 million tonnes of hydrogen currently produced per annum,

however, approximately 96% are derived from the reforming of fossil fuel feedstocks (49% natural gas, 29% liquid hydrocarbons, and 18% coal), resulting in high indirect CO<sub>2</sub> emissions [2]. The remaining 4% is produced *via* the electrolysis of water, which is only considered as a low-carbon source if low-carbon electricity with low embodied emissions is used [3,4]. Furthermore, renewable energy-based processes cannot produce hydrogen at a price or scale that is competitive with fossil fuels [5,6]. A major hindrance to the economic production of renewable-based hydrogen is the substantial capital expenditure (CAPEX)

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required [7]. The upfront financial burden combined with the low capacity factors of renewable energy assets make such processes prohibitively expensive to compete with incumbent technologies [8,9]. However, as the long-term costs associated with externalities, i.e., indirect costs linked to environmental impacts, of fossil fuels are typically excluded from such comparisons, the “real” total cost of hydrogen production remains unclear.

Some works studied the merits of alternative hydrogen production pathways considering direct production costs and emissions (CO<sub>2</sub>-equivalent). Dincer et al. [10] compared 19 different hydrogen production pathways based on renewable and non-renewable sources in terms of environmental impact, cost, energy, and exergy efficiencies. Their study quantified the social cost of carbon (\$/t CO<sub>2</sub>-equivalent) to evaluate the economic consequences of CO<sub>2</sub>-equivalent emissions. Their findings suggested that hybrid nuclear thermochemical cycles are promising candidates for low-cost and low-environmental impact hydrogen. Ewan et al. [11] compared 14 hydrogen production technologies according to CO<sub>2</sub> emissions, power density, land use, and production costs using an overall Figure of Merit. The study found that ‘high energy density’ technologies using primary energy sources (i.e., nuclear, natural gas, and coal) had an order of magnitude higher ‘merit values’. Machhammer et al. [12] studied six hydrogen production technologies in terms of cost and carbon footprint, concluding that methane pyrolysis is the most promising technology to produce low-cost and low-carbon footprint hydrogen. Speirs et al. [13] investigated the costs and greenhouse gas emissions of nine hydrogen production routes with a focus on studying the supply chain contributions to the total process emissions. They found that low-carbon hydrogen supply chains had highly variable and non-negligible emissions contributions to the life cycle total. Parkinson et al. [5] investigated the cradle-to-gate life cycle emissions and costs of 12 hydrogen production routes, comparing each route to steam methane reforming (SMR) via the Levelised Cost of Carbon Mitigation and a set of decarbonisation metrics. The results showed that the most cost-effective methods of decarbonisation still utilised fossil-feedstocks, but only achieved moderate levels of decarbonisation.

Other works have explicitly focussed on quantifying the environmental impacts of hydrogen production technologies through life-cycle assessments (LCA). Valente et al. [14] conducted comparative LCAs of 23 hydrogen production routes from non-renewable sources (coal, natural gas, oil, and nuclear) and renewable sources (wind, solar, hydropower, biomass, and geothermal), with a focus on their acidification potential. The authors recommended using harmonised life-cycle impacts covering the global warming potential (GWP), cumulative non-renewable energy demand, and acidification potential indicators in the evaluation of these systems. Moreno et al. [15] carried out an LCA of hydrogen production using different biomass feedstocks in Spain, focussing on global warming potential, acidification potential, eutrophication potential, and energy consumption (MJ/kgH<sub>2</sub>). The authors identified wastes from forestry as the most promising raw materials for hydrogen from biomass gasification (BG) routes. Utgikar et al. [16] also conducted an LCA of hydrogen production via high-temperature electrolysis from nuclear energy, compared with SMR, biomass gasification, solar photovoltaics (PV), and wind electrolysis. The LCA comparison focused on two environmental indicators, i.e., global warming potential and acidification potential, identifying hydrogen production from high-temperature electrolysis as a promising route relative to the SMR. Koroneos et al. [17] performed an LCA of six hydrogen production routes, comparing SMR with water electrolysis with energy supplied via solar PV, wind, biomass gasification, hydropower, and solar thermal. The LCA covered four environmental categories, namely global warming potential, acidification potential, eutrophication potential, and winter smog effect. The study concluded that, of the technologies assessed, solar PV electrolysis exhibited the worst environmental impacts due to the high acidification potential in the manufacturing phase of the PV panels and the very low efficiency of PV systems [17].

LCA-based approaches have been widely adopted to build strong cases, rooted in quantitative analysis, to replace fossil fuel-based technologies by ‘greener’ alternatives. However, LCA studies often focus on a reduced subset of technologies and tend to overlook environmental impacts beyond climate change. Notably, the LCA studies previously reported have typically focussed on global warming potential and energy consumption as environmental indicators of interest. Unfortunately, ‘burden-shifting,’ i.e., improving one impact at the expense of worsening others (or the same impact at a global level when considering the entire life cycle of the product), often arises in science and engineering [18]. Hence, when trade-offs are present between impact metrics, the severity of burden-shifting must be further investigated using tailored approaches applied to the standard LCA results.

Two recent studies by Valente et al. [19] and González et al. [20] enlarged the scope of conventional LCA’s applied to hydrogen generation to include the costs of environmental externalities. The study by Valente et al. [19] was the first to monetise the environmental externalities of hydrogen production routes (SMR and biomass gasification). To this end, it applied the ‘eco-efficiency’ concept and the monetisation factors for human health (HH) and climate change reported in the CASES project dataset by Porchia and Bigano [21]. They concluded that biomass gasification is a promising alternative to the conventional SMR production pathway [19]. Gonzalez et al. [20] assessed the environmental impacts of hydrogen production from non-fossil routes (wind, solar, biomass, and nuclear) as a feedstock for methanol production using data from Ecoinvent [22] accessed via SimaPro [23]. They performed a monetisation analysis based on the ReCiPe 2016 [24] and applied the recently developed concept of planetary boundaries to demonstrate that fossil methanol is globally unsustainable.

Previous studies have focused on the ranges and variations of the levelised cost of hydrogen (LCOH), life cycle emissions, and subsets of other environmental indicators from various stages of production. These works have led to various conclusions of the ‘best’ hydrogen production route depending on the environmental factors included. The studies have highlighted, however, that ‘low-environmental impacts’, even for the renewable-based routes, are not guaranteed when the full supply chain is evaluated. In this context, the transition to more sustainable hydrogen generation systems should be underpinned by sound assessments of the available technologies accounting for the additional costs of the environmental impacts over the entire supply chain and point of generation. So far, however, no single work has presented a comprehensive assessment of the most promising hydrogen production technologies considering simultaneously their cost and externalities due to impacts on human health, ecosystem quality (EQ), and resources depletion (RD).

To contribute to filling this gap, herein a detailed assessment of hydrogen production is presented covering ten different technologies (Table 1), i.e., methane, coal, and biomass gasification (with and without carbon capture and storage), methane pyrolysis, and electrolysis (from wind, nuclear and solar), and spanning impacts on HH, EQ,

**Table 1**  
Production technologies investigated in this analysis and their technology readiness level (TRL), as described in Ref. [25].

