Supporting Information for

Future environmental impacts of global hydrogen production

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1. Unit process data of nine H_2 technologies

The unit process data of nine H_2 technologies are shown in below. Inputs, which are supplied from own processes, i.e. processes not already contained in the premise pLCI database, are marked with an asterisk (*).

Table S1. Life cycle inventory of gaseous H_2 production (1 kg, 30 bar, 99.8% purity) by CG.

Exchanges	Amount	Unit	Data source
Economic flows			
market for chemical factory, organics	7.00E-10	unit	1
market for hard coal	8.51	kilogram	2
market for lime, packed	1.68E-01	kilogram	1
market for liquid storage tank, chemicals, organics	3.97E-09	unit	1
market group for transport, freight train	1.14	ton kilometer	1
market for water, deionised	11.28	kilogram	2
market group for transport, freight, inland waterways, barge	4.24E-01	ton kilometer	1
market (group) for electricity, low voltage	-3.18	kilowatt hour	2
treatment of hard coal ash, residual material landfill	-5.05E-01	kilogram	1
treatment of waste gypsum, inert material landfill	-2.28E-01	kilogram	1
Environmental flows			
Ammonia (to air)	6.93E-03	kilogram	1
Carbon dioxide, fossil (to air)	21.42	kilogram	2
Hydrogen chloride (to air)	1.04E-02	kilogram	1

Table S2. Life cycle inventory of gaseous H_2 production (1 kg, 30 bar, 99.8% purity) by CG CCS.

Exchanges	Amount	Unit	Data source
Economic flows			
CO_2 storage/at H_2 production plant, pre, pipeline 400km, storage 3000m	20.39	kilogram	3
market for chemical factory, organics	7.00E-10	unit	1
market for hard coal	9.7	kilogram	3
market for lime, packed	1.68E-01	kilogram	1
market for liquid storage tank, chemicals, organics	3.97E-09	unit	1
market group for transport, freight train	1.14	ton kilometer	1
market for water, deionised	38.08	kilogram	3
market (group) for electricity, high voltage	1.36	kilowatt hour	3
market group for transport, freight, inland waterways, barge	4.24E-01	ton kilometer	1
treatment of hard coal ash, residual material landfill	-5.05E-01	kilogram	1
treatment of waste gypsum, inert material landfill	-2.28E-01	kilogram	1
Selexol (Dimethylether of polyethylene glycol)[a]*	1.43E-04	kilogram	4
market for heat pump, heat and power co-generation unit, 160kW electrical[a]	2.01E-07	unit	4
market for absorption chiller, 100kW[a]	4.02E-07	unit	4
market for gas turbine, 10MW electrical[a]	2.01E-07	unit	4
market for liquid storage tank, chemicals, organics[a]	5.57E-08	unit	4
market for pump, 40W[a]	2.01E-07	unit	4
treatment of spent solvent mixture, hazardous waste incineration[a]	-1.43E-04	kilogram	4
Environmental flows			

Water, cooling, unspecified natural origin (natural resource, in water)[a]	1.70E+00	cubic meter	4
Ammonia (to air)	6.93E-03	kilogram	1
Carbon dioxide, fossil (to air)	2.27	kilogram	3
Hydrogen chloride (to air)	1.04E-02	kilogram	1

a. These processes are used for CO_2 capture. The values are corresponding to capturing 20.39 kg CO_2.

Table S3. Life cycle inventory of Selexol (1 kg).

Exchanges	Amount	Unit
Economic flows		
market for dimethyl sulfate	0.96	kilogram
market for methanol	0.16	kilogram
market for transport, freight train	0.6	ton kilometer
market for transport, freight, lorry, unspecified	0.05	ton kilometer
market for triethylene glycol	0.62	kilogram

Source: Volkart, Bauer, and Boulet[4]

Table S4. Life cycle inventory of gaseous H_2 production (1 kg, 25 bar, 99.97% purity) by NG SMR.

Exchanges	Amount	Unit
Economic flows		
market for chemical factory, organics	5.35E-10	unit
market for aluminium oxide, metallurgical	5.33E-04	kilogram
market for chromium oxide, flakes	3.60E-05	kilogram
market for copper oxide	3.62E-04	kilogram
market for liquid storage tank, chemicals, organics	2.55E-09	unit
market for magnesium oxide	2.80E-05	kilogram
market for molybdenum trioxide	1.67E-05	kilogram
market for nickel, class 1	2.03E-04	kilogram
market for portafer	3.12E-04	kilogram
market for quicklime, milled, packed	4.80E-05	kilogram
market for silica sand	1.16E-05	kilogram
market for water, deionised	7.54E+00	kilogram
market for zeolite, powder	8.83E-04	kilogram
market for zinc oxide	3.71E-04	kilogram
market (group) for electricity, high voltage	-1.23331	kilowatt hour
market for natural gas, high pressure	3.919176	cubic meter
Environmental flows		
Acetaldehyde (to air)	3.07E-08	kilogram
Acetic acid (to air)	4.6E-06	kilogram
Benzene (to air)	1.23E-05	kilogram
Benzo(a)pyrene (to air)	3.07E-10	kilogram
Butane (to air)	2.15E-05	kilogram
Carbon dioxide, fossil (to air)	8.922294	kilogram
Carbon monoxide, fossil (to air)	6.44E-05	kilogram
Dinitrogen monoxide (to air)	3.07E-06	kilogram
Formaldehyde (to air)	3.07E-06	kilogram
Mercury (to air)	9.2E-10	kilogram

Methane, fossil (to air)	6.14E-05	kilogram
Nitrogen oxides (to air)	5.49E-04	kilogram
PAH, polycyclic aromatic hydrocarbons (to air)	3.07E-07	kilogram
Particulates, < 2.5 um (to air)	6.14E-06	kilogram
Pentane (to air)	3.68E-05	kilogram
Propane (to air)	6.14E-06	kilogram
Propionic acid (to air)	6.14E-07	kilogram
Sulfur dioxide (to air)	1.69E-05	kilogram
Toluene (to air)	6.14E-06	kilogram
Water, cooling, unspecified natural origin (natural resource, in water)	3.80E-01	cubic meter

Source: Antonini et al.[5]

Table S5. Life cycle inventory of gaseous H_2 production (1 kg, 25 bar, 99.97% purity) by NG SMR CCS.

Exchanges	Amount	Unit
Economic flows		
CO_2 storage/at H_2 production plant, pre, pipeline 400km, storage 3000m	5.664958	kilogram
market for chemical factory, organics	5.35E-10	unit
market for aluminium oxide, metallurgical	5.33E-04	kilogram
market for chromium oxide, flakes	3.60E-05	kilogram
market for copper oxide	3.62E-04	kilogram
market for diethanolamine	1.93E-04	kilogram
market for liquid storage tank, chemicals, organics	2.55E-09	unit
market for magnesium oxide	2.80E-05	kilogram
market for molybdenum trioxide	1.67E-05	kilogram
market for nickel, class 1	2.03E-04	kilogram
market for portafer	3.12E-04	kilogram
market for quicklime, milled, packed	4.80E-05	kilogram
market for silica sand	1.16E-05	kilogram
market for water, deionised	7.54E+00	kilogram
market for zeolite, powder	8.83E-04	kilogram
market for zinc oxide	3.71E-04	kilogram
market (group) for electricity, high voltage	-2.00E-01	kilowatt hour
market for natural gas, high pressure	3.856157	cubic meter
Environmental flows		
Acetaldehyde (to air)	2.82E-08	kilogram
Acetic acid (to air)	4.23E-06	kilogram
Benzene (to air)	1.13E-05	kilogram
Benzo(a)pyrene (to air)	2.82E-10	kilogram
Butane (to air)	1.97E-05	kilogram
Carbon dioxide, fossil (to air)	3.119275	kilogram
Carbon monoxide, fossil (to air)	5.92E-05	kilogram
Dinitrogen monoxide (to air)	2.82E-06	kilogram
Formaldehyde (to air)	2.82E-06	kilogram
Mercury (to air)	8.45E-10	kilogram
Methane, fossil (to air)	5.63E-05	kilogram
Nitrogen oxides (to air)	5.04E-04	kilogram
PAH, polycyclic aromatic hydrocarbons (to air)	2.82E-07	kilogram

Particulates, < 2.5 um (to air)	5.63E-06	kilogram
Pentane (to air)	3.38E-05	kilogram
Propane (to air)	5.63E-06	kilogram
Propionic acid (to air)	5.63E-07	kilogram
Sulfur dioxide (to air)	1.55E-05	kilogram
Toluene (to air)	5.63E-06	kilogram
Water, cooling, unspecified natural origin (natural resource, in water)	3.80E-01	cubic meter

Source: Antonini et al.[5]

Table S6. Life cycle inventory of gaseous H_2 production (1 kg, 26 bar, 99.97% purity) by BG.

Exchanges	Amount	Unit
Economic flows		
market for liquid storage tank, chemicals, organics	2.55E-09	unit
market for water, deionised	15.90552	kilogram
market for wood chips, wet, measured as dry mass	11.6966	kilogram
market (group) for electricity, low voltage	1.368832	kilowatt hour
synthetic gas factory construction	5.35E-10	unit
treatment of wastewater, average, capacity 1E9l/year	-1.24E-02	cubic meter
Environmental flows		
Carbon dioxide, non-fossil (to air)	21.19664	kilogram

Source: Antonini et al.[6]

Table S7. Life cycle inventory of gaseous H_2 production (1 kg, 26 bar, 99.97% purity) by BG CCS.

Exchanges	Amount	Unit	Data source
Economic flows			
CO_2 storage/at H_2 production plant, pre, pipeline 400km, storage 3000m	18.02775	kilogram	6
market for liquid storage tank, chemicals, organics	2.55E-09	unit	6
market for water, deionised[a]	16.3391	kilogram	6, 7
market for wood chips, wet, measured as dry mass	11.6966	kilogram	6
market (group) for electricity, low voltage	4.756841	kilowatt hour	6
market for diethanolamine	1.76E-04	kilogram	7
synthetic gas factory construction	5.35E-10	unit	6
treatment of wastewater, average, capacity 1E9l/year[a]	-1.29E-02	cubic meter	6, 7
Environmental flows			
Water, cooling, unspecified natural origin (from natural resource)[a]	1.496476	cubic meter	7
Carbon dioxide, non-fossil (to air)	3.168898	kilogram	6

a. The added amounts compared with the BG process are corresponding to capturing 18.02775 CO_2.

Table S8. Life cycle inventory of gaseous H_2 production (1 kg, 30 bar, 99.99% purity) by AE powered by grid electricity.

Exchanges	Amount	Unit	Data source
Economic flows			
electrolyzer, AE, Balance of Plant*	2.99E-07	unit	Calculation
electrolyzer, AE, Stack*	8.97E-07	unit	Calculation
market for potassium hydroxide	3.70E-03	kilogram	8
market (group) for electricity, low voltage[a]	49.75	kilowatt hour	Calculation

market for water, deionised	12	kilogram	9
Environmental flows			
Water, cooling, unspecified natural origin (natural resource, in water)	0.0881	cubic meter	8
Oxygen (to air)	8	kilogram	8

a. In the sensitivity analysis, for solar PV, onshore wind and hydro power, the processes of power generation “electricity production, photovoltaic, 570kWp open ground installation, multi-Si”, “electricity production, wind, 1-3MW turbine, onshore” and “electricity production, hydro, reservoir, tropical region (alpine region)” are used. If the process of hydro power from reservoir is not available in specific region, the process of “electricity production, hydro, run-of-river” is used.

Table S9. Life cycle inventory of AE’s BoP production (1 MW).

