### Supplementary Information (SI) for Green Chemistry. This journal is © The Royal Society of Chemistry 2025

Supporting information

#### Ehrhardt and Rothenberg

## List of abbreviations

Autothermal reforming				
Alkaline Water Electrolysis				
Carbon Capture and Storage				
Coal Gasification				
Levelized Cost Of Electricity				
Proton Exchange Membrane (water electrolysis)				
Steam Methane Reforming				
Solid Oxide Electrolysis Cell				
Hydrogen produced through water electrolysis, using renewable energy.				
h Hydrogen produced through fossil-carbon based methods, where carbon capture and storage is applied to (partially) abate emissions.				

Method for calculating of the cost of hydrogen. Table S1 shows the data used for calculating the hydrogen costs per process and the various data sources. To be able to compare the fossilcarbon based hydrogen production and the electrolytic hydrogen production on the same scale, we calculate the capital expenditure (CapEx) per kW of hydrogen produced, which equals 0,03 kg H<sub>2</sub> per second (LHV = 33,6 kWh/kg). In the case of electrolysis, the CapEx is represented per kW of electrolyzer capacity. For processes based on fossil-carbon sources, the annual cost is calculated by dividing the CapEx by the plant lifetime in years, T<sub>plant</sub>, and adding the operational costs (OpEx), represented as a percentage of CapEx. This results in eq S1.

Annual cost = 
$$\frac{CapEx}{T_{plant}} + OpEx$$
 (S1)

There are no large-scale electrolysis plants, so we assume that the lifetime of such a plant is longer than that of the electrolysis stacks (the stacks are replaced a few times during the plant lifetime, depending on the stack lifetime, Tstack. The stacks are assumed to cost half of the CapEx, so the total annual cost of the electrolysis plant is given by eq S2,

Annual cost = 
$$\frac{0.5 \times CapEx}{T_{plant}} + \frac{0.5 \times CapEx}{T_{stack}} + OpEx$$
 (S2)

Assuming that all plants operate for 300 days per year, regardless of whether they run on electrolysis or using fossil carbon, the fixed cost per kg hydrogen can be calculated from eq S3,

$$FixedCost_{kgH2} = \frac{annual\,cost \times 33,6}{300 \times 24}$$
(S3)

From this FixedCost<sub>kgH2</sub> and the cost of the resources used (e.g., coal, natural gas, or electricity), we can calculate the total cost per kg hydrogen using eq S4,

$$TotalCost_{kgH2} = \frac{FixedCost_{kgH2}}{F_{capacity}} + C_{energy} \times C_{cost} + E_{energy} \times E_{cost} + W_{amount} \times W_{cost}$$
(S4)

10

where C<sub>energy</sub> is amount of fossil fuel, expressed as energy, C<sub>cost</sub> is the cost of the fossil fuel in J/GJ,  $E_{energy}$  is the electricity consumed in the production of 1 kg hydrogen in kWh,  $E_{cost}$  is the cost of electricity in \$/KWh, W<sub>amount</sub> is the amount of water consumed in the process for making 1 kg of hydrogen, in kg, and W<sub>cost</sub> is the cost of water in \$/kg. F<sub>capacity</sub> is a capacity factor that accounts for the intermittent supply of renewable solar and wind energy. When the plant cannot run consistently, the fixed cost per kg hydrogen increases. Therefore fixed cost is divided by this capacity factor, taken to be 100% when using conventional power, or when producing hydrogen using fossil-carbon based methods.

Carbon taxation can be included by adding another term, which accounts for the CO<sub>2</sub> emissions per kg of hydrogen multiplied by the tax per kg of CO<sub>2</sub>, as shown in eq S5,

\_. .

$$TotalCost_{kgH2} = \frac{FixedCost_{kgH2}}{F_{capacity}} + C_{energy} \times C_{cost} + E_{energy} \times E_{cost} + W_{amount} \times W_{cost} + C_{emit} \times C_{tax}$$
(S5)

where C<sub>emit</sub> is the amount of CO<sub>2</sub> emitted per kg of hydrogen produced, in kg, and C<sub>tax</sub> is the carbon tax, in \$/kg CO<sub>2</sub>