No.	Technology name	Short name	TRL
1	Steam methane reforming	SMR	9
2	Steam methane reforming with CCS	SMR + CCS	7–8
3	Coal gasification	CG	9
4	Coal gasification with CCS	CG + CCS	6–7
5	Methane pyrolysis	CH <sub>4</sub> pyrolysis	3–5
6	Biomass gasification	BG	5–6
7	Biomass gasification with CCS	BG + CCS	3–5
8	Electrolysis from wind energy	Wind	9
9	Electrolysis from solar PV energy	Solar PV	9
10	Electrolysis from nuclear energy	Nuclear	9

CCS = carbon capture and storage. PV = photovoltaics.

and RD. The latter are monetised to uncover the real cost of every technological route, which allows identifying the ‘lowest total cost’ pathway for at-scale hydrogen production. Hence, no previous studies have performed such an analysis covering the breadth of technologies considered here for a cradle-to-gate, pressurized hydrogen supply. Notably, the study focuses on identifying if the ranges of additional costs incurred, when environmental externalities are accounted for, contribute significantly to the total cost of hydrogen (TCH). Therefore, we address the following questions:

- i. What are the real costs of a proposed hydrogen production technology compared with SMR (business as usual) considering the future (often unaccounted for) costs of environmental externalities?
- ii. How do the ranges in monetised life cycle emissions values affect the total cost of production of a technology?
- iii. What are the barriers for potential technologies in terms of their TCH to compete with SMR?

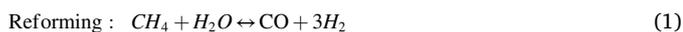
## 2. Materials and methods

### 2.1. Selected hydrogen production technologies:

We consider ten representative technologies for H<sub>2</sub> production (Table 1, data in Table 2). A short description of each route is given next. Note that hydrogen is supplied by all routes at a minimum pressure of 30 bar to be practicable for any downstream uses.

#### 2.1.1. Steam methane reforming with and without carbon capture and storage

The SMR process is a two-step process, as shown in Eq. (1) and (2):



Natural gas is the main feedstock for SMR, which mostly comprises methane, mixed with various hydrocarbons and CO<sub>2</sub>. During the reforming, the feedstock reacts with steam at high temperature (Eq. (1)). Thereafter, carbon monoxide (CO) and hydrogen are produced together with the unreacted natural gas. Next, additional steam is introduced to react with CO to recover additional hydrogen and convert CO to CO<sub>2</sub> in a water-gas shift reaction (WGSR – Eq. (2)). The overall process efficiency

is approximately 76% (CH<sub>4</sub> to H<sub>2</sub> on a higher heating basis) [26]. The SMR process emits large amounts of CO<sub>2</sub>, which can be reduced by deploying a carbon capture and storage system, where the flue gases are removed and separated from the products stream. Thereafter, 90% of the CO<sub>2</sub> is absorbed with an amine solvent (monoethanolamine - MEA). The treated flue gas stream is vented into the atmosphere. CO<sub>2</sub> is thereafter thermally desorbed and compressed at 110 bar for storage [27]. The energy efficiency for SMR + CCS is 68% (CH<sub>4</sub> to H<sub>2</sub> on a higher heating basis), mainly due to the energy required to regenerate the MEA and the electricity required for compression. Thus, relative to the base case without CCS, the additional energy consumption expressed in heat provided by methane (assuming methane was used as a heat source for the stripper of the CCS plant and to produce the electricity for compression) amounts to 3.79 MJ CH<sub>4</sub>/kg CO<sub>2</sub> captured. This figure fits within the range stated in the literature (from 3.6 to 4 MJ CH<sub>4</sub>/kg CO<sub>2</sub> captured [28–30]). Furthermore, the CO<sub>2</sub> emissions from the capture process amount to 0.21 kg CO<sub>2</sub>/kg CO<sub>2</sub> captured, based on the work by Farajzadeh *et al.* [31]. Further details on the calculations are available in section 2 in the Electronic Supplementary Information (ESI).

In both cases (with and without CCS), hydrogen is further purified to 99.99% after the WGSR in a pressure swing adsorption unit, which is also used in the coal gasification (CG) and BG technologies [26].

#### 2.1.2. Methane pyrolysis

Pyrolysis processes decompose hydrocarbons into solid carbon and hydrogen (Eq. (3)) at high temperatures (thermally or catalytically) [32]. As no oxygen is present, no carbon oxides are formed, potentially eliminating the need for secondary processing steps such as the WGSR and reducing the CAPEX and operational expenditures (OPEX) compared to SMR [33]. The higher H<sub>2</sub> concentration of the product gas stream also has considerable potential for minimising downstream clean-up processes [5]. The cost of methane pyrolysis is strongly dependant on the processing route, the price of natural gas, and the by-product solid carbon [5]. Several pyrolysis processes including plasma-based, high-temperature thermal (thermal black), solid catalytic, and molten metal catalytic systems have been proposed and developed, a detailed discussion can be found in [34]. Here we assume a catalytic molten metal process (TRL 3-5, Table 1). From a carbon-storage perspective, pyrolysis processes offer the advantage of storing a solid C-product as opposed to gaseous CO<sub>2</sub> – Eq. (3).



**Table 2**

Life cycle inventories (LCI) of the investigated technologies to produce 1 kg of hydrogen at a minimum of 30 bar. Further information on the embodied inputs can be found in Table S2 in the ESI.

Embodied Inputs	Unit	SMR	SMR + CCS	CH <sub>4</sub> Pyrolysis	CG	CG + CCS	BG	BG + CCS	Nuclear	Solar PV	Wind
Natural Gas	kg	3.36	3.76	4.86	–	–	–	–	–	–	–
Electricity	kWh	0.31	1.11	–	–	1.36	–	3.58	54.2	54.2	54.2
Water	kg	21.90	23.70	8.08	11.28	38.08	47.48	47.96	10.00	10.00	10.00
Coal	kg	–	–	–	8.51	9.70	–	–	–	–	–
Biomass Feedstock	kg	–	–	–	–	–	36.28	36.34	–	–	–
Biomass transport	t.km	–	–	–	–	–	2.90	2.93	–	–	–
Direct Emissions											
CO <sub>2</sub>	kg	9.26	1.03	2.50	22.00	4.13	32.84	16.77	–	–	–
CH <sub>4</sub>	kg	–	–	–	2.66x10 <sup>-02</sup>	3.22x10 <sup>-02</sup>	–	–	–	–	–
N <sub>2</sub> O	kg	–	–	–	6.97x10 <sup>-06</sup>	1.87x10 <sup>-05</sup>	–	–	–	–	–
NO <sub>2</sub>	kg	–	–	–	–	–	0.01	7.74x10 <sup>-3</sup>	–	–	–
Co-product											
Solid Carbon	kg	–	–	3.00	–	–	–	–	–	–	–
Electricity	kWh	–	–	–	3.18	–	2.07	–	–	–	–
Reference		[27,55]			[37]	[38]	[42]	[43]	[16]	[56]	[57]
LCOH	USD2019 <sup>b</sup>	1.35	2.01	1.87	1.48	2.32	2.40	3.71 <sup>a</sup>	4.95	9.49	5.61
Reference		[5]						[5,58]	[5]		
Product											
Hydrogen	kg	1.00									

<sup>a</sup> An average value of \$4.67 and \$2.27/kg H<sub>2</sub> from [5,58].