Exchanges	Amount	Unit	Data source
Economic flows			
market for cast iron	716.1	kilogram	8
market for concrete, 35MPa	7.7	cubic meter	8
market for electronics, for control units	100	kilogram	8
market for ethylene glycol	7	kilogram	8
market for extrusion, plastic pipes	464.6	kilogram	8
market for glass fibre	464.6	kilogram	8
market for injection moulding	3	kilogram	8
market for aluminium, wrought alloy	160	kilogram	8
market for copper, cathode	616.7	kilogram	8
market for polyethylene, low density, granulate	467.4	kilogram	8
market for reinforcing steel	5134.4	kilogram	8
market for sheet rolling, aluminium	100	kilogram	8
market for sheet rolling, chromium steel	6697.8	kilogram	8
market for sheet rolling, steel	10130	kilogram	8
market for steel, chromium steel 18/8, hot rolled	6697.8	kilogram	8
market for steel, low-alloyed, hot rolled	6075.6	kilogram	8
market for tube insulation, elastomere	207.9	kilogram	8
market for welding, arc, steel	29	meter	8
market for wire drawing, copper	616.7	kilogram	8
market (group) for electricity, low voltage	37113.5	kilowatt hour	8
Environmental flows			
Transformation, from industrial area (natural resource, land)	135	square meter	10
Transformation, to industrial area (natural resource, land)	135	square meter	10
Occupation, industrial area (natural resource, land)	2700	square meter-year	10

Source: Gerloff[8]

Table S10. Life cycle inventory of AE’s stack production (1 MW).

Exchanges	Amount	Unit
Economic flows		
market for sheet rolling, chromium steel	20194.4	kilogram
market for steel, chromium steel 18/8, hot rolled	20194.4	kilogram
market for nickel, class 1	2884.9	kilogram
market for tetrafluoroethylene	144.2	kilogram
market for polysulfone	48.8	kilogram
market for zirconium oxide	73	kilogram

market (group) for electricity, low voltage	95553.3	kilowatt hour

Source: Gerloff[8]

Table S11. Life cycle inventory of gaseous H_2 production (1 kg, 30 bar, 99.99% purity) by PEM powered by grid electricity.

Exchanges	Amount	Unit	Data source
Economic flows			
electrolyzer, PEM, Balance of Plant*	3.45E-07	unit	Calculation
electrolyzer, PEM, Stack*	1.04E-06	unit	Calculation
market (group) for electricity, low voltage	57.47	kilowatt hour	Calculation
market for water, deionised	12	kilogram	9
Environmental flows			
Water, cooling, unspecified natural origin (natural resource, in water)	0.0881	cubic meter	8
Oxygen	8	kilogram	8

Table S12. Life cycle inventory of PEM's BoP production (1 MW).

Exchanges	Amount	Unit	Data source
Economic flows			
market for aluminium, wrought alloy	260	kilogram	8
market for cast iron	600	kilogram	8
market for copper, anode	345	kilogram	8
market for electronics, for control units	100	kilogram	8
market for ethylene glycol	7	kilogram	8
market for extrusion, plastic pipes	464.6	kilogram	8
market for injection moulding	300	kilogram	8
market for lubricating oil	100	kilogram	8
market for polyethylene, low density, granulate	464.6	kilogram	8
market for polypropylene, granulate	300	kilogram	8
market for reinforcing steel	3312.3	kilogram	8
market for sheet rolling, aluminium	200	kilogram	8
market for sheet rolling, chromium steel	4327	kilogram	8
market for sheet rolling, copper	100	kilogram	8
market for sheet rolling, steel	5382.3	kilogram	8
market for steel, chromium steel 18/8, hot rolled	4327	kilogram	8
market for steel, low-alloyed	3150	kilogram	8
market for tube insulation, elastomere	115	kilogram	8
market for welding, arc, steel	29	meter	8
market for wire drawing, copper	245	kilogram	8
market for zeolite, powder	100	kilogram	8
market for concrete, 35MPa	2.3	cubic meter	8
market (group) for electricity, low voltage	50000	kilowatt hour	8
Environmental flows			
Transformation, from industrial area (natural resource, land)	105	square meter	10
Transformation, to industrial area (natural resource, land)	105	square meter	10
Occupation, industrial area (natural resource, land)	2100	square meter-year	10

Table S13. Life cycle inventory of PEM's stack production (1 MW).

Exchanges	Amount	Unit	Data source
Economic flows			
market for titanium	528	kilogram	11
market for aluminium, wrought alloy	27	kilogram	11
market for sheet rolling, aluminium	27	kilogram	11
market for steel, chromium steel 18/8, hot rolled	100	kilogram	11
market for sheet rolling, chromium steel	100	kilogram	11
market for copper, anode	4.5	kilogram	11
market for sheet rolling, copper	4.5	kilogram	11
market for activated carbon, granular	9	kilogram	11
market for tetrafluoroethylene	9.184	kilogram	11, 12
market for sulfuric acid	6.816	kilogram	11, 12
market for platinum	0.075	kilogram	11
market for synthetic rubber	4.8	kilogram	8
market for iridium*	0.75	kilogram	11
market (group) for electricity, low voltage	103890.8	kilowatt hour	8

Table S14. Life cycle inventory of market for iridium (1 kg).

Exchanges	Amount	Unit
Economic flows		
market for electricity, low voltage	54212.21	kilowatt hour
Environmental flows		
Iridium, in ground (natural resource, in ground)	1	kilogram
Occupation, arable land, unspecified use (natural resource, land)	41.7465	square meter-year
Occupation, forest, unspecified (natural resource, land)	41.7465	square meter-year
Occupation, mineral extraction site (natural resource, land)	635.274	square meter-year
Transformation, from mineral extraction site (natural resource, land)	4.882	square meter
Transformation, to mineral extraction site (natural resource, land)	4.882	square meter
Water, unspecified natural origin (natural resource, in ground)	199.7499	cubic meter
Ethane, 1,1,1-trichloro-, HCFC-140 (to air)	8.02E-10	kilogram
Ethane, 1,2-dichloro- (to air)	4.56E-04	kilogram
Arsenic (to air)	3.38E-03	kilogram
Benzo(a)pyrene (to air)	3.03E-02	kilogram
Benzene (to air)	3.03E-02	kilogram
Lead (to air)	1.81E-02	kilogram
Cadmium (to air)	1.43E-04	kilogram
Methane, trichlorofluoro-, CFC-11 (to air)	1.44E-04	kilogram
Methane, non-fossil (to air)	7.81E-02	kilogram
Methane, fossil (to air)	19.13	kilogram
Hydrocarbons, chlorinated (to air)	8.10E-04	kilogram
Chromium (to air)	6.93E-03	kilogram
Carbon monoxide, fossil (to air)	7.159	kilogram
Carbon dioxide, fossil (to air)	11146.62	kilogram
Carbon dioxide, non-fossil (to air)	412.196	kilogram
Methane, dichloro-, HCC-30 (to air)	8.76E-08	kilogram

Dioxins, measured as 2,3,7,8-tetrachlorodibenzo-p-dioxin (to air)	5.73E-09	kilogram
Ethane (to air)	5.56E-03	kilogram
Particulates, > 2.5 um, and < 10um (to air)	36.7	kilogram
Formaldehyde (to air)	4.86E-02	kilogram
Hydrogen sulfide (to air)	1.91E-02	kilogram
Hydrochloric acid (to air)	4.99E-01	kilogram
Benzene, hexachloro- (to air)	4.70E-09	kilogram
Hydrogen fluoride (to air)	4.87E-02	kilogram
Ethane, 1,1,1,2-tetrafluoro-, HFC-134a (to air)	2.10E-07	kilogram
Copper (to air)	2.56E-02	kilogram
Dinitrogen monoxide (to air)	1.06	kilogram
Ammonia (to air)	3.52E-01	kilogram
Nickel (to air)	2.69E-02	kilogram
NMVOC, non-methane volatile organic compounds, unspecified origin (to air)	26.859	kilogram
Nitrogen oxides (to air)	30.635	kilogram
Polychlorinated biphenyls (to air)	9.52E-10	kilogram
Phenol, pentachloro- (to air)	2.46E-06	kilogram
Perfluoropentane (to air)	3.43E-06	kilogram
PAH, polycyclic aromatic hydrocarbons (to air)	1.50E-03	kilogram
Mercury (to air)	2.62E-04	kilogram
Sulfur hexafluoride (to air)	4.43E-05	kilogram
Sulfur dioxide (to air)	2172.255	kilogram
Methane, tetrachloro-, R-10 (to air)	1.02E-04	kilogram
Zinc (to air)	6.79E-02	kilogram
Arsenic, ion (to water)	2.75E-01	kilogram
Lead (to water)	2.67E-01	kilogram
Cadmium, ion (to water)	2.97E-02	kilogram
Chloride (to water)	34.494	kilogram
Chromium, ion (to water)	5.73E-02	kilogram
Cyanide (to water)	6.65E-01	kilogram
Fluoride (to water)	5.93E-01	kilogram
AOX, Adsorbable Organic Halogen as Cl (to water)	4.48E-05	kilogram
Copper, ion (to water)	8.41E-01	kilogram
Ammonium, ion (to water)	6.54E-02	kilogram
Nickel (to water)	4.51	kilogram
Nitrate (to water)	6.80E-02	kilogram
Tin, ion (to water)	1.50E-05	kilogram
TOC, Total Organic Carbon (to water)	10.576	kilogram
Phenol (to water)	2.00E-03	kilogram
PAH, polycyclic aromatic hydrocarbons (to water)	1.50E-04	kilogram
Mercury (to water)	3.53E-03	kilogram
Suspended solids, unspecified (to water)	6.86E-01	kilogram
Sulfate (to water)	272.715	kilogram
Phosphorus (to water)	1.73E-01	kilogram
Nitrogen (to water)	2.656	kilogram
Zinc, ion (to water)	7.043	kilogram

Source: ProBas[13]

Table S15. Life cycle inventory of gaseous H_2 production (1 kg, 30 bar, 99.9% purity) by SOEC powered by grid electricity.

Exchanges	Amount	Unit	Data source
Economic flows			
electrolyzer, SOEC, Balance of Plant*	2.57E-07	unit	Calculation
electrolyzer, SOEC, Stack*	2.31E-06	unit	Calculation
market (group) for electricity, low voltage	42.73	kilowatt hour	Calculation
market for heat, district or industrial, other than natural gas	18.864	megajoule	8
market for water, deionised	12	kilogram	9
Environmental flows			
Water, cooling, unspecified natural origin (natural resource, in water)	0.6447	cubic meter	8
Oxygen (to air)	8	kilogram	8

Table S16. Life cycle inventory of SOEC's BoP production (1 MW).

Exchanges	Amount	Unit	Data source
Economic flows			
market for cast iron	3000	kilogram	8
market for acrylonitrile-butadiene-styrene copolymer	1.4	kilogram	8
market for concrete, 35MPa	2.3	cubic meter	8
market for electronics, for control units	100	kilogram	8
market for ethylene glycol	35	kilogram	8
market for extrusion, plastic pipes	534	kilogram	8
market for injection moulding	1.4	kilogram	8
market for aluminium, wrought alloy	401	kilogram	8
market for copper, cathode	428.5	kilogram	8
market for polyethylene, low density, granulate	534	kilogram	8
market for reinforcing steel	13730.6	kilogram	8
market for sheet rolling, aluminium	100	kilogram	8
market for sheet rolling, chromium steel	16621.4	kilogram	8
market for sheet rolling, steel	12081.2	kilogram	8
market for steel, chromium steel 18/8, hot rolled	16621.4	kilogram	8
market for steel, low-alloyed, hot rolled	2250	kilogram	8
market for steel, low-alloyed	1503.6	kilogram	8
market for tube insulation, elastomere	176.6	kilogram	8
market for welding, arc, steel	33.3	meter	8
market for wire drawing, copper	428.5	kilogram	8
market (group) for electricity, low voltage	76420.2	kilowatt hour	8
Environmental flows			
Transformation, from industrial area (natural resource, land)	55	square meter	14
Transformation, to industrial area (natural resource, land)	55	square meter	14
Occupation, industrial area (natural resource, land)	1100	square meter-year	14

Table S17. Life cycle inventory of SOEC's stack production (1 MW).