Resource / timeframe	Process	CapEx (\$ / kW <sub>H2</sub> )	OpEx (% of CapEx)	lifetime (y)	Annual cost (\$/kW <sub>H2</sub> )	Fixed cost (\$/kg H <sub>2</sub> )	Natural gas (GJ/kg H2)	Electricity kWh/kg H <sub>2</sub>	CO <sub>2</sub> emssion kg/kg H <sub>2</sub>	Water (L/kg H2)
Natural Gas	SMR	730[1]	5%[1]	25 <sup>[1]</sup>	66	0,31	0,18 <sup>[2]</sup>	0,96 [2]	9,1[3]	15 <sup>[4], j</sup>
	SMR+CCS (95% efficient)	1440 [1]	4% [1]	25 [1]	115	0,49	0,26 <sup>[2]</sup>	4,5 <sup>[2], g</sup>	0,5 <sup>[1,3], h</sup>	15 <sup>[4], j</sup>
	ATR	1282 [2]	6,8%[2]	25 [2]	138	0,59	0,15 <sup>[2]</sup>	2,35 [2]	8,39[2]	7,4 [2]
	ATR+CCS (91% capture)	1807 [2]	5,9% [2]	25 [2]	179	0,76	0,15 <sup>[2]</sup>	3,59 <sup>[2]</sup>	0,62 <sup>[2]</sup>	7,4 [2]
	CH₄ pyrolysis	1345 [2]	14,4% [2]	25 [2]	247	1,05	0,21 [2]	2,23 [2]	1,5 <sup>[5]</sup>	0 [2]
							Coal kg/kg H <sub>2</sub>	CCS cost (\$/t)		
Coal	CG	2680 <sup>[1]</sup>	5% [1]	25 [1]	241	1,03	6,09 <sup>f</sup>	-	20,8[6]	16,8[7]
	CG + CCS (95% efficient)	2790 <sup>[1]</sup>	5%[1]	25 [1]	251	1,07	6,41 <sup>f</sup>	65[8]	1,1 <sup>[1,3,6], i</sup>	16,8 [7]
Electricity		CapEx (\$/ kW <sub>capacity</sub> )	OpEx (% of CapEx)	Lifetime (h)	Annual cost (\$/kW <sub>H2</sub> ) <sup>l</sup>	Fixed cost (\$/kg H <sub>2</sub> ) <sup>1</sup>		Electricity (kWh/kg H <sub>2</sub> )		Water (L/kg H <sub>2</sub> )
Current	AWE	1100 <sup>[9], a</sup>	3% [1]	90000 <sup>[10], c</sup>	109	0,46		50 [11]		11 <sup>[12]</sup>
	PEM	2090 <sup>[9], a</sup>	3% <sup>[1]</sup>	70000 <sup>[13], d</sup>	235	1,00		52,2 [14]		11 <sup>[12]</sup>
	SOEC (water)	2100 [15], ь	3%[1]	48000 [16]	297	1,26		45 [17]		11 <sup>[12]</sup>
	SOEC (steam)	2100 <sup>[15], b</sup>	3%[1]	48000 [16]	297	1,26		40 [18]		11 <sup>[12]</sup>
2030	AWE	767 <sup>[15], b</sup>	3%[1]	130000 <sup>[10], c</sup>	65	0,28		50[11]		11 <sup>[12]</sup>
	PEM	532 <sup>[15], b</sup>	3% [1]	90000 [15]	52	0,22		52,2[14]		11[12]
	SOEC (water)	1266 <sup>[15], b</sup>	3%[1]	60000 <sup>[19], e</sup>	156	0,66		45 [17]		11 <sup>[12]</sup>
	SOEC (steam)	1266 <sup>[15], b</sup>	3%[1]	60000 <sup>[19], e</sup>	156	0,66		40 [18]		11 <sup>[12]</sup>
2040	AWE	636 <sup>[15], b</sup>	3%[1]	175000 <sup>[10], c</sup>	48	0,20		50[11]		11[12]
	PEM	464 <sup>[15], b</sup>	3% [1]	90000 <sup>[13], d</sup>	46	0,20		52,2[14]		11[12]
	SOEC (water)	1090 <sup>[15], b</sup>	3%[1]	90000 <sup>[19], e</sup>	108	0,46		45 [17]		11 <sup>[12]</sup>
	SOEC (steam)	1090 [15], в	3% [1]	90000 <sup>[19], e</sup>	108	0,46		40 [18]		11[12]

# Table S1. Numerical data and sources for estimating the cost of hydrogen.

### **Table notes**

- **a.** Average reported value.<sup>[9]</sup>
- **b.** Data from linear interpolation of data from 2020, 2030, 2050.<sup>[15]</sup>
- c. Advancements assumed to improve the lifetime from lower to upper bound of estimates.<sup>[10]</sup> This means an increase from 10 to 20 years or 90.000 to 175.000h. 2030 as the average of 130.000 h.
- **d.** 8 years <sup>[13]</sup> equals aproximately 70.000h.
- e. For 2030 the lower estimate was used, the upper estimate for 2040.<sup>[19]</sup>
- f. Calculated by dividing the stochiometric carbon used (3 kg/kg H<sub>2</sub>), divided by efficiency reported (76% without, and 69% with CCS), and assuming coal with 92% carbon content. <sup>[1]</sup>
- g. Value for 85% capture.<sup>[2]</sup>
- h. Calculated with efficiency decrease from standard SMR, and 95% CO<sub>2</sub> capture.<sup>[1,3]</sup>
- i. Calculated with efficiency decrease from 60% to 58%, assuming 95% CO<sub>2</sub> capture.<sup>[1]</sup>
- j. Calculated from stoichiometry, with a 3:1 ratio used. <sup>[4]</sup>
- k. Assuming stacks are replaced after lifetime, and total plant lifetime is 25 years, with stack cost representing 50% of total CAPEX.