<sup>b</sup> LCOH was converted from 2016 to 2019 using 1.07 inflation conversion factor.

### 2.1.3. Coal gasification with and without carbon capture and storage

In this route, coal is partially oxidised in the presence of oxygen or air to produce a syngas mixture ( $\text{CO}$ ,  $\text{H}_2$ ,  $\text{CO}_2$ , and unreacted  $\text{CH}_4$ ) at high temperatures (800–1300 °C) and pressures of 30–70 bar [35]. The syngas is further enriched by the WGSR to recover more hydrogen. Coal gasification is less efficient than SMR (55%) but offers higher single-train capacities [36]. The overall reaction is presented in Eq. (4). The lower carbon to hydrogen ratio in coal relative to natural gas results in significantly higher direct  $\text{CO}_2$  emissions from the process. The inventory data for both coal gasification routes (without and with CCS) are taken from the works by Ruthowski and Vickers, respectively [37,38].



### 2.1.4. Biomass gasification with and without carbon capture and storage

Biomass resources can be used for hydrogen production [39]. Similar to coal, gasification is the most convenient pathway for biomass feedstocks as biomass gasification provides the highest yield taking place at high temperatures, typically at 500–1400 °C [40]. The overall reaction is shown in Eq. (5) [5].



There is a wealth of interdependent research related to LCAs that investigate biomass-to-hydrogen processes differing in the biomass feedstock and system configurations [40]. This study considers poplar and covers the plantation phase of the biomass, fertilisers requirements, and water consumption following the work by Peters et al. [41]. Biomass gasification can be also integrated with CCS to yield a negative carbon balance. The inventory data for both biomass gasification systems without and with CCS are taken from Susmozas et al. [42,43], respectively. Further details on the inventory data of the poplar can be found in Table S3 in the ESI.

### 2.1.5. Electrolysis-based routes

High purity hydrogen ( $\approx 100\%$  hydrogen) can be produced from water electrolysis as described by Eq. (6). Alkaline and proton exchange membrane (PEM) electrolyzers operate at low temperatures (70–90 °C), while solid oxide electrolysis cells can work at high temperatures (650–850 °C) [44]. In this study, a PEM electrolyser is considered as it provides a faster start, higher flexibility and can work with intermittent power technologies such as solar and wind, attaining an efficiency as high as 85% [45]. Furthermore, the PEM electrolyser produces hydrogen at 30 bar, which enables a consistent comparison between the investigated production routes [46]. Our study compares electricity from nuclear, wind, and solar to cover the electrolyser's energy needs. The inventory data for the electrolysis process is taken from Colella et al. [46].



## 2.2. Environmental assessment

The study herein comprises six steps consistent with the general LCA methodology. The first three steps correspond to the goal and scope definition, inventory analysis, and impact assessment phases, with the remaining steps connected to the interpretation phase using external-

An LCA of the selected technologies using the ISO14040 standards was performed [47]. Concerning step I, the goal of this work is to assess the environmental impacts of hydrogen production routes from several different feedstocks, including fossil, biomass, and carbon-free based sources. Hydrogen end-use applications are excluded from this study; however, such applications may warrant further investigation to match supply-demand profiles accurately. Accordingly, the functional unit corresponds to one kilogram of hydrogen product pressurised to a minimum of 30 bar to ensure a consistent comparison between the fossil and carbon-free processes as well as to satisfy hydrogen end uses. For electrolytic routes where  $\text{O}_2$  is generated, no value or burden allocation was assigned to the  $\text{O}_2$  by-product. The motivation for this assumption is twofold. First,  $\text{O}_2$  would have to be compressed before being sold, which would increase the energy needs and, consequently, the environmental impact of the process. Second, the market would be very likely unable to absorb the amount of  $\text{O}_2$  produced at a large scale, assuming a high  $\text{H}_2$  demand. A cradle-to-gate scope that encompasses all the embodied input burdens (upstream), production, and additional pressurization (if required) has been adopted (Table 2). The system boundaries are illustrated in Fig. 1. Other LCA assumptions and limitations are discussed in the ESI. The location of this study was based on the United States (US).

Second (II), the life cycle inventory (LCI) of each technological route was quantified from the raw materials (feedstock) requirements, energy consumption or generation, waste, and emissions to air, soil, and water. The life cycle inventory data for all the investigated technologies and their respective sources are shown in Table 2. For the embodied burdens, inventories were taken from Ecoinvent v3.4 accessed via SimaPro v9. Further details on the inventory flows can be found in Table S2 in the ESI. Wind power in the US was assumed to be 100% from onshore, according to IRENA [48].

Third (III), the LCI's were used in a life-cycle impact assessment (LCIA) following the ReCiPe 2016 method [24], which translates all the LCI data into 18 environmental impacts at the midpoint level; these are further aggregated into damage to human health, ecosystem quality and resources depletion at the endpoint level. All the calculations were implemented in SimaPro v9. The three environmental impacts in the endpoints areas of protection were monetised using the values reported by Fantke et al. [49], which enables consistent comparisons of process alternatives [50]. The monetary values for the human health and ecosystem quality impacts are 74,000 €/DALY and  $9.5 \times 10^6$  €/Species yr, respectively. All the monetised values were adjusted to USD2019 by inflation. Further details on the monetisation conversion calculations are available in Table S1 in the ESI. Note that the endpoint environmental impacts are the primary focus of this work, while additional information regarding the impacts at the midpoint level are presented in Figures S1a, S1b, and S1c in the ESI.

Fourth (IV), the monetised cost of environmental externalities was combined with the levelised cost of hydrogen (Eq. (7)) to generate estimates of the TCH. Variations in direct hydrogen production costs are often large, heavily dependent on the process variables, and the financial modelling assumptions used. These have been studied in exhaustive detail elsewhere and are not the main-focus here [51–54]. The average production costs for each technological pathway reported by Parkinson et al. have been used here [5]. Thus, the TCH from any production route can be represented by Eq. (7):

$$\text{TCH} \left( \frac{\$}{\text{kgH}_2} \right) = \text{MonetisedIndicators} \left( \frac{\$}{\text{Impact}} \right) \times \text{LCIAImpact} \left( \frac{\text{Impact}}{\text{kgH}_2} \right) + \text{LCOH} \left( \frac{\$}{\text{kgH}_2} \right) \quad (7)$$

ities and considering as well the main uncertainties affecting the calculations. The six steps are described below.