Exchanges	Amount	Unit
Economic flows		
market for aluminium oxide, metallurgical	6.4	kilogram

market for barium oxide	6.4	kilogram
market for boric oxide	6.4	kilogram
Lanthanum strontium manganite (LSM)*	2.1	kilogram
market for cerium oxide	91.5	kilogram
market for nickel, class 1	144.1	kilogram
market for praseodymium oxide	9	kilogram
market for samarium-europium-gadolinium oxide	37.7	kilogram
market for sheet rolling, chromium steel	8976.1	kilogram
market for silicone product	6.4	kilogram
market for steel, chromium steel 18/8, hot rolled	8976.1	kilogram
market for zirconium oxide	170.7	kilogram
market (group) for electricity, low voltage	122224.4	kilowatt hour

Source: Gerloff [8]

Table S18. Life cycle inventory of LSM production (1 kg).

Exchanges	Amount	Unit
Economic flows		
market for lanthanum oxide	5.04E-01	kilogram
market for manganese	8.62E-02	kilogram
market for strontium carbonate	5.51E-01	kilogram
market for nitric acid, without water, in 50% solution state	1.3181	kilogram
market for chloroacetic acid	1.667388	kilogram
market for ammonia, anhydrous, liquid	3.00E-01	kilogram
market for water, deionised	8.833922	kilogram
market group for electricity, low voltage	15.68021	kilowatt hour

Source: Staffell et al.[15]

For the delivery purity and pressure of the H_2 from water electrolysis, only the information about PEM (industry grade N5.0-99.999% and 30 bar) can be available from the refence Bareiß et al.[11] that we directly used. We further checked other references to clarify these information about AE and SOEC and made a comparison to ensure the value used in our paper is reasonable. The H_2 produced by AE is delivered at 99.999% purity and 30 bar pressure with the system electrical efficiency of 53-70%, as mentioned in the Table5-1 in the report of Smolinka et al.[16] This electrical efficiency was cited in the research of Zhang et al.,[17] which is the main source reference of the AE's stack and BoP in the Gerloff.[8] Purity requirements vary significantly from different applications.[18] Although 99.999% purity of H_2 produced by AE and PEM can be achieved based on the electrical efficiency used in this paper, the mid-range value of 99.99% (N4.0) purity from manufacturer (between 99.9%-N3.0 and 99.999%) [19-22] was used as the target purity due to lack of specific users. Gerloff[8] used Häfele et al.[23]'s LCI of SOEC's stack, whose operating pressure is 1 bar, and added H_2 compressors in SOEC's BoP. In other references using the similar SOEC system, the generated H_2 (99.9% purity) is generally compressed from 1 bar to 30 bar, with the system electrical efficiency of SOEC between 75% and 88%.[24-27] The target delivery purity and pressure of the H_2 produced by water electrolysis are shown in Table S19.

Table S19. The system electrical efficiency of the target H_2 product of the water electrolysis.

Parameters	AE	PEM	SOEC
Electrical efficiency used in this paper (%)	67	58	78
Delivery pressure of H_2 (bar)	30	30	30
Delivery purity of H_2 (%)	99.99	99.99	99.9
Electrical efficiency for the target H_2 product (%)	53-70	50-70	75-88

Table S20. LCI of 1 MW PEM stack production in the Middle East and the USA in 2030 and 2050 broken down into technology improvements (likely material reductions), regional variations (where the regional electricity mix is used), and other inputs that do not change over time and region.

Economic flows	Unit	Location	Amount in 2030	Amount in 2050
Technology improvements				
market for titanium	kg	GLO	213.69	35
market for steel, chromium steel 18/8, hot rolled	kg	GLO	73.68	40
market for sheet rolling, chromium steel	kg	GLO	73.68	40
market for activated carbon, granular	kg	GLO	7.14	4.5
market for tetrafluoroethylene (Nafion)	kg	GLO	4.59	1.148
market for sulfuric acid (Nafion)	kg	RoW	3.41	0.852
market for platinum	kg	GLO	0.05	0.02
market for iridium	kg	GLO	0.26	0.03
Regional variations				
market for electricity, low voltage	kWh	MEA/USA	103890.8	103890.8
Others				
market for aluminium, wrought alloy	kg	GLO	27	27
market for sheet rolling, aluminium	Kg	GLO	27	27
market for copper, anode	kg	GLO	4.5	4.5
market for sheet rolling, copper	kg	GLO	4.5	4.5
market for synthetic rubber	kg	GLO	4.8	4.8

2. Global H_2 markets across regions

2.1 Current H_2 production across regions (2020)

For the IEA's regions where no data of H_2 production by CG and NG SMR in 2020 was available, the following assumptions were made:

Coal is used as the feedstock of H_2 production in limited regions including China, India, Japan, Southeast Asia, Africa and Rest of Asia Pacific.[28] For Southeast Asia, Africa and Rest of Asia Pacific, where there is no data of H_2 production amount of CG, their values are generated by multiplying the remaining global total H_2 production amount by CG excluding the known amount of China, India and Japan, by the ratios of their respective coal supply amount in 2020.[29]

Australia's hydrogen production was around 0.65 Mt and virtually all of this H_2 is made using NG SMR.[30] For the 1.8 Mt H_2 produced and used in Korea in 2020, 40% was produced from NG SMR, with the remaining 60% obtained as by-product from various sources.[31] The NG SMR proportion in the H_2 market of Rest of Asia Pacific was set as the same as the weighted average value for Australia and Korea, which are dominated by H_2 producing countries in this region. Russia has no official statistics of its H_2 market,[32] but what can be confirmed is that there is practically no government or industry program for producing H_2 from coal.[33] Thus, the H_2 market of Russia is assumed to consist of only NG SMR technology excluding the by-product H_2. The Rest of Eurasia has a similar situation. So the global remaining H_2 production amount of NG SMR excluding other 13 regions were proportionally assigned to Russia and the Rest of Eurasia according their respective total H_2 production amount.

2.2 Future H_2 production across regions (until 2050)

The future regional dedicated H_2 production volumes in the IEA's STEPS, APS and NZE scenarios were derived via the following steps. For the H_2 production volumes from 2020 to 2050 in the STEPS and APS, the IEA provides global total H_2 production volumes and specific values of CG CCS, NG SMR CCS, water electrolysis and bioenergy (lacking CG and NG SMR), as well as the total production volumes including by-product H_2 of 15 regions.[29] At first, the fraction of the global H_2 production volumes of CG and NG SMR in 2020 was used to distinguish between CG and NG SMR in the residual production volumes (excluding by-product H_2, which was considered unchanged in the future). After getting the production volumes of different H_2 technologies at the global level, we can then assign these values to 15 regions.

Our further assumption is that the regional fractions in CG and NG SMR after 2020 will change with the same trend of their total H_2 production volumes[29] (The regional fractions are shown in Table S20-S23). Thus, the production volume of CG and NG SMR after 2020 in each region can be obtained by multiplying the global total production volume of CG and NG SMR with regional fractions. Above fractions were also used for assigning the production volume of CG CCS and NG SMR CCS. For bioenergy-based H_2 technology, the regional fraction of the total H_2 production volume was used to assign it due to lack of starting values in 2020 and reference basis. At last, the production volume of water electrolysis in each region over time can be obtained by subtracting the above known amount and by-product H_2 from the regional total H_2 production volume. Water electrolysis includes AE, PEM and SOEC. If there is no clear classification for one region in 2020, the global average proportion, 61%, 31% and 8% for AE, PEM and SOEC would be adopted as the alternative.[31] PEM is currently one of the two commercially available electrolyzer technologies together with AE.[34] On the one hand, the share of AE in the total installed capacity of announced projects remains at around 60% for the next five years, but decreases afterwards, so that by 2030 the total capacity could be equally split between AE and PEM electrolyzers.[35] On the other hand, Schmidt et al.[36] found that experts believed PEM would be the dominant electrolysis technology by as early as 2030. Moreover, PEM has a simpler balance of plant and produces H_2 at a higher pressure than AE, which means lower energy requirements for compression.[10] Studies also show that PEM might be more future-proof than AE; for example, PEM electrolyzers exhibit a higher power-density per footprint ratio compared to AE electrolyzers, making the overall system footprint less space-consuming,[37] and PEM is shown to exhibit higher flexibility and can be installed with variable power (solar photovoltaic and wind) without impacting the electrolyzer performance.[38] Thus, a conservative market share of 60% for PEM in water electrolysis in 2050 is assumed. The SOEC is simply assumed to increase 1% every 5 years from 2020 to 2050. At the same time, the remaining proportion is AE's market share.

For the NZE scenario, only the global H_2 production volume by fossil fuel, CCS, bioenergy, water electrolysis and by-product is available and there is no regional data.[39] Thus, the source of coal and natural gas in fossil fuel and CCS were distinguished by the fractions used in the APS scenario. At the same time, the reginal fractions of the global H_2 production from 2020 to 2050 of the APS scenario were used to get the regional total production volumes in the NZE scenario. Other steps were also consistent with the APS scenario. BG CCS was only adopted in the NZE scenario from 2040 with a fraction of 1% in bioenergy-based H_2 production volume and can achieve no more than 5% by 2050.[29] The annual H_2 production volumes by various technologies in 15 regions between 2020 and 2050 under three scenarios are shown in Figure S1.

Table S21. The regional fraction of CG and CG CCS between 2020 and 2050 in the STEPS scenario.

Regions	2020	2025	2030	2035	2040	2045	2050
Africa	1.7%	1.9%	2.0%	2.2%	2.4%	2.5%	2.7%
China	84.7%	84.3%	83.9%	82.6%	81.3%	80.1%	79.1%
India	7.2%	7.5%	7.8%	8.6%	9.4%	10.1%	10.7%
Japan	0.5%	0.5%	0.5%	0.5%	0.5%	0.6%	0.6%
Southeast Asia	2.9%	3.0%	3.0%	3.2%	3.4%	3.5%	3.7%
Rest of Asia Pacific	3.0%	2.9%	2.7%	2.9%	3.0%	3.2%	3.3%

Table S22. The regional fraction of CG and CG CCS between 2020 and 2050 in the APS and NZE scenario.

	2020	2025	2030	2035	2040	2045	2050
Africa	1.7%	1.8%	1.9%	2.1%	2.3%	2.4%	2.5%
China	84.7%	84.6%	84.4%	81.7%	79.9%	78.6%	77.7%
India	7.2%	7.2%	7.1%	8.1%	8.8%	9.2%	9.5%
Japan	0.5%	0.6%	0.6%	0.8%	0.9%	0.9%	1.0%
Southeast Asia	2.9%	2.9%	2.9%	3.2%	3.4%	3.5%	3.6%
Rest of Asia Pacific	3.0%	3.0%	3.0%	4.1%	4.8%	5.3%	5.7%

Table S23. The regional fraction of NG SMR and NG SMR CCS between 2020 and 2050 in the STEPS scenario.