Understanding the model limitations. Our model was designed to estimate costs for a wide array of technologies. It does therefore not take into account differences in regional fixed cost. This effect is usually small, as the main contributor to the cost of hydrogen is the raw material cost (e.g., coal or natural gas). Regional fixed costs can depend on local salaries, but also on distances from required infrastructure, pipelines, railways, and underground  $CO_2$  storage facilities. The model assumes that the fossil-carbon based fixed costs are constant, but in practice these processes also use some electricity that can vary in price depending on the location. Data from peer-reviewed publications were applied where possible. For regional and accumulative data, the most reliable sources are non-commercial intergovernmental organisations such as the International Energy Agency (IEA), which have a long-term reputation for data quality and impartiality, and publish their findings open-access.

**Including salt cavern storage**. The temporary  $H_2$  storage in salt caverns, which is needed for building a reliable renewable hydrogen infrastructure, comes at an additional cost. The cost of hydrogen including salt cavern storage is based on a cost of 0.8 \$/kg H<sub>2</sub> for storage, multiplied by the fraction that needs to be stored, shown in eq S6,<sup>[20]</sup>

$$S_{cavern} = 0.8 \times (100\% - F_{capacity}) \tag{S6}$$

where  $S_{cavern}$  is the cost of hydrogen storage per kg of hydrogen produced, in \$/kg. The cost effects of salt cavern storage are shown in Table S2, using the scenarios published by the International Energy Agency. We use the example of alkaline water electrolysis (AWE) in table S2, as this is the most mature and cost-effective technology

While other methods of hydrogen storage are available, underground hydrogen storage in salt caverns is most economical for creating a buffer for reliable offtake, and provides sufficient scale. Chemical storage of hydrogen in carriers such as ammonia, liquid organic hydrogen carriers or (complex) metal hydrides is more suited for application close to the end-users, or for long term storage, where benefits of compact storage or safety outweigh the decreased energy efficiency due to required chemical binding and release of hydrogen.<sup>[21]</sup>

	Region	Wind energy type	LCOE (\$/MWh)	F <sub>capacity</sub>	production cost (\$/kg H <sub>2</sub> )	with salt cavern storage (\$/kg H <sub>2</sub> )
2023	EU	Onshore wind	60	29%	4,78	5,35
	US	Onshore wind	40	42%	3,24	3,70
	China	Onshore wind	45	24%	4,40	5,01
2030	EU	Offshore wind	45	55%	2,83	3,19
	US	Onshore wind	35	43%	2,48	2,94
	China	Onshore wind	40	27%	3,23	3,81

*Table S2.* Current and projected cost of green hydrogen using wind power + AWE per region.

2040	EU	Offshore wind	40	56%	2,43	2,77
	US	Onshore wind	35	44%	2,29	2,74
	China	Onshore wind	37,5	26%	2,89	3,48

**Conversion table**. For calculations, values of different units are converted into standard units. The conversion values of these numbers are given in table S1. Currency conversion from Euro to US dollars was done with an exchange rate of 1.1 \$ per euro (December 2024). <sup>[22]</sup>

Table S3: Conversion values of different units of energy to joules.

value in Joules
1
3600
$4.1868 \times 10^{10}$
1055
$3.73 \times 10^{7}$

### **Example calculation: Cost of SMR in Figure 2.**

First, the annual cost in \$/kW of hydrogen produced is calculated using the values from Table S1, and substituting these into equation S1.