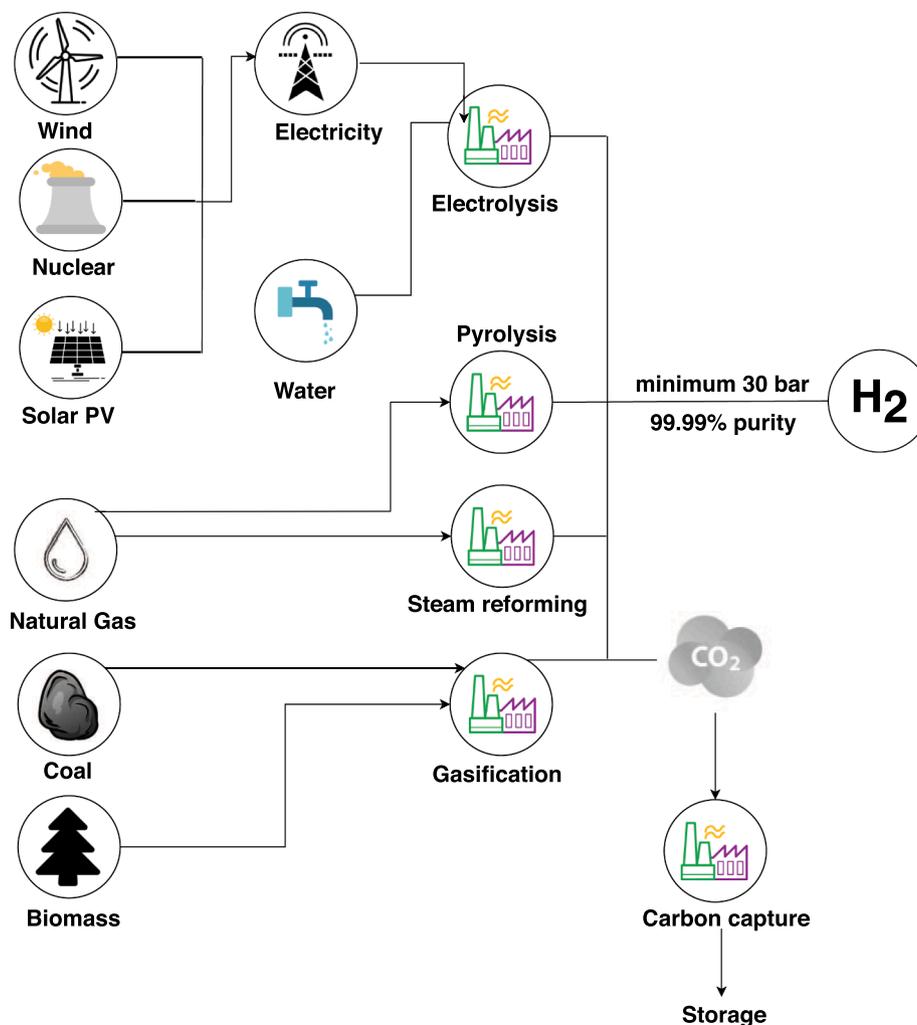


Fig. 1. Production processes considered in this analysis to produce 1 kg of hydrogen at a minimum of 30 bar and 99.99% purity.

Fifth (V), the combined results of the monetised LCIA and levelised cost of hydrogen (TCH) were used to identify stages in the life-cycle of each process contributing the most to the environmental impact. This analysis allows us to draw meaningful insights and recommendations for the systems studied.

Six (VI), the main uncertainties affecting the LCA calculations, mainly in the life cycle inventory entries, were assessed and quantified. To this end, 1000 scenarios were generated using the Monte Carlo sampling method implemented in SimaPro v9, each entailing different values of the endpoint indicators. The reported monetisation values were applied to each such scenario to obtain a range of monetised impacts for the range of life cycle inventory entries. Further details on the uncertainty analysis can be found in section 5 in the ESI.

### 3. Results and discussion

The results of the study are presented in three main sections. First, the LCA endpoint indicators and individual breakdowns for each technology are discussed. Second, global warming potential results are presented. Third, the total cost of hydrogen for each production route is assessed by combining the levelised cost of hydrogen and monetised environmental impacts.

#### 3.1. Environmental impacts in endpoint area of protection

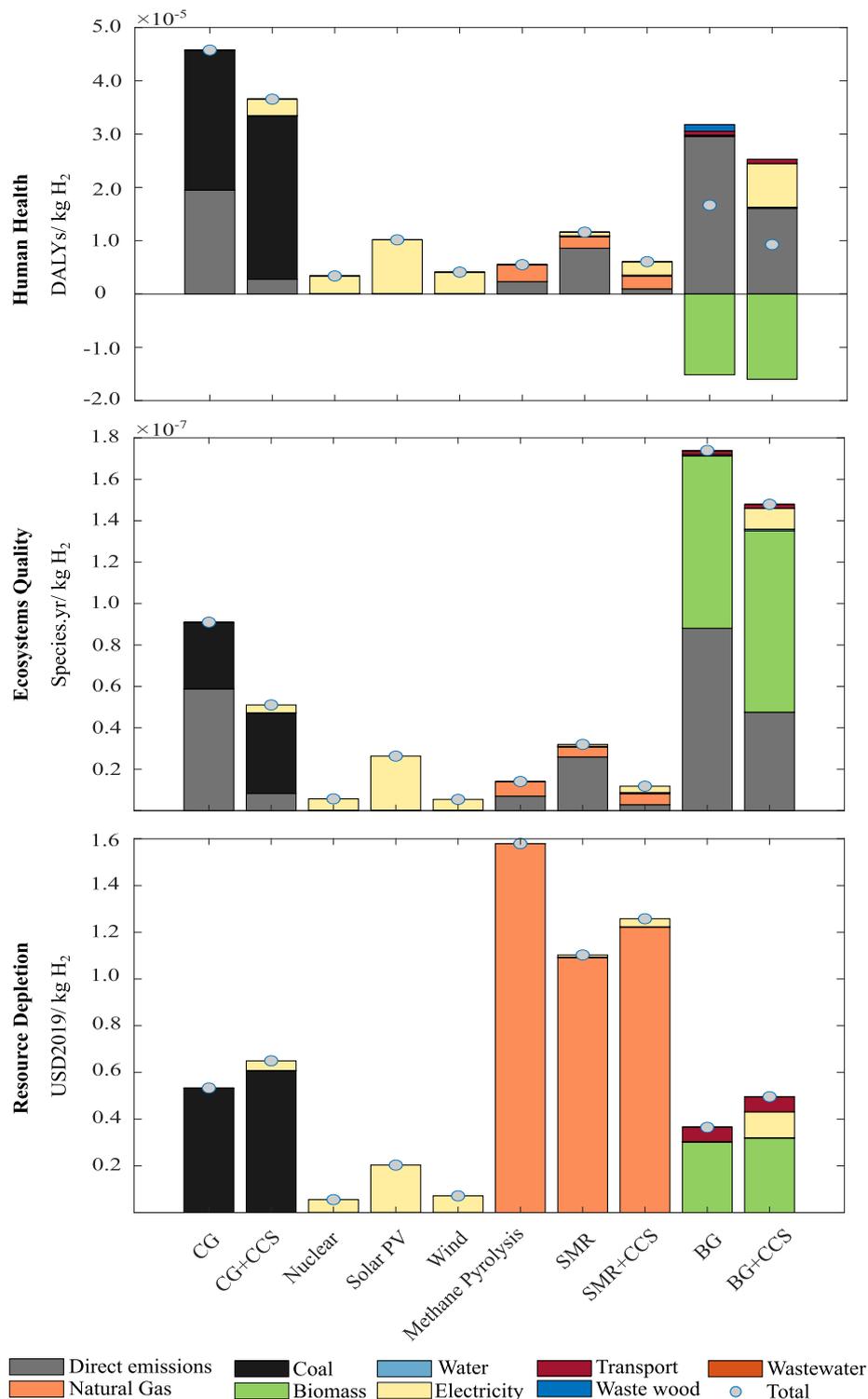
The endpoint environmental impacts on human health, ecosystem

quality, and resources depletion for each hydrogen production route are shown in Fig. 2. Further breakdowns for each endpoint (damage-oriented) indicators in terms of their midpoint-level (problem-oriented) indicators are available in Figure S1 in the ESI.