	2020	2025	2030	2035	2040	2045	2050
United States	17.9%	17.4%	16.9%	16.7%	16.5%	16.4%	16.2%
Rest of North America	4.7%	4.4%	4.2%	4.1%	4.0%	3.9%	3.9%
Brazil	0.3%	0.5%	0.6%	0.7%	0.8%	0.9%	1.0%
Rest of Central and South America	4.2%	4.3%	4.4%	4.8%	5.1%	5.3%	5.6%
European Union	8.8%	7.7%	6.9%	6.4%	6.0%	5.7%	5.4%
Rest of Europe	2.4%	2.4%	2.3%	2.3%	2.3%	2.3%	2.3%
Africa	4.7%	5.1%	5.5%	5.8%	6.1%	6.4%	6.6%
Middle East	18.3%	20.0%	21.3%	20.9%	20.6%	20.3%	20.0%

Russia	5.2%	4.5%	4.0%	3.8%	3.6%	3.5%	3.3%
Rest of Eurasia	0.4%	0.4%	0.4%	0.4%	0.3%	0.3%	0.3%
China	11.4%	11.3%	11.2%	10.6%	10.2%	9.8%	9.4%
India	11.5%	12.1%	12.4%	13.3%	14.1%	14.7%	15.3%
Japan	1.7%	1.6%	1.5%	1.5%	1.6%	1.6%	1.6%
Southeast Asia	4.0%	4.1%	4.2%	4.3%	4.4%	4.5%	4.5%
Rest of Asia Pacific	4.7%	4.4%	4.2%	4.3%	4.4%	4.5%	4.5%

Table S24. The regional fraction of NG SMR and NG SMR CCS between 2020 and 2050 in the APS and NZE scenario.

	2020	2025	2030	2035	2040	2045	2050
United States	17.9%	19.4%	20.4%	21.6%	22.3%	22.8%	23.2%
Rest of North America	4.7%	4.3%	4.0%	3.5%	3.2%	3.0%	2.8%
Brazil	0.3%	0.6%	0.8%	1.1%	1.3%	1.4%	1.5%
Rest of Central and South America	4.2%	4.6%	4.9%	4.9%	5.0%	5.0%	5.0%
European Union	8.8%	9.2%	9.6%	9.3%	9.1%	9.0%	8.9%
Rest of Europe	2.4%	2.9%	3.2%	3.3%	3.3%	3.3%	3.4%
Africa	4.7%	4.8%	4.8%	5.1%	5.4%	5.5%	5.6%
Middle East	18.3%	18.4%	18.4%	15.8%	14.3%	13.2%	12.5%
Russia	5.2%	3.9%	3.1%	2.4%	1.9%	1.7%	1.4%
Rest of Eurasia	0.4%	0.4%	0.3%	0.3%	0.2%	0.2%	0.2%
China	11.4%	10.8%	10.3%	9.6%	9.1%	8.8%	8.6%
India	11.5%	10.9%	10.5%	11.5%	12.0%	12.4%	12.7%
Japan	1.7%	1.8%	1.9%	2.2%	2.4%	2.5%	2.6%
Southeast Asia	4.0%	3.8%	3.6%	3.8%	4.0%	4.1%	4.1%
Rest of Asia Pacific	4.7%	4.4%	4.3%	5.6%	6.4%	7.0%	7.3%

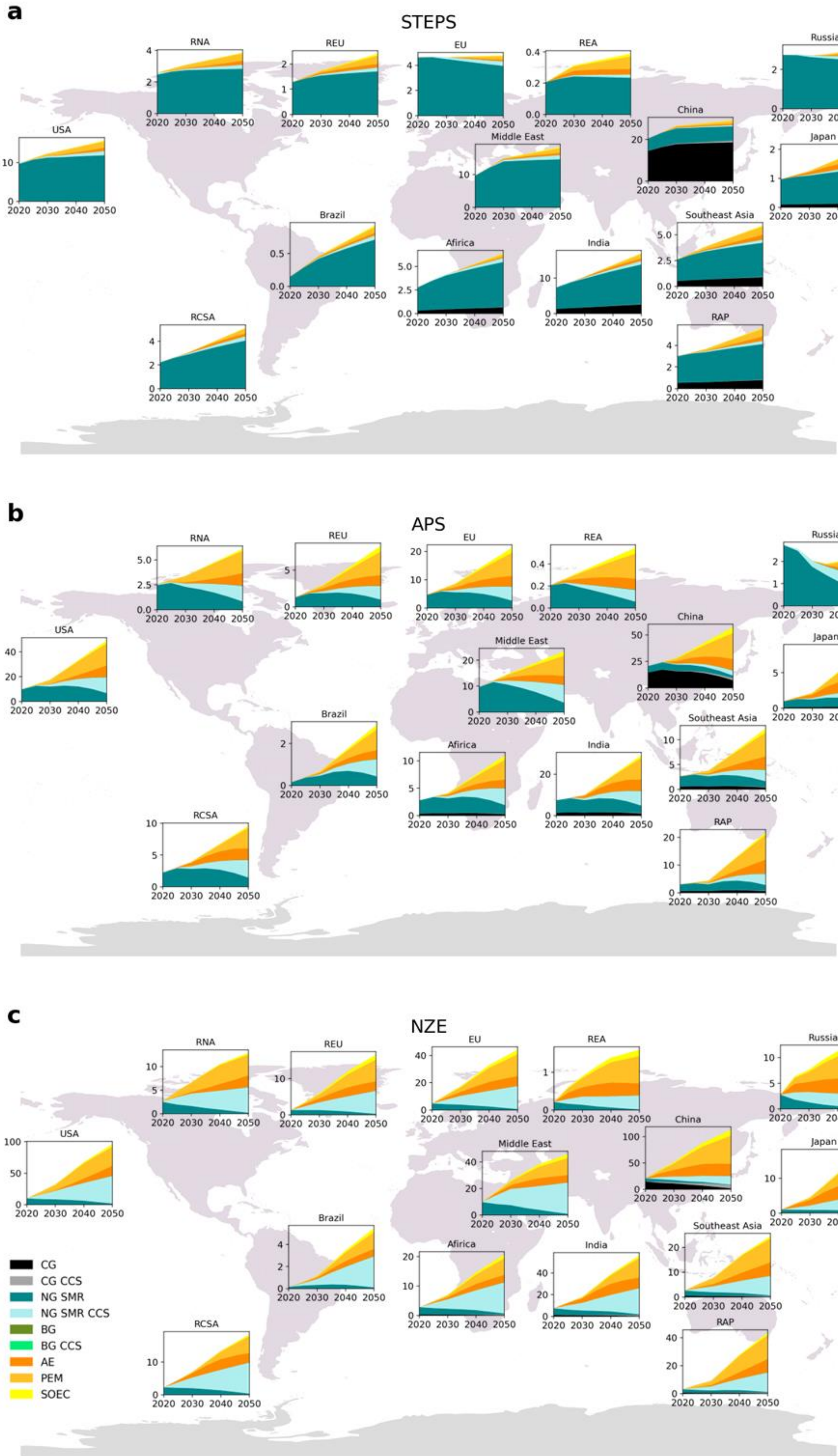

Figure S1. H_2 production volumes in 15 regions from 2020 to 2050 in the STEPS, APS and NZE scenarios. In the figure, RNA= Rest of North America, REU= Rest of Europe, REA= Rest of Eurasia, RCSA= Rest of Central and South America and RAP= Rest of Asia Pacific. The unit of the stacked area charts is Mt per year.

3. Regional scope

Table S25. The region matching between IEA and REMIND models.

No.	IEA regions	REMIND regions
1	Brazil	LAM
2	Rest of Central and South America	LAM
3	Southeast Asia	OAS
4	Rest of Asia Pacific	OAS
5	Africa	SSA
6	European Union (EU)	EUR
7	Rest of Europe	NEU
8	Middle East	MEA
9	Russia	REF
10	Rest of Eurasia	REF
11	Rest of North America	CAZ
12	China	CHA
13	India	IND
14	Japan	JPN
15	USA	USA

Table S26. IEA regions and countries (ISO alpha-3 code).

No.	IEA Regions	ISO code of countries belonging to this region
1	Brazil	BRA
2	Rest of Central and South America	ABW, AIA, ARG, ATG, BES, BHS, BLM, BLZ, BMU, BOL, BRB, BVT, CHL, COL, CRI, CUB, CUW, CYM, DMA, DOM, ECU, FLK, GLP, GRD, GTM, GUF, GUY, HND, HTI, JAM, KNA, LCA, MAF, MSR, MTQ, NIC, PAN, PER, PRI, PRY, SGS, SLV, SUR, SXM, TCA, TTO, URY, VCT, VEN, VGB and VIR
3	Southeast Asia	BRN, IDN, KHM, LAO, MMR, MYS, PHL, SGP, THA and VNM
4	Rest of Asia Pacific	AFG, ASM, ATF, AUS, BGD,BTN, CCK, COK, CXR, FJI, FSM, GUM, HMD, IOT, KIR, KOR, LKA, MDV, MHL, MNG, MNP, NCL, NFK, NIU, NPL, NRU, NZL, PAK, PCN, PLW, PNG, PRK, PYF, SLB, TKL, TLS, TON, TUV, TWN, UMI, VUT, WLF, WSM and MAC
5	Africa	AGO, BDI, BEN, BFA, BWA, CAF, CIV, CMR, COD, COG, COM, CPV, DJI, DZA, EGY, ERI, ESH, ETH, GAB, GHA, GIN, GMB, GNB, GNQ, KEN, LBR, LBY, LSO, MAR, MDG, MLI, MOZ, MRT, MUS, MWI, MYT, NAM, NER, NGA, REU, RWA, SDN, SEN, SHN, SLE, SOM, SSD, STP, SWZ, SYC, TCD, TGO, TUN, TZA, UGA, ZAF, ZMB and ZWE
6	EU	AUT, BEL, BGR, CYP, CZE, DEU, DNK, ESP, EST, FIN, FRA, GRC, HRV, HUN, IRL, ITA, LTU, LUX, LVA, MLT, NLD, POL, PRT, ROU, SVK, SVN and SWE
7	Rest of Europe	ALA, ALB, AND, BIH, BLR, CHE, FRO, GBR, GGY, GIB, GRL, IMN, ISL, LIE, JEY, MCO, MDA, MKD, MNE, NOR, SJM, SMR, SRB, TUR, UKR, VAT, ISR and PSE,
8	Middle East	ARE, BHR, IRN, IRQ, JOR, KWT, LBN, OMN, QAT, SAU, SYR and YEM
9	Russia	RUS
10	Rest of Eurasia	ARM, AZE, GEO, KAZ, KGZ, TJK, TKM and UZB
11	Rest of North America	CAN, SPM and MEX
12	China	CHN and HKG
13	India	IND
14	Japan	JPN
15	USA	USA

Source: IEA[40]

Table S27. REMIND regions and countries (ISO alpha-3 code).

No.	REMIND regions	ISO code of countries belonging to this region
1	LAM	ABW, AIA, ARG, ATA, ATG ,BES, BHS, BLM, BLZ, BMU, BOL, BRA, BRB, BVT, CHL, COL, CRI, CUB, CUW, CYM, DMA, DOM, ECU, FLK, GLP, GRD, GTM, GUF, GUY, HND, HTI, JAM, KNA, LCA, MAF, MEX, MSR, MTQ, NIC, PAN, PER, PRI, PRY, SGS, SLV, SUR, SXM, TCA, TTO, URY, VCT, VEN, VGB, and VIR
2	OAS	AFG, ASM, ATF, BGD, BRN, BTN, CCK, COK, CXR, FJI, FSM, GUM, IDN, IOT, KHM, KIR, KOR, LAO, LKA, MDV, MHL, MMR, MNG, MNP, MYS, NCL, NFK, NIU, NPL, NRU, PAK, PCN, PHL, PLW, PNG, PRK, PYF, SGP, SLB, THA, TKL, TLS, TON, TUV, UMI, VNM, VUT, WLF, and WSM
3	SSA	AGO, BDI, BEN, BFA, BWA, CAF, CIV, CMR, COD, COG, COM, CPV, DJI, ERI, ETH, GAB, GHA, GIN, GMB, GNB, GNQ, KEN, LBR, LSO, MDG, MLI, MOZ, MRT, MUS, MWI, MYT, NAM, NER, NGA, REU, RWA, SEN, SHN, SLE, SOM, SSD, STP, SWZ, SYC, TCD, TGO, TZA, UGA, ZAF, ZMB, and ZWE
4	EUR	ALA, AUT, BEL, BGR, CYP, CZE, DEU, DNK, ESP ,EST, FIN, FRA, FRO, GBR, GGY, GIB, GRC, HRV, HUN, IMN, IRL, ITA, JEY, LTU, LUX, LVA, MLT, NLD, POL, PRT, ROU, SVK, SVN, and SWE
5	NEU	ALB, AND, BIH, CHE, GRL, ISL, LIE, MCO, MKD, MNE, NOR, SJM, SMR, SRB, TUR, and VAT
6	MEA	ARE, BHR, DZA, EGY, ESH, IRN, IRQ, ISR, JOR, KWT, LBN, LBY, MAR, OMN, PSE, QAT, SAU, SDN, SYR, TUN, and YEM
7	REF	ARM, AZE, BLR, GEO, KAZ, KGZ, MDA, RUS, TJK, TKM, UKR, and UZB
8	CAZ	AUS, CAN, HMD, NZL, and SPM
9	CHA	CHN, HKG, MAC, and TWN
10	IND	IND
11	JPN	JPN
12	USA	USA

Source: Baumstark et al.[41]

4. Supplementary results

4.1 Prospective environmental impacts of H_2 production

Table S28. The contribution of various drivers to GHG emissions reduction from 2020 to 2050 of per kg H_2 produced by grid-powered water electrolysis.