Annual cost = 
$$\frac{CapEx}{T_{plant}} + OpEx = \frac{730}{25} + (5\% \times 730) = 66 \, \text{\$/kW}_{H2}$$

The fixed cost per kg of hydrogen is then calculated using equation S3.

$$FixedCost_{kgH2} = \frac{annual\ cost * 33,6}{300 * 24} = \frac{66 * 33,6}{300 * 24} = 0.31 \ \text{\$/kg_{H2}}$$

The plot in Figure 2, based on equation S4, takes the form y = mx + b. Here, m is the natural gas consumption per kg H<sub>2</sub> (C<sub>energy</sub>), and x is the cost of natural gas (C<sub>cost</sub>). The capacity factor F<sub>capacity</sub> is equal to 1, as natural gas is a continuous energy source. Used electricity and water costs (E<sub>cost</sub> and W<sub>cost</sub>) were 0,127 \$/kWh, and 0,33 \$/m<sup>3</sup> respectively. Substituting the values from Table S1 into equation S4 results in the plotted line represented as SMR in figure 2.

$$\begin{split} TotalCost_{kgH2} = & \frac{FixedCost_{kgH2}}{F_{capacity}} + C_{energy} \times C_{cost} + E_{energy} \times E_{cost} + W_{amount} \times W_{cost} = \frac{0,31}{1} \\ & + 0.96 \times 0.127 + 0.33 \times 0.015 = 0.18 \times C_{cost} + 0.437 \end{split}$$

### References

- [1] Global Hydrogen Review 2023, IEA, 2023.
- [2] A. O. Oni, K. Anaya, T. Giwa, G. Di Lullo, A. Kumar, Energy Conversion and Management 2022, 254, 115245.
- [3] P. Sun, B. Young, A. Elgowainy, Z. Lu, M. Wang, B. Morelli, T. Hawkins, *Environmental Science & Technology* **2019**, *53*, 7103–7113.
- [4] J. G. Speight, *The Refinery of the Future*, Gulf Professional Publishing, Cambridge, MA, 2020, **2020**.
- [5] B. Parkinson, J. W. Matthews, T. B. McConnaughy, D. C. Upham, E. W. McFarland, *Chemical Engineering & Technology* **2017**, *40*, 1022–1030.
- [6] "IEA, Comparison of the emissions intensity of different hydrogen production routes," can be found under https://www.iea.org/data-and-statistics/charts/comparison-of-the-emissions-intensity-of-different-hydrogen-production-routes-2021, **2021**. Accessed 13-2-2025
- [7] K. Sturgess, Water for the Hydrogen Economy, 2020.
- [8] IEA, "Indicative CO<sub>2</sub> capture costs for coal and gas-fired power plants by capture rate," can be found under https://www.iea.org/data-and-statistics/charts/indicative-co2-capturecosts-for-coal-and-gas-fired-power-plants-by-capture-rate, 2020. Accessed 13-2-2025
- [9] M. El-Shafie, *Results in Engineering* 2023, 20, 101426.
- [10] C. Graves, S. D. Ebbesen, M. Mogensen, K. S. Lackner, *Renewable and Sustainable Energy Reviews* **2011**, *15*, 1–23.
- [11] "Nel, Atmospheric Alkaline Electrolyser," can be found under https://nelhydrogen.com/product/atmospheric-alkaline-electrolyser-a-series/, 2024 Accessed 13-2-2025
- [12] X. Shi, X. Liao, Y. Li, *Renewable Energy* **2020**, *154*, 786–796.
- [13] B. Yang, R. Zhang, Z. Shao, C. Zhang, *International Journal of Hydrogen Energy* **2023**, *48*, 13767–13779.
- [14] "Hydrogen and Power-to-X solutions," can be found under siemensenergy.com/electrolyzer, **2024**. Accessed 8-1-2025
- [15] H. Z. Böhm Andreas Goers, Sebastian Tichler, Robert Kroon, Pieter, *Innovative Large-Scale Energy Storage Technologies and Power-to-Gas Concepts after Optimization, Report on Experience Curves and Economies of Scale*, **2018**.
- [16] L. Wang, M. Chen, R. Küngas, T.-E. Lin, S. Diethelm, F. Maréchal, J. Van herle, *Renewable and Sustainable Energy Reviews* **2019**, *110*, 174–187.
- [17] A. Chmielewski, J. Kupecki, L. Szablowski, K. Fijalkowski, K. Bogdzinski, O. Kulik, T. Adamczewski, *Currently Available and Future Methods of Energy Storage*, WWF, Poland, 2020.
- [18] G. Jiménez-Martín, X. Judez, M. Aguado, I. Garbayo, International Journal of Hydrogen Energy 2024, S0360319924054466.
- [19] O. Schmidt, A. Gambhir, I. Staffell, A. Hawkes, J. Nelson, S. Few, *International Journal of Hydrogen Energy* **2017**, *42*, 30470–30492.
- [20] M. Talukdar, P. Blum, N. Heinemann, J. Miocic, *iScience* 2024, 27, 108771.
- [21] T. Amirthan, M. S. A. Perera, *Journal of Natural Gas Science and Engineering* **2022**, *108*, 104843.
- [22] "Euro to US dollars Historical Exchange Rates," can be found under https://wise.com/gb/currency-converter/eur-to-usd-rate/history, **2024.** Accessed 7-1-2025