Unabated coal gasification shows the highest impact on human health, generally followed by coal gasification with carbon capture and storage and unabated biomass gasification, then SMR, solar PV, biomass gasification with carbon capture and storage, SMR with carbon capture and storage, methane pyrolysis, and finally wind and nuclear technologies. For ecosystem quality, biomass gasification shows the highest impact, followed closely by biomass gasification with carbon capture and storage, coal gasification, coal gasification with carbon capture and storage, SMR, and solar PV. Then, methane pyrolysis, SMR with carbon capture and storage, nuclear and wind. Finally, fossil-utilising technologies, especially natural gas, exhibit the highest levels of resources depletion while wind and nuclear electrolysis have the lowest resources depletion impacts.

A deeper analysis of the midpoint-level indicators (Figures S1a, S1b, and S1c in the ESI) reveals that the high human health and ecosystem quality impacts are driven mainly by the high global warming potential, the formation of fine particulate matter (FPMF), land-use and water consumption.

For SMR, the integration of carbon capture and storage reduces the impacts on human health by 48% and ecosystem quality by 63%. The same applies to coal gasification with carbon capture and storage, which improves by 20% in human health and 44% in ecosystem quality

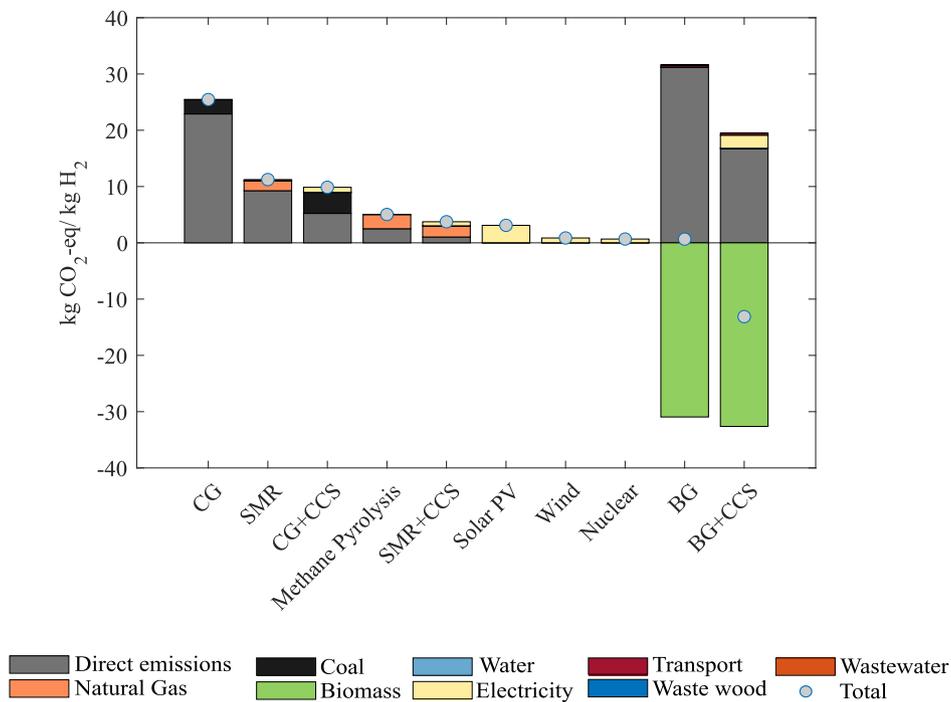


**Fig. 2.** Breakdown of the endpoint environmental impacts for the assessed hydrogen production processes considered in the analysis. The electricity contribution in the renewables refers to electricity generated from the specified form of energy, i.e., power technology.

compared to the unabated coal gasification. Notably, methane pyrolysis shows very close human health and ecosystem quality results to SMR with carbon capture and storage due to low direct CO<sub>2</sub> emissions in both cases. Furthermore, the impacts on resources depletion associated with the SMR with carbon capture and storage and methane pyrolysis routes are higher than in the SMR, and mainly driven by the nature of the feedstock consumed (natural gas).

For biomass routes, although biomass gasification with carbon

capture and storage shows a lower human health compared to SMR, this technology route didn't show negative human health compared to the negative global warming potential (Fig. 3). The negative CO<sub>2</sub> emissions are accredited to carbon fixation during the biomass growth phase and storage with carbon capture and storage. The same credit is not observed for unabated biomass gasification, as the fixated carbon source is re-released to the atmosphere. The high impact on human health in the biomass gasification and biomass gasification with carbon capture and



**Fig. 3.** Breakdown of the global warming potential (GWP) for the evaluated processes. The technologies are ranked from highest to lowest with respect to their GWP values.

storage routes relates to the water consumption at the midpoint level (Figure S1a in the ESI). Similarly, the high impact on ecosystem quality in these routes is driven by the high land-use change and water consumption linked to the biomass plantation phase (Figure S1c in the ESI), often neglected when assessing only the global warming potential.

For electrolysis routes, the high human health and ecosystem quality of solar PV electrolysis are predominately driven by the manufacturing phase and the crystalline silicon requirements for the production of the photovoltaic panels [59]. For nuclear and wind electrolysis, the human health and ecosystem quality impacts embodied in electricity are the main dominant factor. This impact is strongly connected to the manufacturing phase of the electricity generation facilities that power water electrolysis. For wind electrolysis, the impact is mainly due to the materials for construction for the wind turbine, of which steel and iron materials are the major contributors to the environmental impacts [57]. For nuclear electrolysis, the mining of uranium and the production of nuclear fuel are the main contributors to the environmental impacts [60].

### 3.2. Global warming potential of the evaluated hydrogen production technologies

Fig. 3 provides the total greenhouse gas emissions per 1 kg of hydrogen produced. Biomass gasification with carbon capture and storage shows the lowest global warming potential value ( $-13.11$  kg CO<sub>2</sub>-eq/kg H<sub>2</sub>), as carbon capture and storage leads to a net-negative carbon balance). This global warming potential value is in good agreement with the only LCA study reported for biomass gasification with carbon capture and storage, i.e.,  $-14.63$  kg CO<sub>2</sub>-eq/kg H<sub>2</sub> [43]. This technology is followed by the unabated biomass gasification process ( $0.65$  kg CO<sub>2</sub>-eq/kg H<sub>2</sub>), where both global warming potential values (biomass gasification and biomass gasification with carbon capture and storage) fit well within the range previously reported [5]. The biomass routes are then followed by water electrolysis by nuclear and wind energies, i.e.,  $0.67$  and  $0.86$  kg CO<sub>2</sub>-eq/kg H<sub>2</sub>, respectively, and then solar PV ( $3.1$  kg CO<sub>2</sub>-eq/kg H<sub>2</sub>). In all of the cases, the electricity source supplied to the electrolyser is the main contributor to the total global