Scenario	Region	Technology	Electricity decarbonization (%)	Efficiency improvement (%)	Material demand decrease (%)	Lifespan extension (%)
STEPS	China	AE-Grid	99.57	0.27	0.08	0.09
		PEM-Grid	99.45	0.48	0.05	0.02
		SOEC-Grid	99.62	0.13	0.10	0.14
	USA	AE-Grid	99.42	0.27	0.14	0.16
		PEM-Grid	99.36	0.52	0.09	0.03
		SOEC-Grid	99.45	0.09	0.19	0.26
	EU	AE-Grid	98.69	0.87	0.21	0.24
		PEM-Grid	98.26	1.56	0.13	0.05
		SOEC-Grid	98.87	0.46	0.27	0.40
APS	China	AE-Grid	99.60	0.24	0.07	0.09
		PEM-Grid	99.50	0.44	0.05	0.02
		SOEC-Grid	99.65	0.12	0.10	0.14
	USA	AE-Grid	99.40	0.30	0.14	0.16
		PEM-Grid	99.32	0.56	0.09	0.03
		SOEC-Grid	99.44	0.11	0.19	0.26
	EU	AE-Grid	98.73	0.84	0.20	0.23

		PEM-Grid	98.32	1.50	0.13	0.05
		SOEC-Grid	98.91	0.44	0.27	0.39
NZE	China	AE-Grid	99.62	0.21	0.08	0.09
		PEM-Grid	99.54	0.39	0.05	0.02
		SOEC-Grid	99.66	0.10	0.10	0.14
	USA	AE-Grid	99.92	-0.23	0.14	0.16
		PEM-Grid	100.22	-0.34	0.09	0.03
		SOEC-Grid	99.81	-0.23	0.19	0.24
	EU	AE-Grid	99.22	0.35	0.20	0.23
		PEM-Grid	99.16	0.67	0.12	0.05
		SOEC-Grid	99.26	0.11	0.26	0.36

Table S29. Environmental impacts of per kg H_2 in the global H_2 market in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq $\times 10^{-2}$)	1.3	1.6	1.6	2.3	1.4	2.8	1.3
Ecotoxicity: freshwater (CTUe)	171.9	187.2	177.2	208.2	135.4	196.6	123.7
Resource use: energy carriers (MJ, net calorific value)	157.4	163.7	148.4	170.5	86.7	171.2	90.4
Eutrophication: aquatic freshwater (kg PO_4-eq $\times 10^{-3}$)	1.0	1.3	1.2	2.0	0.8	1.9	0.7
Eutrophication: aquatic marine (kg N-eq $\times 10^{-3}$)	1.7	2.3	2.2	3.5	1.9	4.1	1.9
Eutrophication: terrestrial (mol N-eq $\times 10^{-2}$)	3.8	4.3	3.9	5.0	2.3	4.9	2.2
Human toxicity: cancer effects (CTUh $\times 10^{-9}$)	1.5	1.8	2.2	2.9	4.7	4.1	4.6
Human toxicity: non- cancer effects (CTUh $\times 10^{-9}$)	3.2	4.3	5.1	7.3	9.6	9.8	9.2
Ionising radiation: human health (kBq U^{235}-eq)	0.4	0.5	0.6	1.2	1.6	2.2	1.8
Land use (dimensionless)	11.8	15.4	26.6	28.8	84.6	44.2	81.8
Resource use: minerals and metals (kg Sb-eq $\times 10^{-5}$)	2.2	2.8	4.6	5.7	14.4	9.7	13.8
Ozone depletion (kg CFC-11-eq $\times 10^{-7}$)	6.9	6.7	6.1	6.9	4.2	7.1	4.5
Particulate matter (disease incidence $\times 10^{-7}$)	3.7	4.0	3.5	4.0	1.8	3.1	1.5
Photochemical ozone formation (kg NMVOC-eq $\times 10^{-2}$)	1.3	1.5	1.3	1.7	0.9	1.9	0.9
Water use (m^3 world eq. deprived)	0.2	0.6	1.0	1.9	2.9	3.2	3.2
Climage change (kg CO_2-eq)	13.6	13.8	12.0	12.9	3.7	9.4	2.3

Table S30. Environmental impacts of per kg H_2 in the H_2 market of China in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq $\times 10^{-2}$)	2.5	2.9	1.9	3.2	1.9	3.7	1.7
Ecotoxicity: freshwater (CTUe)	394.5	427.7	212.9	437.9	212.9	370.0	175.2
Resource use: energy carriers (MJ, net calorific value)	156.0	168.1	101.8	173.6	101.8	166.9	91.6
Eutrophication: aquatic freshwater (kg PO_4-eq $\times 10^{-3}$)	2.4	2.7	1.3	2.8	1.3	2.9	1.1
Eutrophication: aquatic marine (kg N-eq $\times 10^{-3}$)	2.4	3.3	2.4	4.2	2.4	5.4	2.1
Eutrophication: terrestrial (mol N-eq $\times 10^{-2}$)	8.3	9.0	3.6	9.0	3.6	7.6	2.7
Human toxicity: cancer effects (CTUh $\times 10^{-9}$)	1.5	1.9	5.5	3.1	5.5	5.6	5.8
Human toxicity: non- cancer effects (CTUh $\times 10^{-7}$)	0.4	0.6	1.2	1.0	1.2	1.5	1.3

Ionising radiation: human health (kBq U^{235}-eq)	-0.07	0.03	2.7	0.6	2.7	1.7	2.9
Land use (dimensionless)	27.6	30.9	121.5	48.1	121.5	86.0	125.2
Resource use: minerals and metals (kg Sb-eq $\times 10^{-4}$)	0.2	0.2	1.8	0.6	1.8	1.4	1.9
Ozone depletion (kg CFC-11-eq $\times 10^{-7}$)	2.5	2.6	2.5	2.8	2.5	3.8	2.6
Particulate matter (disease incidence $\times 10^{-6}$)	1.1	1.2	0.4	1.2	0.4	0.8	0.3
Photochemical ozone formation (kg NMVOC-eq $\times 10^{-2}$)	0.7	1.0	0.7	1.2	0.7	1.6	0.7
Water use (m^3 world eq. deprived)	0.6	0.8	1.4	1.1	1.4	1.6	1.5
Climage change (kg CO_2-eq)	19.1	20.0	5.2	19.1	5.2	13.5	2.4

Table S31. Environmental impacts of per kg H_2 in the H_2 market of USA in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq $\times 10^{-2}$)	1.3	1.4	1.3	1.9	1.3	1.6	1.4
Ecotoxicity: freshwater (CTUe)	114.4	114.3	117.8	139.8	117.8	133.7	119.8
Resource use: energy carriers (MJ, net calorific value)	147.1	150.4	69.6	162.8	69.6	156.3	84.3
Eutrophication: aquatic freshwater (kg PO_4-eq $\times 10^{-3}$)	-0.1	0.2	0.5	1.9	0.5	0.4	0.5
Eutrophication: aquatic marine (kg N-eq $\times 10^{-3}$)	1.8	2.0	1.6	3.0	1.6	2.4	1.7
Eutrophication: terrestrial (mol N-eq $\times 10^{-2}$)	2.1	2.1	1.7	2.9	1.7	2.6	1.9
Human toxicity: cancer effects (CTUh $\times 10^{-9}$)	2.4	2.7	4.5	3.5	4.5	3.8	4.3
Human toxicity: non- cancer effects (CTUh $\times 10^{-8}$)	2.4	3.1	8.0	5.6	8.0	5.7	7.2
Ionising radiation: human health (kBq U^{235}-eq)	0.8	1.2	0.7	1.9	0.7	2.6	1.0
Land use (dimensionless)	3.3	7.5	75.5	20.5	75.5	29.3	69.3
Resource use: minerals and metals (kg Sb-eq $\times 10^{-4}$)	0.3	0.3	1.2	0.6	1.2	0.8	1.1
Ozone depletion (kg CFC-11-eq $\times 10^{-7}$)	5.8	5.8	3.4	5.6	3.4	5.4	3.8
Particulate matter (disease incidence $\times 10^{-7}$)	0.9	1.0	1.1	1.3	1.1	1.2	1.1
Photochemical ozone formation (kg NMVOC-eq $\times 10^{-2}$)	1.8	1.9	1.0	2.0	1.0	1.8	1.2
Water use (m^3 world eq. deprived)	0.2	0.3	0.8	0.8	0.8	1.1	1.0
Climage change (kg CO_2-eq)	10.4	10.4	3.4	10.1	3.4	6.6	2.4

Table S32. Environmental impacts of per kg H_2 in the H_2 market of EU in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq $\times 10^{-2}$)	0.7	0.6	1.2	1.1	1.2	1.3	1.2
Ecotoxicity: freshwater (CTUe)	59.0	57.0	106.8	93.4	106.8	110.4	106.0
Resource use: energy carriers (MJ, net calorific value)	170.7	168.6	75.1	169.9	75.1	161.3	81.4
Eutrophication: aquatic freshwater (kg PO_4-eq $\times 10^{-4}$)	3.3	1.7	5.8	3.6	5.8	4.6	5.4
Eutrophication: aquatic marine (kg N-eq $\times 10^{-3}$)	2.0	1.9	2.1	2.8	2.1	3.1	2.2
Eutrophication: terrestrial (mol N-eq $\times 10^{-2}$)	2.2	2.1	2.3	3.1	2.3	3.4	2.5
Human toxicity: cancer effects (CTUh $\times 10^{-9}$)	1.7	1.7	5.1	3.3	5.1	4.1	4.9
Human toxicity: non- cancer effects (CTUh $\times 10^{-8}$)	2.5	2.3	9.2	5.6	9.2	7.4	8.7
Ionising radiation: human health (kBq U^{235}-eq)	1.1	1.1	0.8	2.7	0.8	3.5	0.9
Land use (dimensionless)	3.4	3.9	50.4	22.8	50.4	34.4	54.0
Resource use: minerals and metals (kg Sb-eq $\times 10^{-4}$)	0.3	0.3	1.4	0.7	1.4	1.0	1.3

Ozone depletion (kg CFC-11-eq $\times10^{-6}$)	1.9	1.9	0.8	1.6	0.8	1.3	0.9
Particulate matter (disease incidence $\times10^{-7}$)	0.5	0.5	1.1	1.0	1.1	1.2	1.1
Photochemical ozone formation (kg NMVOC-eq $\times10^{-2}$)	1.6	1.6	1.0	1.6	1.0	1.5	1.1
Water use (m^3 world eq. deprived)	0.3	0.3	1.4	1.4	1.4	1.9	1.6
Climage change (kg CO_2-eq)	11.4	11.2	3.6	8.8	3.6	5.5	2.7

Table S33. Environmental impacts of per kg H_2 in the H_2 market of Brazil in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq $\times10^{-2}$)	0.4	0.6	1.0	0.9	1.0	1.0	1.0
Ecotoxicity: freshwater (CTUe)	35.8	45.0	88.9	61.1	88.9	66.9	79.4
Resource use: energy carriers (MJ, net calorific value)	161.9	155.6	78.9	138.0	78.9	129.8	92.8
Eutrophication: aquatic freshwater (kg PO_4-eq $\times10^{-4}$)	0.1	1.6	4.9	2.5	4.9	3.5	4.1
Eutrophication: aquatic marine (kg N-eq $\times10^{-3}$)	1.3	1.5	1.6	1.8	1.6	1.9	1.6
Eutrophication: terrestrial (mol N-eq $\times10^{-2}$)	1.4	1.7	1.7	2.0	1.7	2.1	1.9
Human toxicity: cancer effects (CTUh $\times10^{-9}$)	0.9	1.3	3.8	2.1	3.8	2.4	3.3
Human toxicity: non- cancer effects (CTUh $\times10^{-8}$)	1.8	2.6	7.7	4.1	7.7	4.6	6.5
Ionising radiation: human health (kBq U^{235}-eq)	0.03	0.1	0.2	0.2	0.2	0.3	0.2
Land use (dimensionless)	4.3	11.6	87.3	28.7	87.3	29.8	76.3
Resource use: minerals and metals (kg Sb-eq $\times10^{-4}$)	0.2	0.3	1.2	0.6	1.2	0.7	1.0
Ozone depletion (kg CFC-11-eq $\times10^{-6}$)	2.0	1.9	1.0	1.6	1.0	1.5	1.1
Particulate matter (disease incidence $\times10^{-8}$)	1.6	3.6	9.5	6.3	9.5	7.2	8.9
Photochemical ozone formation (kg NMVOC-eq $\times10^{-3}$)	6.3	7.0	6.2	7.5	6.2	7.6	6.5
Water use (m^3 world eq. deprived)	-0.8	1.6	7.1	6.1	7.1	8.2	8.5
Climage change (kg CO_2-eq)	10.1	9.5	3.6	7.9	3.6	5.3	2.5

Table S34. Environmental impacts of per kg H_2 in the H_2 market of Rest of Central and South America in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq $\times10^{-3}$)	4.1	5.5	9.7	8.1	9.7	9.4	9.2
Ecotoxicity: freshwater (CTUe)	36.2	40.1	85.6	57.1	85.6	65.4	77.4
Resource use: energy carriers (MJ, net calorific value)	161.9	160.6	79.6	141.7	79.6	130.8	92.2
Eutrophication: aquatic freshwater (kg PO_4-eq $\times10^{-4}$)	0.2	1.2	4.7	2.3	4.7	3.3	3.9
Eutrophication: aquatic marine (kg N-eq $\times10^{-3}$)	1.3	1.5	1.5	1.7	1.5	1.8	1.5
Eutrophication: terrestrial (mol N-eq $\times10^{-2}$)	1.4	1.6	1.6	1.9	1.6	2.0	1.8
Human toxicity: cancer effects (CTUh $\times10^{-9}$)	0.9	1.0	3.8	2.0	3.8	2.4	3.3
Human toxicity: non- cancer effects (CTUh $\times10^{-8}$)	1.9	2.2	7.5	3.8	7.5	4.5	6.5
Ionising radiation: human health (kBq U^{235}-eq)	0.03	0.06	0.2	0.2	0.2	0.3	0.2
Land use (dimensionless)	4.3	6.3	86.5	25.1	86.5	28.9	76.4
Resource use: minerals and metals (kg Sb-eq $\times10^{-4}$)	0.2	0.3	1.2	0.5	1.2	0.7	1.0
Ozone depletion (kg CFC-11-eq $\times10^{-6}$)	2.0	1.9	1.0	1.7	1.0	1.6	1.1
Particulate matter (disease incidence $\times10^{-8}$)	1.7	2.7	8.0	5.3	8.0	6.4	7.8
Photochemical ozone formation (kg NMVOC-eq $\times10^{-3}$)	6.4	6.8	6.0	7.3	6.0	7.5	6.3

Water use (m^3 world eq. deprived)	-0.7	0.3	7.0	5.2	7.0	8.0	8.6
Climage change (kg CO_2-eq)	10.1	9.8	3.5	8.1	3.5	5.3	2.4

Table S35. Environmental impacts of per kg H_2 in the H_2 market of Rest of North America in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq $\times10^{-2}$)	1.8	1.8	1.2	1.7	1.2	1.6	1.3
Ecotoxicity: freshwater (CTUe)	31.2	38.5	61.0	50.4	61.0	62.6	60.7
Resource use: energy carriers (MJ, net calorific value)	139.2	136.5	67.2	130.1	67.2	119.6	76.9
Eutrophication: aquatic freshwater (kg PO_4-eq $\times10^{-4}$)	-3.7	1.5	2.6	1.6	2.6	3.2	2.2
Eutrophication: aquatic marine (kg N-eq $\times10^{-3}$)	2.3	2.5	1.7	2.4	1.7	2.3	1.7
Eutrophication: terrestrial (mol N-eq $\times10^{-2}$)	2.6	2.7	1.8	2.6	1.8	2.4	1.9
Human toxicity: cancer effects (CTUh $\times10^{-9}$)	1.9	2.0	3.0	2.3	3.0	2.5	2.7
Human toxicity: non- cancer effects (CTUh $\times10^{-8}$)	1.7	2.2	4.0	2.7	4.0	3.1	3.5
Ionising radiation: human health (kBq U^{235}-eq)	-0.1	0.4	0.6	1.1	0.6	2.1	1.0
Land use (dimensionless)	6.5	9.2	36.2	8.1	36.2	5.6	32.7
Resource use: minerals and metals (kg Sb-eq $\times10^{-5}$)	2.2	2.6	5.5	3.2	5.5	3.8	4.6
Ozone depletion (kg CFC-11-eq $\times10^{-6}$)	1.4	1.3	0.7	1.1	0.7	1.0	0.7
Particulate matter (disease incidence $\times10^{-7}$)	1.0	1.0	0.9	1.0	0.9	1.0	0.9
Photochemical ozone formation (kg NMVOC-eq $\times10^{-2}$)	1.0	1.0	0.7	1.0	0.7	0.9	0.7
Water use (m^3 world eq. deprived)	-0.5	2.1	10.5	6.5	10.5	12.0	14.9
Climage change (kg CO_2-eq)	9.3	8.9	2.9	7.5	2.9	4.3	2.1

Table S36. Environmental impacts of per kg H_2 in the H_2 market of Rest of Europe in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq $\times10^{-2}$)	0.6	1.2	0.9	0.7	0.9	4.3	0.9
Ecotoxicity: freshwater (CTUe)	26.8	35.9	92.9	64.7	92.9	81.2	84.2
Resource use: energy carriers (MJ, net calorific value)	161.0	152.9	60.3	122.0	60.3	134.5	69.6
Eutrophication: aquatic freshwater (kg PO_4-eq $\times10^{-3}$)	0.3	1.0	0.5	0.3	0.5	4.6	0.5
Eutrophication: aquatic marine (kg N-eq $\times10^{-3}$)	1.2	1.5	1.2	1.3	1.2	3.0	1.2
Eutrophication: terrestrial (mol N-eq $\times10^{-2}$)	1.3	1.4	1.3	1.4	1.3	2.3	1.3
Human toxicity: cancer effects (CTUh $\times10^{-9}$)	1.0	1.5	3.8	2.4	3.8	3.4	3.6
Human toxicity: non- cancer effects (CTUh $\times10^{-8}$)	1.8	3.0	8.5	4.7	8.5	8.1	7.8
Ionising radiation: human health (kBq U^{235}-eq)	0.9	0.9	0.4	0.9	0.4	1.2	0.5
Land use (dimensionless)	1.9	2.6	8.3	3.6	8.3	3.8	9.0
Resource use: minerals and metals (kg Sb-eq $\times10^{-4}$)	0.2	0.4	1.4	0.7	1.4	0.9	1.3
Ozone depletion (kg CFC-11-eq $\times10^{-6}$)	1.2	1.1	0.5	1.0	0.5	0.9	0.6
Particulate matter (disease incidence $\times10^{-8}$)	2.5	3.6	6.1	4.5	6.1	9.0	5.8
Photochemical ozone formation (kg NMVOC-eq $\times10^{-3}$)	4.0	4.7	4.2	4.3	4.2	8.9	4.2
Water use (m^3 world eq. deprived)	0.3	3.0	11.6	10.5	11.6	13.3	11.4
Climage change (kg CO_2-eq)	9.8	9.2	2.6	6.8	2.6	6.0	2.0

Table S37. Environmental impacts of per kg H_2 in the H_2 market of Africa in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq $\times 10^{-2}$)	1.1	1.0	1.3	2.8	1.3	1.4	1.2
Ecotoxicity: freshwater (CTUe)	116.9	115.6	120.7	172.6	120.7	122.6	109.8
Resource use: energy carriers (MJ, net calorific value)	152.6	151.6	73.9	159.1	73.9	135.5	85.3
Eutrophication: aquatic freshwater (kg PO_4-eq $\times 10^{-3}$)	1.3	1.3	0.9	2.4	0.9	0.9	0.6
Eutrophication: aquatic marine (kg N-eq $\times 10^{-3}$)	1.6	1.6	1.6	3.0	1.6	1.9	1.5
Eutrophication: terrestrial (mol N-eq $\times 10^{-2}$)	2.5	2.4	1.9	3.7	1.9	2.3	1.8
Human toxicity: cancer effects (CTUh $\times 10^{-9}$)	1.0	1.0	4.7	2.4	4.7	2.4	4.0
Human toxicity: non- cancer effects (CTUh $\times 10^{-8}$)	3.3	3.3	9.2	8.4	9.2	6.0	8.1
Ionising radiation: human health (kBq U^{235}-eq)	0.09	0.08	0.08	0.2	0.09	0.2	0.1
Land use (dimensionless)	7.7	8.5	92.8	21.2	92.8	24.8	77.1
Resource use: minerals and metals (kg Sb-eq $\times 10^{-4}$)	0.2	0.2	1.3	0.5	1.3	0.7	1.1
Ozone depletion (kg CFC-11-eq $\times 10^{-7}$)	6.7	6.7	4.2	6.5	4.2	6.7	4.7
Particulate matter (disease incidence $\times 10^{-7}$)	0.6	0.5	1.2	1.0	1.2	0.9	1.0
Photochemical ozone formation (kg NMVOC-eq $\times 10^{-2}$)	0.7	0.7	0.7	1.1	0.7	0.9	0.7
Water use (m^3 world eq. deprived)	0.1	0.1	3.3	3.3	3.3	5.3	3.8
Climage change (kg CO_2-eq)	11.4	11.1	3.9	11.2	3.9	7.0	2.8