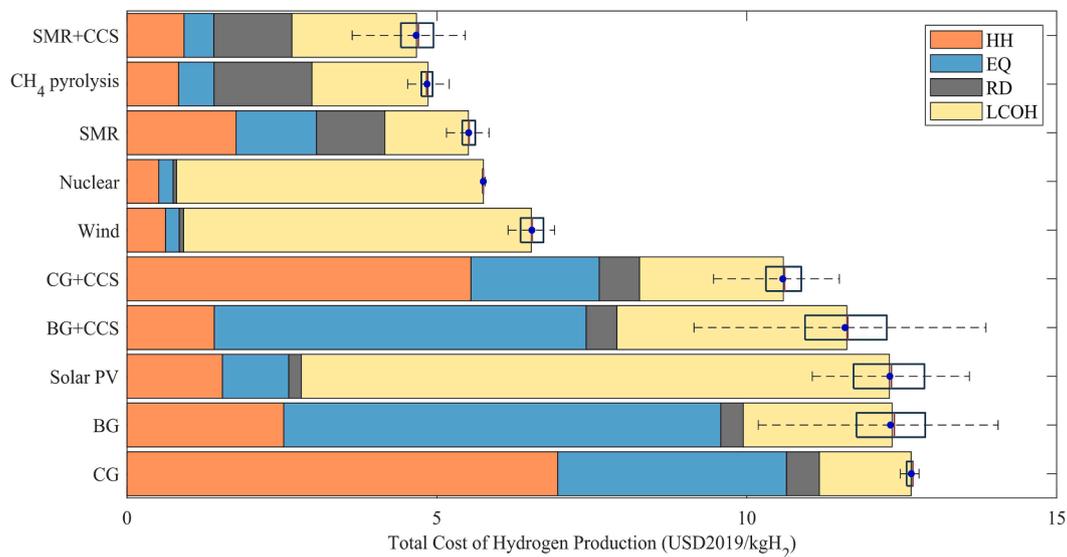
warming potential. These technologies are followed by SMR with carbon capture and storage, methane pyrolysis and coal gasification with carbon capture and storage, and, finally, coal gasification and SMR, which show the highest global warming potential values ( $25.24$  and  $11.24$  kg CO<sub>2</sub>-eq/kg H<sub>2</sub>, respectively). Note that all the global warming potential values obtained herein are consistent with the values reported elsewhere [5].

Our results, therefore, show that assessing global warming potential only could potentially lead to misleading conclusions. For example, when omitting land use and water consumption for the biomass cases, they emerge as superior; however, the same biomass technologies display the worst ecosystem quality impact values. Therefore, covering the endpoint metrics is crucial to ensure a meaningful assessment relative to the fossil pathway.

### 3.3. Total cost of hydrogen production

The TCH production (Fig. 4) was calculated from Eq. (7) by combining the monetised environmental impacts shown in Fig. 2 with the average LCOH for each production route from Parkinson et al. [5]. The average monetised environmental impacts account for significant fractions of the TCH for fossil-based routes (76% in SMR, 57% in SMR with carbon capture and storage, 62% in methane pyrolysis, 88% in coal gasification, 78% in coal gasification with carbon capture and storage). Meanwhile, the direct production costs (LCOH) dominate the TCH in the electrolytic routes (86%, 77%, 86% for nuclear, solar, and wind electrolysis, respectively). Furthermore, the externalities account for 68% and 81% of the TCH for the BG with and without carbon capture and storage, respectively. Hence, our results show that externalities can represent a significant fraction of the TCH and, consequently, should be accounted for in the economic assessment.

The uncertainty ranges of the TCH shown by the superimposed box plots in Fig. 4 were generated by Monte-Carlo analysis of 1000 scenarios (see details in section 2.2 – sixth step). The endpoint indicators were subsequently obtained for each such scenario and monetised accordingly to evaluate the robustness of the findings. Further information on the uncertainty analysis is provided in section 5 in the ESI. Note that the



**Fig. 4.** Total cost of the assessed H<sub>2</sub> production routes (TCH) in terms of externalities (HH, EQ, and RD) and LCOH. For the uncertainty analysis of externalities, the boxplot bars represent the 95% confidence interval assuming that the uncertain parameters follow lognormal distributions. The dot represents the mean TCH and the red line represents the median. HH refers to the monetised human health indicator, EQ refers to the monetised ecosystem quality indicator, RD refers to the monetised resources depletion and LCOH refers to the levelised cost of hydrogen. All indicators are expressed in USD2019 per kg H<sub>2</sub>.

LCOH variables were not varied in Fig. 4.

The lowest TCH value corresponds to the natural-gas blue hydrogen fossil routes (SMR with carbon capture and storage and methane pyrolysis), despite their higher CO<sub>2</sub> emissions compared with electrolytic routes. Notably, SMR with carbon capture and storage is the most cost-effective production route (considering externalities) despite its larger LCOH compared with the unabated SMR [ $\$1.88$  /kgH<sub>2</sub> and  $1.26$  /kgH<sub>2</sub> for SMR with carbon capture and storage and SMR, respectively]. More precisely, the TCH value for unabated SMR is  $\$5.51$  /kgH<sub>2</sub> compared with SMR + CCS at  $\$4.67$  /kgH<sub>2</sub>, highlighting the influence of the monetised environmental externalities on the TCH. The large externality costs are mainly driven by the higher global warming potential (Figure S1 in the ESI) in the former route. The question of how to improve the TCH of the hydrogen routes, which was addressed elsewhere [54,61,62], falls beyond the scope of this work. In contrast, opportunities for improving the environmental performance are discussed next.

### 3.3.1. Steam methane reforming with carbon capture and storage

SMR and SMR with carbon capture and storage show very similar supply chains but differ in their fuel usage and direct emissions. In the SMR with carbon capture and storage, improving the capture rate above 90% would decrease the impact on the human health and ecosystem quality categories due to the associated reduction in direct CO<sub>2</sub> emissions, which is the major contributor to those categories. The OPEX and CAPEX are also linked to the capture rates, with higher capture rates requiring greater fuel duty and additional equipment [63]. As demonstrated, removal rates are often around 80%, while the costs of deep decarbonisation (>90%) remain unclear [27,64]. Replacing the MEA solvent used in the post-combustion absorption of the flue gas by other means of capture, such as adsorption, could improve the capture rate and the environmental impacts while offering potential cost reductions [65]. Metal-organic frameworks (MOF) are a promising family of porous crystalline adsorbents, which are still at pilot/ research stages. MOFs can act as capture and storage materials for CO<sub>2</sub> due to their high surface area and pore volumes [66]. MOF materials could, therefore, help to address the limitations of the conventional storage currently used [67].

The resources depletion category is the other major contributor to the total cost of environmental externalities. Approximately 70% of the resources depletion impact arises from the natural gas feedstock, with

the remaining 30% given by the process fuel requirements [68,69]. The latter contribution could be reduced by using waste energy streams through process integration, though this will likely lead to additional integration costs [70]. Hence, whilst SMR with carbon capture and storage currently offers the lowest total cost solution, the opportunities for reduced environmental impacts are limited over the medium-long term.