Table S38. Environmental impacts of per kg H_2 in the H_2 market of India in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq $\times 10^{-2}$)	-0.2	1.4	1.5	4.9	1.5	6.1	1.3
Ecotoxicity: freshwater (CTUe)	103.9	150.3	143.7	249.4	143.7	268.1	129.2
Resource use: energy carriers (MJ, net calorific value)	135.9	152.4	130.0	187.3	130.0	201.8	130.1
Eutrophication: aquatic freshwater (kg PO_4-eq $\times 10^{-3}$)	0.6	1.5	1.0	3.3	1.0	3.6	0.7
Eutrophication: aquatic marine (kg N-eq $\times 10^{-3}$)	-0.2	1.9	2.1	6.3	2.1	7.8	1.8
Eutrophication: terrestrial (mol N-eq $\times 10^{-2}$)	1.2	3.3	2.2	7.7	2.2	8.7	1.9
Human toxicity: cancer effects (CTUh $\times 10^{-9}$)	0.8	1.3	4.4	2.9	4.4	4.0	4.1
Human toxicity: non- cancer effects (CTUh $\times 10^{-7}$)	0.2	0.5	1.1	1.1	1.1	1.4	1.0
Ionising radiation: human health (kBq U^{235}-eq)	-0.03	0.08	5.3	1.3	5.3	3.1	5.0
Land use (dimensionless)	6.7	10.3	21.4	17.8	21.4	18.2	19.5
Resource use: minerals and metals (kg Sb-eq $\times 10^{-4}$)	0.2	0.3	1.6	0.6	1.6	0.9	1.4
Ozone depletion (kg CFC-11-eq $\times 10^{-7}$)	6.2	6.2	4.3	6.1	4.3	6.3	4.5
Particulate matter (disease incidence $\times 10^{-7}$)	0.4	0.7	1.3	1.4	1.3	1.7	1.1
Photochemical ozone formation (kg NMVOC-eq $\times 10^{-2}$)	0.2	0.8	0.7	2.0	0.7	2.5	0.7
Water use (m^3 world eq. deprived)	-0.2	0.1	6.7	2.2	6.7	5.0	6.7
Climage change (kg CO_2-eq)	10.8	11.8	3.8	12.9	3.8	10.0	2.6

Table S39. Environmental impacts of per kg H_2 in the H_2 market of Japan in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050

Acidification (mol H+-eq $\times10^{-2}$)	2.4	2.7	1.9	3.9	1.9	3.2	1.8
Ecotoxicity: freshwater (CTUe)	137.9	150.1	132.3	191.9	132.3	178.5	131.9
Resource use: energy carriers (MJ, net calorific value)	177.1	184.2	90.4	210.6	90.4	211.8	91.4
Eutrophication: aquatic freshwater (kg PO_4-eq $\times10^{-3}$)	1.1	1.3	0.8	2.4	0.8	1.3	0.6
Eutrophication: aquatic marine (kg N-eq $\times10^{-3}$)	3.8	4.5	3.2	6.6	3.2	5.6	3.0
Eutrophication: terrestrial (mol N-eq $\times10^{-2}$)	4.8	5.4	3.9	7.6	3.9	6.2	3.9
Human toxicity: cancer effects (CTUh $\times10^{-9}$)	2.5	3.0	5.6	4.4	5.6	5.0	5.4
Human toxicity: non- cancer effects (CTUh $\times10^{-7}$)	0.6	0.7	1.0	1.1	1.0	1.1	1.0
Ionising radiation: human health (kBq U^{235}-eq)	0.1	1.1	2.6	3.3	2.6	5.6	2.7
Land use (dimensionless)	17.8	27.3	79.0	50.3	79.0	39.1	82.6
Resource use: minerals and metals (kg Sb-eq $\times10^{-4}$)	0.3	0.5	1.5	0.9	1.5	1.2	1.4
Ozone depletion (kg CFC-11-eq $\times10^{-7}$)	1.8	2.1	2.1	3.1	2.1	3.6	2.0
Particulate matter (disease incidence $\times10^{-7}$)	1.1	1.3	1.6	1.9	1.6	1.9	1.6
Photochemical ozone formation (kg NMVOC-eq $\times10^{-2}$)	1.6	1.7	1.1	2.2	1.1	1.9	1.0
Water use (m^3 world eq. deprived)	0.3	0.7	1.9	1.7	1.9	2.4	2.1
Climage change (kg CO_2-eq)	13.1	12.4	0.9	11.4	0.9	7.3	-1.0

Table S40. Environmental impacts of per kg H_2 in the H_2 market of Southeast Asia in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq $\times10^{-2}$)	1.2	1.6	1.3	2.2	1.3	2.3	1.2
Ecotoxicity: freshwater (CTUe)	91.8	111.8	119.3	138.0	119.3	156.7	114.8
Resource use: energy carriers (MJ, net calorific value)	153.5	159.6	65.9	167.5	65.9	167.3	70.0
Eutrophication: aquatic freshwater (kg PO_4-eq $\times10^{-3}$)	1.9	3.1	0.9	4.7	0.9	4.1	0.7
Eutrophication: aquatic marine (kg N-eq $\times10^{-3}$)	1.6	2.6	1.6	3.8	1.6	4.1	1.5
Eutrophication: terrestrial (mol N-eq $\times10^{-2}$)	3.0	3.6	1.9	4.4	1.9	4.2	1.6
Human toxicity: cancer effects (CTUh $\times10^{-9}$)	1.0	1.7	4.6	2.6	4.6	3.7	4.4
Human toxicity: non- cancer effects (CTUh $\times10^{-7}$)	0.4	0.6	1.0	0.8	1.0	1.0	0.9
Ionising radiation: human health (kBq U^{235}-eq)	0.1	0.3	0.5	0.7	0.5	1.5	0.8
Land use (dimensionless)	11.6	23.4	121.4	39.4	121.4	63.1	113.7
Resource use: minerals and metals (kg Sb-eq $\times10^{-4}$)	0.2	0.4	1.5	0.6	1.5	1.0	1.4
Ozone depletion (kg CFC-11-eq $\times10^{-7}$)	6.1	6.1	3.6	6.1	3.6	6.4	3.7
Particulate matter (disease incidence $\times10^{-7}$)	0.7	1.1	1.1	1.6	1.1	1.8	1.0
Photochemical ozone formation (kg NMVOC-eq $\times10^{-2}$)	0.7	0.9	0.6	1.1	0.6	1.3	0.6
Water use (m^3 world eq. deprived)	0.2	1.2	2.7	2.5	2.7	4.9	3.2
Climage change (kg CO_2-eq)	12.4	12.4	3.4	12.3	3.4	9.0	2.1

Table S41. Environmental impacts of per kg H_2 in the H_2 market of Rest of Asia Pacific in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq $\times10^{-2}$)	1.1	1.4	1.3	2.2	1.3	2.4	1.2
Ecotoxicity: freshwater (CTUe)	90.3	101.3	117.3	138.0	117.3	156.8	114.7
Resource use: energy carriers (MJ, net calorific value)	152.9	156.0	65.1	167.6	65.1	167.4	69.7

Eutrophication: aquatic freshwater (kg PO_4-eq ×10^{-3})	1.7	2.4	0.9	4.6	0.9	4.1	0.7
Eutrophication: aquatic marine (kg N-eq ×10^{-3})	1.6	2.1	1.6	3.8	1.6	4.1	1.4
Eutrophication: terrestrial (mol N-eq ×10^{-2})	2.9	3.2	1.9	4.4	1.9	4.1	1.6
Human toxicity: cancer effects (CTUh ×10^{-9})	1.0	1.4	4.6	2.6	4.6	3.7	4.5
Human toxicity: non- cancer effects (CTUh ×10^{-7})	0.4	0.5	1.0	0.8	1.0	1.0	0.9
Ionising radiation: human health (kBq U^{235}-eq)	0.1	0.2	0.5	0.7	0.5	1.6	0.8
Land use (dimensionless)	11.0	18.3	122.3	39.6	122.3	63.5	113.9
Resource use: minerals and metals (kg Sb-eq ×10^{-4})	0.2	0.3	1.5	0.5	1.5	1.0	1.4
Ozone depletion (kg CFC-11-eq ×10^{-7})	6.2	6.2	3.7	6.2	3.7	6.4	3.7
Particulate matter (disease incidence ×10^{-7})	0.6	0.9	1.0	1.6	1.0	1.8	1.0
Photochemical ozone formation (kg NMVOC-eq ×10^{-2})	0.7	0.8	0.6	1.1	0.6	1.3	0.6
Water use (m^3 world eq. deprived)	0.2	0.8	2.7	2.6	2.7	5.0	3.2
Climage change (kg CO_2-eq)	12.2	12.1	3.3	12.2	3.3	9.0	2.1

Table S42. Environmental impacts of per kg H_2 in the H_2 market of Middle East in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq ×10^{-2})	0.5	0.6	1.0	0.9	1.0	1.2	1.0
Ecotoxicity: freshwater (CTUe)	39.7	44.4	89.4	64.4	89.4	74.1	80.9
Resource use: energy carriers (MJ, net calorific value)	177.1	178.7	90.1	184.0	90.1	177.3	99.7
Eutrophication: aquatic freshwater (kg PO_4-eq ×10^{-4})	1.9	2.1	5.4	2.4	5.4	3.5	4.7
Eutrophication: aquatic marine (kg N-eq ×10^{-3})	1.4	1.5	1.6	2.0	1.6	2.3	1.6
Eutrophication: terrestrial (mol N-eq ×10^{-2})	1.5	1.6	1.7	2.2	1.7	2.5	1.9
Human toxicity: cancer effects (CTUh ×10^{-9})	1.3	1.5	3.9	2.1	3.9	2.5	3.7
Human toxicity: non- cancer effects (CTUh ×10^{-8})	2.7	3.1	8.5	4.6	8.5	5.5	7.5
Ionising radiation: human health (kBq U^{235}-eq)	1.1	1.1	0.7	1.1	0.7	1.0	0.7
Land use (dimensionless)	2.6	5.8	110.7	19.4	110.7	31.1	102.9
Resource use: minerals and metals (kg Sb-eq ×10^{-4})	0.2	0.3	1.3	0.5	1.3	0.7	1.1
Ozone depletion (kg CFC-11-eq ×10^{-7})	4.7	5.0	3.2	6.2	3.2	6.5	3.3
Particulate matter (disease incidence ×10^{-7})	0.7	0.7	1.1	0.9	1.1	1.0	1.1
Photochemical ozone formation (kg NMVOC-eq ×10^{-2})	3.2	3.2	1.8	3.0	1.8	2.9	2.0
Water use (m^3 world eq. deprived)	0.2	0.3	0.7	0.6	0.7	0.8	0.7
Climage change (kg CO_2-eq)	12.3	12.2	4.6	11.9	4.6	9.3	3.1

Table S43. Environmental impacts of per kg H_2 in the H_2 market of Russia in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq ×10^{-2})	0.9	0.8	1.3	0.8	1.3	7.1	1.8
Ecotoxicity: freshwater (CTUe)	110.2	108.7	133.9	108.4	133.9	247.4	154.4
Resource use: energy carriers (MJ, net calorific value)	185.2	183.7	132.2	183.1	132.2	315.8	106.7
Eutrophication: aquatic freshwater (kg PO_4-eq ×10^{-4})	3.2	2.3	5.5	2.3	5.5	3.6	7.
Eutrophication: aquatic marine (kg N-eq ×10^{-3})	2.3	2.2	2.7	2.2	2.7	8.1	3.4
Eutrophication: terrestrial (mol N-eq ×10^{-2})	2.	2.4	2.8	2.4	2.8	8.0	3.9

Human toxicity: cancer effects (CTUh ×10^{-9})	2.6	2.6	4.8	2.6	4.8	6.4	6.5
Human toxicity: non- cancer effects (CTUh ×10^{-7})	0.3	0.3	0.9	0.3	0.9	1.4	1.2
Ionising radiation: human health (kBq U^{235}-eq)	1.3	1.2	2.0	1.2	2.0	6.7	3.5
Land use (dimensionless)	5.2	6.8	23.2	9.1	23.2	15.5	80.9
Resource use: minerals and metals (kg Sb-eq ×10^{-4})	0.3	0.3	1.2	0.3	1.2	1.3	1.8
Ozone depletion (kg CFC-11-eq ×10^{-6})	1.4	1.4	0.9	1.4	0.9	1.6	0.5
Particulate matter (disease incidence ×10^{-7})	0.8	0.8	1.6	0.8	1.6	3.2	2.6
Photochemical ozone formation (kg NMVOC-eq ×10^{-2})	2.7	2.7	2.0	2.7	2.0	4.4	1.5
Water use (m^3 world eq. deprived)	0.4	0.3	1.6	0.3	1.6	4.0	2.9
Climage change (kg CO_2-eq)	12.6	12.3	5.9	11.7	5.9	15.7	-0.1

Table S44. Environmental impacts of per kg H_2 in the H_2 market of Rest of Eurasia in three scenarios.