### 3.3.2. Methane pyrolysis

Methane pyrolysis is the second cheapest total cost route. It emits less direct CO<sub>2</sub> emissions and less FPMF (Figure S1a in the ESI) than SMR, which leads to lower human health and ecosystem quality impacts. However, methane pyrolysis consumes more natural gas per unit of H<sub>2</sub> than SMR, which increases the resources depletion costs. In this route, human health and ecosystem quality account for 17% and 12%, respectively, of the TCH. These impacts are mainly driven by the natural gas supply chain emissions and the required heat for the process, which is assumed to be sourced from natural gas. Notably, the sweetening of natural gas and the fugitive methane emissions are the main contributors to the natural gas supply chain emissions. The higher supply chain impacts due to larger natural gas consumption are offset by the lower direct emissions of methane pyrolysis. Other means of heat sources could further reduce the environmental impacts. For the resources depletion category, about 18% of the natural gas is used for heating in the process with an overall efficiency of 53% [54]. Finding alternative heat sources could help reduce the impacts in this category, although this would likely increase the process costs.

Cost reduction opportunities for methane pyrolysis are mostly direct production cost-related (38% of the TCH – Fig. 4). Similarly, as with SMR and SMR with carbon capture and storage, there might be limited opportunities for additional reductions in externalities. The levelised cost of hydrogen of this route is highly sensitive to the natural gas prices and the opportunities for selling the solid carbon produced. For the current analysis, no value was assigned to the solid carbon; hence, finding potential carbon markets and applications would bring the levelised cost of hydrogen down [54]. Currently, solid carbon produced by high-temperature methane pyrolysis is commercially used in tires and electrical equipment; however, the physical and electrical properties determine its suitability to higher value market applications [54]. Another important aspect to highlight is that this technology still

exhibits a relatively low TRL [3–5], with only early-stage pilot plants in operation [54]. Thus, additional technological developments and learning curves may further reduce its TCH.

### 3.3.3. Coal gasification with and without carbon capture and storage

Despite the low costs of the coal feedstock, coal gasification has the highest TCH [\$12.65 /kgH<sub>2</sub>] because of the high environmental externalities (88% of the overall TCH). When coupled with carbon capture and storage, the TCH for coal gasification [\$10.59 /kgH<sub>2</sub>] is improved by 16%, primarily driven by the decrease in the human health and ecosystem quality impacts linked to lower direct CO<sub>2</sub> emissions (81% reduction with capture rates of 86.85%[38]). Carbon capture and storage, however, cannot reduce the environmental impacts associated with the coal feed; these are mainly linked to the methane emissions in the mining and pre-treatment stages (~70%, 36 kg CO<sub>2</sub>-eq/kg CO<sub>2</sub> [24]). Hence, the potential improvements of carbon capture and storage are mainly focused on the direct emissions of the gasification plant.

### 3.3.4. Biomass gasification with and without carbon capture and storage

Both the LCOH and externality impacts are high contributors toward the TCH for the biomass gasification and biomass gasification with carbon capture and storage technologies. Carbon capture and storage reduces the impact on human health substantially, as it is strongly linked to CO<sub>2</sub> emissions. In contrast, the impact on ecosystem quality is not significantly reduced when deploying carbon capture and storage because it is mainly connected to the biomass feedstock (due to the high contributions of the water consumption and land use impacts) (Figure S1c in the ESI).

The LCOH estimates for biomass gasification with carbon capture and storage available in the literature are scarce; only two LCOH values were found [\$2.27 /kgH<sub>2</sub> and 4.6 /kgH<sub>2</sub>] [5,58]. The average of those two values used in the nominal case represents 32% of the TCH of this technology. Since the TRL of this route is still at the research phase [3–5], there is significant uncertainty in the cost estimations in the medium to long terms. Hence, this topic should be the subject of further investigation.

Notably, our analysis is quite sensitive to the biomass feedstock type as land use impacts, water consumption, fertilisers for feedstock plantation, and the transport of the biomass to the point-of-conversion vary spatially. Hence, the former information should be taken into consideration when performing further studies in biomass-based hydrogen production pathways.

The obtained results are aligned with previous studies concerning the midpoint impacts, i.e., biomass gasification emits approximately 0.39 kgCO<sub>2</sub>/kgH<sub>2</sub> [42] and –14.63 kgCO<sub>2</sub>/kgH<sub>2</sub> when equipped with carbon capture and storage [43]. For the ecosystem quality impact, the biomass feedstock is the main contributor to the total impact due to the land utilisation and water consumption in the biomass plantations (Figure S1c in the ESI). Despite the potentially low environmental impacts of biomass gasification with carbon capture and storage, one of the main limitations of biomass routes is the relatively low hydrogen yields from biomass [6–12 wt% H<sub>2</sub>/kg biomass] [71]. For example, a hydrogen yield of 7.97 wt%/kg biomass would require ~48% of the US agricultural crop area to satisfy the current global H<sub>2</sub> demand of 60 million tonnes per annum [26]. Thus, despite the relatively low global warming potential of this route (Fig. 3), there is significant uncertainty in the future potential of such conversion routes at scale.

### 3.3.5. Electrolysis-based routes

Electrolysis-based hydrogen may benefit substantially from future cost reductions (the levelised cost of hydrogen represents at present between 77 and 86% of the TCH for solar PV, wind, and nuclear electrolysis routes, respectively). Bearing this in mind, wind and nuclear electrolysis would emerge as potentially attractive options because their TCH is 4–18% higher than the TCH of SMR (and 39–23% higher than the TCH of SMR with carbon capture and storage). Consequently, a decline

in electricity costs and/or the capital investment of the electrolyser may make them economically competitive [2,8].

Environmental costs are mainly driven by the electricity source – wind, nuclear and solar PV. Although the electrolysis process has zero direct emissions, the supply chain emissions of each electricity source are not negligible [60]. Opportunities for reducing the environmental impacts further might be very limited for the case of wind and nuclear, where externalities represent, in turn, a small percentage of the TCH [~14%]. For solar PV, the environmental impacts are dominated by the manufacturing phase of the panels, currently made of crystalline silicon. Hence, reducing the required materials of a panel or finding alternative materials with lower embodied emissions would improve the environmental performance of this route.

The LCOH is highly dependent on the electricity cost, electrolyser's capital cost, and the capacity factor of the power technology [2]. The capital cost of nuclear power plants, as well as the cost of the uranium fuel, are the main dominant factors in the nuclear route to hydrogen [72]. This is reflected in a range of levelised cost of electricity of [0.08–0.12 \$/kWh] with an average value of [0.1 \$/kWh] [5]. Furthermore, this route benefits from the clean nature of the uranium source and its higher capacity factor compared to wind and solar PV (95% vs. 33% and 20%, respectively). Additionally, the electrolyser's capital cost, currently in the range of [400–1000 \$/kW] with an average of 800 \$/kW, is another major contributor to the total cost [5]. Thus, a reduction in the electrolyser's CAPEX would significantly improve the cost competitiveness of the electrolytic hydrogen. It is worth highlighting in Fig. 4 that SMR with carbon capture and storage shows a higher uncertainty range compared to SMR. This can be attributed to the uncertainties stemming from the additional electricity needs of carbon capture and storage. The severity of this effect varies with the grid infrastructure across countries. This applies as well to coal gasification

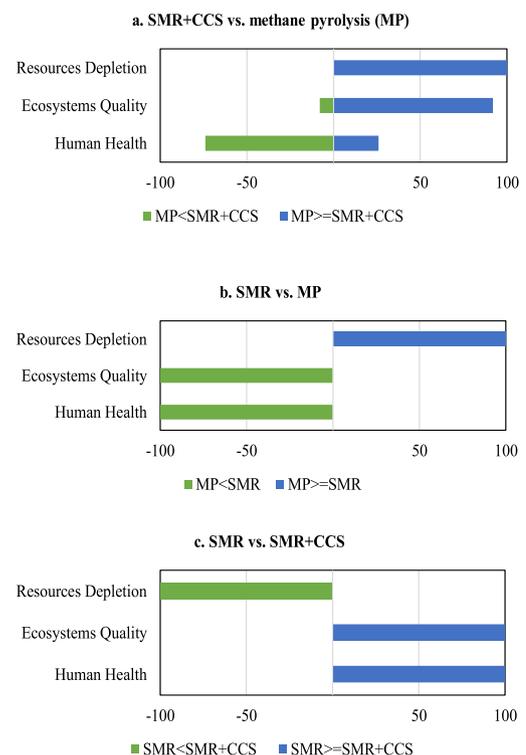


Fig. 5. Pair-wise comparisons between the three cheapest technologies in terms of their TCH (i.e., probability of technology A being higher than that of B in a given category):(a) SMR + CCS versus methane pyrolysis, (b) SMR versus methane pyrolysis, and (c) SMR versus SMR + CCS. Comparisons are shown per impact category at the endpoint areas of protection.

with carbon capture and storage and biomass gasification with carbon capture and storage. The large variation in TCH for the biomass gasification and biomass gasification with carbon capture and storage, depicted by the superimposed box plots, is driven by the variation in biomass source and type, plantation requirements for different crops, and water consumption during the growth phase.

On the other hand, methane pyrolysis shows tighter uncertainty ranges compared to SMR, as its impact is mainly driven by the natural gas feedstock (no electricity input is required). Hence, this technology might be appealing to underpin a transition phase until greener, electrolytic hydrogen becomes more economically competitive. Nuclear-based hydrogen shows good performance and a narrow uncertainty range. However, its cost, together with public acceptability issues, are the main barriers at this stage.

Finally, Fig. 5 shows the results of a set of pair-wise comparisons of those technologies displaying the lowest TCH (SMR with carbon capture and storage and methane pyrolysis). This analysis is carried out to shed further light on their performance, as they show similar mean costs accompanied by uncertainty ranges that overlap in Fig. 4. Notably, to further address the significance of the uncertainty differences between the two technologies, a Monte Carlo analysis for each of the two pathways was performed. The results were generated by repeating the comparison between the two pathways for 1000 scenarios (Fig. 5). In Fig. 5a, the blue bars represent the number of times that technology A is worse than B (i.e., A has a larger impact in that category), while the green bars show the probability of the converse. Thus, there is a 100% probability that methane pyrolysis is worse than SMR with carbon capture and storage in the resources depletion category, 26% in human health, and 92% in ecosystem quality. Furthermore, Fig. 5b and Fig. 5c show that methane pyrolysis outperforms SMR in human health and ecosystem quality (100% probability) and is worse in resources depletion (100% probability too). Finally, SMR with carbon capture and storage outperforms SMR in all the categories (100% probability) except for resources depletion, mainly due to its lower CO<sub>2</sub> emissions but larger energy requirements.

#### 4. Conclusions

This work presented a detailed economic and environmental analysis of hydrogen production processes based on grey (fossil, including coal and natural gas), blue (fossil with carbon capture and storage), and green (renewable and from green sources) hydrogen. LCA principles were applied to assess the environmental performance, while the TCH, defined as the LCOH plus the monetised environmental impacts, was selected to quantify the economic performance.

The results demonstrated that environmental externalities could represent a large percentage of the total hydrogen cost (in the range 14–88%), which highlights the importance of including them in the assessment. SMR with carbon capture and storage emerged as the lowest-total cost hydrogen production method, mainly due to its low production cost and lower direct greenhouse gas emissions (relative to SMR without carbon capture and storage), followed closely by methane pyrolysis. The latter route shows similar total costs compared to SMR with carbon capture and storage, yet its future LCOH is unclear due to the relatively low TRL and uncertain market opportunities for the solid carbon produced as a by-product. These fossil routes are followed by wind and nuclear electrolysis, which could become competitive if the

electrolyser's CAPEX and electricity generation costs decreased significantly. Solar PV electrolysis is more expensive than wind and nuclear and shows also larger externalities due to the crystalline silicon panel manufacturing, thereby resulting in worse total economic performance. Finally, coal and biomass can be perceived as relatively cheap feedstocks, yet, in practice, their “real” cost is significantly higher due to their large externalities. Carbon capture and storage can decrease their direct CO<sub>2</sub> emissions substantially (which, in turn, reduces their externalities). However, carbon capture and storage cannot make them economically competitive compared to SMR, methane pyrolysis, or water electrolysis from nuclear and wind. We note that the results for the case of biomass, emerging as superior when impacts beyond climate change are omitted, strongly depend on the biomass feedstock and its location.

While the economic weights employed to monetise the environmental impacts might be controversial, the LCA results highlight that alternative hydrogen technologies may outperform the standard SMR technology when the full life cycle costs are included. Furthermore, while carbon capture and storage improves the environmental performance of the SMR technology substantially, in a broad sense, this technology might not be regarded as an entirely sustainable solution in the long-term. The reason is that SMR coupled with carbon capture and storage transforms fossil carbon into CO<sub>2</sub>, which would then be stored in reservoirs with limited capacity that would be exhausted at some point. The same applies to coal gasification that is based also on fossil carbon.

Future work should complement the analysis of externalities with other methods, with emphasis on absolute sustainability assessments based on the planetary boundaries. Furthermore, more precise monetisation values should be established, which should be the focus of future research together with a better characterization of the uncertainties in the emissions and cost data.

Overall, the analysis undertaken herein widens the scope of the evaluation of hydrogen production systems to ultimately provide a more transparent assessment of alternative technologies based on sound criteria.

#### CRediT authorship contribution statement

**Amjad Al-Qahtani:** Conceptualization, Formal analysis, Investigation, Methodology, Writing - original draft, Writing - review & editing, Visualization. **Brett Parkinson:** Conceptualization, Formal analysis, Investigation, Writing - review & editing, Visualization. **Klaus Hellgardt:** Writing - review & editing. **Nilay Shah:** Writing - review & editing. **Gonzalo Guillen-Gosalbez:** Conceptualization, Methodology, Writing - review & editing, Supervision.

#### Declaration of Competing Interest

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

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## Appendix

## Nomenclature

Acronym	Meaning
BG	Biomass gasification
CAPEX	Capital expenditure
CCS	Carbon capture and storage
CG	Coal gasification
DALYS	Disabled adjusted lost years
EQ	Ecosystem quality
ESI	Electronic supplementary information
FPMF	Fine particulate matter formation
GWP	Global warming potential
HH	Human health
LCA	Life cycle assessments
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
LCOH	Levelised cost of hydrogen
MEA	Monoethanolamine
MOF	Metal-organic framework
OPEX	Operational expenditure
PEM	Proton exchange membrane
PV	Photovoltaics
RD	Resources depletion
SMR	Steam methane reforming
TCH	Total cost of hydrogen
TRL	Technology readiness level
WGSR	Water-gas shift reaction

## Appendix A. Supplementary material

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.apenergy.2020.115958>.

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