Environmental impact categories (unit)	STEPS			APS		NZE	
	2020	2030	2050	2030	2050	2030	2050
Acidification (mol H+-eq ×10^{-2})	0.9	5.2	1.5	7.8	1.5	7.5	1.8
Ecotoxicity: freshwater (CTUe)	110.2	175.5	148.5	213.1	148.5	255.8	154.3
Resource use: energy carriers (MJ, net calorific value)	185.2	233.3	108.4	259.0	108.4	323.8	106.8
Eutrophication: aquatic freshwater (kg PO_4-eq ×10^{-3})	0.3	2.7	0.7	4.3	0.7	3.8	0.8
Eutrophication: aquatic marine (kg N-eq ×10^{-3})	2.3	5.3	2.9	7.0	2.9	8.5	3.4
Eutrophication: terrestrial (mol N-eq ×10^{-2})	2.5	5.3	3.0	6.8	3.0	8.4	3.9
Human toxicity: cancer effects (CTUh ×10^{-9})	2.6	4.0	6.0	4.8	6.0	6.6	6.5
Human toxicity: non- cancer effects (CTUh ×10^{-7})	0.3	0.8	1.2	1.1	1.2	1.4	1.2
Ionising radiation: human health (kBq U^{235}-eq)	1.3	2.7	2.4	3.7	2.4	7.0	3.5
Land use (dimensionless)	5.2	10.7	23.3	14.8	23.3	16.0	80.8
Resource use: minerals and metals (kg Sb-eq ×10^{-4})	0.3	0.6	1.7	0.8	1.7	1.3	1.8
Ozone depletion (kg CFC-11-eq ×10^{-6})	1.4	1.5	0.7	1.4	0.7	1.6	0.5
Particulate matter (disease incidence ×10^{-7})	0.8	2.0	2.1	2.5	2.1	3.3	2.6
Photochemical ozone formation (kg NMVOC-eq ×10^{-2})	2.7	3.5	1.6	3.9	1.6	4.5	1.5
Water use (m^3 world eq. deprived)	0.4	1.7	2.2	2.5	2.2	4.2	2.8
Climage change (kg CO_2-eq)	12.6	15.4	4.6	16.6	4.6	16.1	-0.1

4.2 Cumulative GHG emissions of H_2 production

As shown in Figure S2, in the STESP, APS and NZE scenarios, China emits 16 Gt CO_2-eq, 14 Gt CO_2-eq, and 15 Gt CO_2-eq GHG emissions from 2020 to 2050. Although China will produce four times more H_2 in 2050 in the NZE scenario compared to the STEPS scenario, the cumulative GHG emissions between 2020 and 2050 in the NZE can be lower than that in the STEPS due to the large-scale use of water electrolysis. In the USA, these cumulative emissions in these scenarios will be 3.9 Gt CO_2-eq, 5.2 Gt CO_2-eq, and 6.1 Gt CO_2-eq. The H_2 demand in the USA in 2050 in the NZE scenario is close to that in China. However, since the US has a lower emission intensity of electricity, the cumulative GHG emissions are lower than China.

Contrary to the decreasing trend of H_2 production in the STEPS scenario, the EU is expected to produce more H_2 in the APS and NZE scenarios. In the EU, the cumulative GHG emissions of H_2 production will be 1.6 Gt CO_2-eq, 2.4 Gt CO_2-eq, and 3.1 Gt CO_2-eq in three scenarios. The high increase of H_2 production in the APS and NZE scenarios makes the cumulative GHG emissions in these scenarios higher than those in the STEPS scenario. The overall H_2 production related GHG emissions of China, the USA and the EU in the NZE scenario could use 2.5-8.6%, 1.0-3.4% and 0.5-1.7% of the residual carbon budget between 2020 and 2050 to limit global warming to 1.5°C with 67% certainty.[42] Overall, in the NZE scenario, the cumulative GHG emissions of H_2 production in most regions will always be higher than in the STEPS scenario. Their H_2 production mixes in the NZE scenario need a more significant and faster transition to reverse this trend.

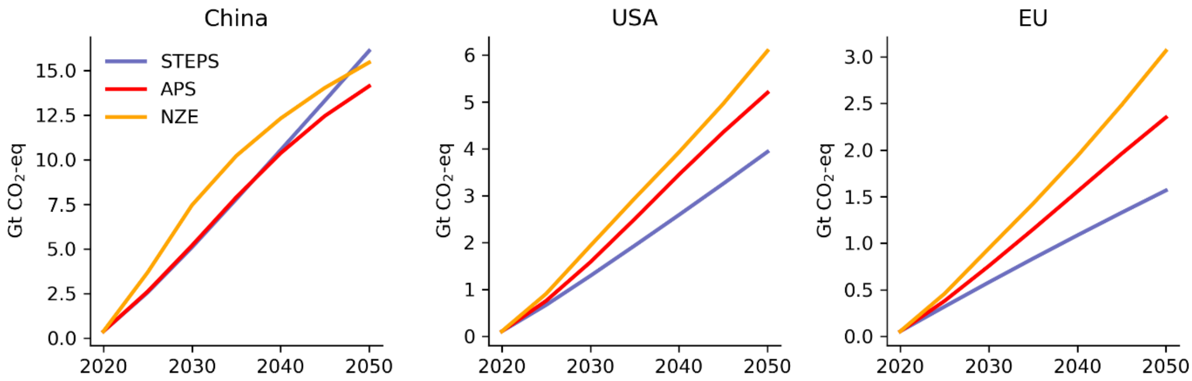

Figure S2. The cumulative GHG emissions of H_2 production in China, USA and EU in three scenarios.

4.3 Sensitivity analysis

This sensitivity analysis assumes the use of dedicated renewable electricity generation from solar photovoltaic (PV), on-shore wind, and hydropower, as currently planned and listed in IEA's H_2 production projects database.[43] We modeled these as the electricity source for water electrolysis. The proportion of H_2 production amount of water electrolysis powered by renewable electricity in water electrolysis is further assumed as 100% to quantify their impacts on the global and regional cumulative GHG emissions of H_2 production by 2050. In addition, NG SMR CCS is further assumed to be replaced by water electrolysis powered by 100% renewables to quantify the GHG emissions reduction potential of radically transitioning H_2 production to green H_2 technologies.

As shown in Figure S3, the 100% renewable electricity-powered water electrolysis and its substitution for NG SMR CCS have a limited impact on cumulative GHG emissions of H_2 production at regional and global levels in the STEPS scenario (declining 3.5% at the most). STEPS assumes a limited amount of H_2 production from water electrolysis and NG CCS. As water electrolysis plays a more critical role in the APS and NZE scenarios, the impact of the electricity source of water electrolysis on cumulative GHG emissions by 2050 becomes more significant. In the APS scenario, the global cumulative GHG emissions of H_2 production by 2050 can decrease by 5.4-10.9%, if 100% of electricity from renewable sources are used in water electrolysis. Using water electrolysis powered

100% renewables to further replace NG SMR CCS, the cumulative GHG emissions of H_2 production can be reduced by 10.8%-18.0%. In the NZE scenario, the global cumulative GHG emissions of H_2 production by 2050 can decrease by 9.8-21.9% and 30.7-49.8% corresponding to these two assumptions. Unlike in China and the USA, the scale-up of water electrolysis using dedicated electricity from solar PV will not cause a significant decrease in cumulative GHG emissions of H_2 production by 2050 in the EU. The EU will decarbonize its electricity production quicker than China and the USA. In the EU, only on-shore wind and hydropower can help water electrolysis to decarbonize further as its grid electricity will move relatively quickly to low carbon emissions. In the USA, the dedicated renewable has a very limited potential to help water electrolysis to decarbonize further due to the adoption of BECCS in its grid electricity.

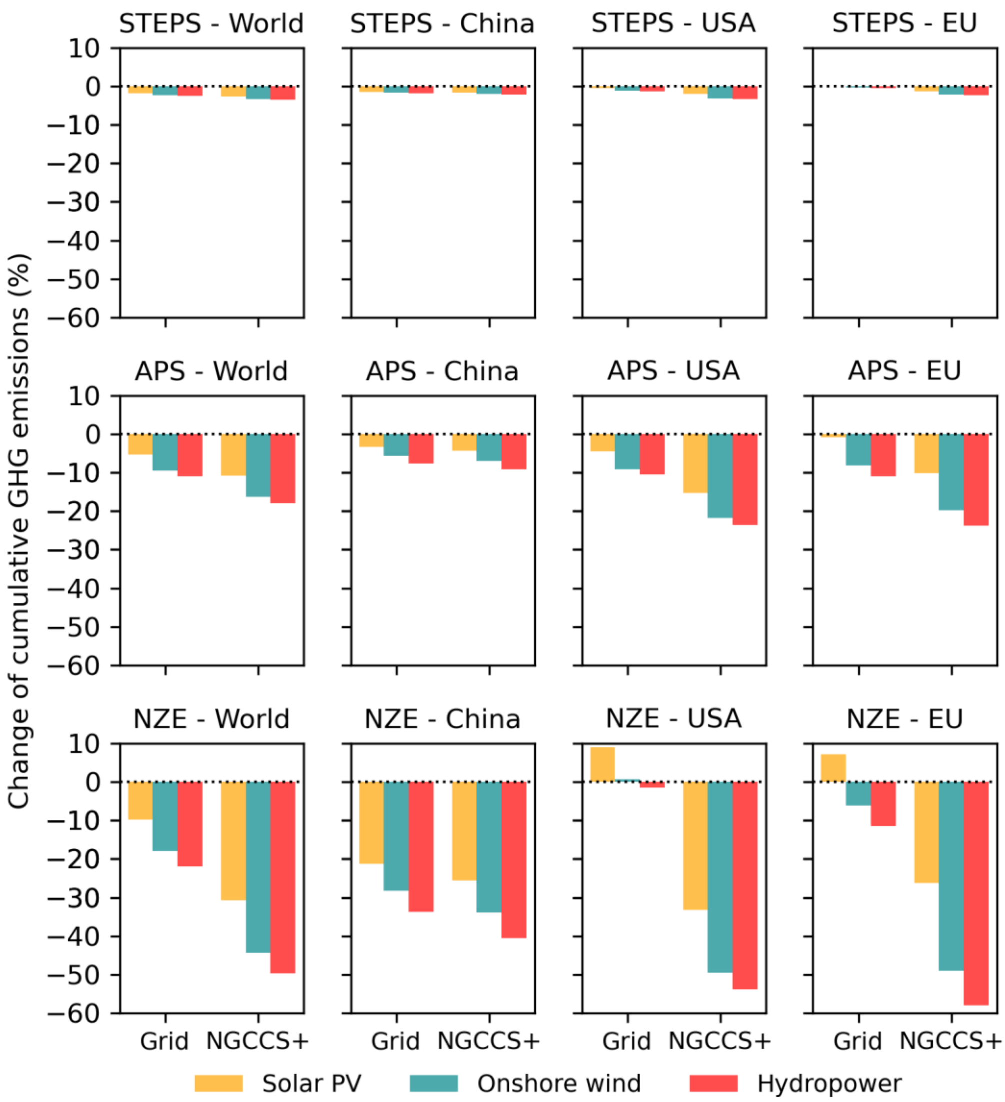

Figure S3. Sensitivity analysis. This figure shows the relative change of global and regional cumulative GHG emissions of H_2 production by 2050 caused by 100% renewable electricity-powered water electrolysis and its further substitution for NG SMR CCS. The "NGCCS+" refers to the grid-connected water electrolysis and NG SMR CCS.

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