Title: Tradeoffs in Life Cycle Water Use and Greenhouse Gas Emissions of Hydrogen Production Pathways

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Abstract: Hydrogen has been promoted as a key component of global decarbonization efforts, with various past studies estimating carbon emissions for several production pathways, but little past work has considered its water resource needs. This life cycle analysis considers hydrogen production on a per-kilogram basis for 11 pathways, fossil and non-fossil. It also includes impacts of treating water to the required quality for hydrogen production. Greenhouse gas emissions results were in a range of -15 to +31 kg CO_2e/kg H_2 produced. Water consumption varied more widely, from about 7 to 55 kg water/kg H_2 for fossil-based pathways and 530 to 3,400 kg water/kg H_2 for biomass-based pathways. Electrolysis with various renewable electricity scenarios were also modeled. Overall, there are challenging tradeoffs to be navigated to achieve a low carbon and water footprint in hydrogen economy.

Keywords: Hydrogen; LCA; GWP; Life Cycle Assessment; Global Warming Potential; Water

Abbreviations: SMR (steam methane reforming); ATR (autothermal reforming); CG (coal gasification); BG/CG (biomass and coal co-gasification); BG (biomass gasification); MP (methane pyrolysis); PEM (proton exchange membrane); SOEC (solid oxide electrolysis cell); CCS (carbon capture and storage); SYP (southern yellow pine); MDEA (methyldiethanolamine); AGR (acid gas removal); DQI (data quality index)

Introduction

Hydrogen is a critical research area in a portfolio of opportunities to replace readily available yet environmentally impactful fossil fuels in support of decarbonization efforts. Hydrogen purports to be "the basis for decarbonizing hard-to-abate applications" [1], including heat-intensive industries like iron and steel production. In 2021, the U.S. Department of Energy (DOE) announced a Hydrogen Energy Earthshot initiative that established goals of reducing clean hydrogen costs to one dollar per one kilogram (kg) in one decade [2]. Globally, about $500 billion of investment in more than 130 large-scale projects are planned by 2030, including many in Europe and China [3].

Meeting decarbonization and other sustainability goals will require hydrogen produced with low environmental impacts. Current low-carbon targets set by DOE correspond to direct process global warming potential (GWP) of 2 kg of carbon dioxide equivalents (CO_2e) per kg of hydrogen delivered [4], or 4 kg CO_2e over the life cycle [5], with similar targets expected in Europe. Considering that conventional routes to hydrogen produce more than 9 kg CO_2e per kg H_2 via the reforming reaction alone, a concerted effort is needed to identify low-carbon hydrogen technologies, evaluate their feasibility, and analyze their complete life cycle environmental impact. Beyond greenhouse gas (GHG) emissions, another key consideration will be the water required to produce hydrogen. A life cycle analysis (LCA) approach can help to consider the total impacts of hydrogen production, including those upstream, across traditional fossil-based and emerging non-fossil pathways [6, 7]. Such approaches use detailed estimates of inputs and outputs of energy, materials, and other resources required for each production process.

This paper begins with a comprehensive review of past LCA literature on hydrogen production, then discusses the data and methods used for an updated LCA for various pathways. Then, GWP and water consumption results for the hydrogen production scenarios will be presented and discussed.

Literature Review

Various studies have provided material, water, or energy inputs relevant to processes used in large-scale hydrogen production. Most past work is techno-economic analyses (TEAs) of the "stack" or direct H_2 production processes, addressing the cost of producing gaseous hydrogen (the purity of which was not always specified). These studies do not typically consider the rest of the life cycle. Analysis of conventional hydrogen profiles is common, as most reports have analyzed steam methane reforming (SMR) or coal gasification (CG) with or without carbon capture and sequestration (CCS) [8, 9, 10]. Several studies have looked at different electrolysis configurations, including proton exchange membrane (PEM) electrolysis and solid oxide electrolyzer cells (SOECs).

Beyond TEAs, several relevant studies have been completed that looked beyond direct process impacts and included various upstream processes such as fuel or electricity production. A past National Energy Technology Laboratory (NETL) study compared six fossil-based pathways in terms of levelized cost of hydrogen and GWP effects over the life cycle [11]. A European study [12] conducted a comparative LCA of SMR, autothermal reforming (ATR), CG, and methane pyrolysis (MP), with integrated CCS attached to the reforming and gasification technologies. The study included raw materials, construction, energy acquisition, and manufacturing. CG with CCS

was shown to have the lowest GHG impact across all scenarios, with a GWP of 0.1 kg CO_2e/Nm^3 H_2.

Çetinkaya et al. evaluated the life-cycle impacts of SMR, CG, wind electrolysis, solar electrolysis, and nuclear thermochemical water splitting with Cu-Cl cycle [13]. CG resulted in a lower GWP than SMR, with 11.3 kg CO_2e/kg H_2 compared to 11.9 kg CO_2e/kg H_2, and wind electrolysis outperformed solar electrolysis with a GWP of 0.97 CO_2e/kg H_2 compared to 2.4 CO_2e/kg H_2. The nuclear pathway was the highest of the study, with a GWP of CO_2e/kg H_2. The wind electrolysis pathway matches the GWP result in a 2004 NREL study [14], and the SMR GWP result is similar to a 2001 NREL report's value of 11.8 kg CO_2e/kg H_2 [15]. The nuclear Cu-Cl cycle result is significantly higher than that of 0.74 kg CO2e/kg H2 reported in Ozbilen et al. [16].

In recent literature, references to fossil fuel-based technologies largely exist in a comparative context to renewable energy-based pathways. The most recent studies have focused on hydrogen production technologies powered by renewable energy sources, such as solar farms co-located with surface feedwater for electrolysis (with a GWP of 5.0 kg CO_2e/kg H_2) [17], or solar thermochemical with seawater desalination [18] (with a GWP of 1.44 kg CO_2e/kg H_2), finding that renewable energy-based solutions could lead to substantial improvements in GWP impacts.

In a review of 21 existing LCA studies focused on electrolysis technologies [19], three types of electrolyzers were identified (alkaline, PEM, and SOEC), but studies were deemed difficult to compare due to their differences in system boundary, geographic region, and data vintage. Electrolysis generally has low GWP impacts, but only if renewable energy is used. The review paper shows an average GWP of ~1 kg CO_2e/kg H_2 for wind electrolysis and ~2 kg CO_2e/kg H_2 for solar electrolysis. Electrolysis using European average grid electricity resulted in GWP impacts over double those of CG or SMR [19].

The only paper to report water impact results was a 2018 study by Mehmeti et al. [20], which compared SMR, coal gasification, biomass gasification, biomass reformation, PEM, SOEC, and three dark fermentation pathways. Among other impact assessment methods, the paper reported water consumption potential and water scarcity footprint. Biomass reformation with corn had the lowest water consumption of 2.25 m^3/kg H_2, and PEM had the highest water consumption of 223 m^3/kg H_2. These same pathways resulted in the lowest and highest water scarcity footprint, with 212 m^3/kg H_2 and 9600 m^3/kg H_2, respectively.

Overall, these past studies show that: fossil-based technology pathways generally have higher stack GHG emissions than non-fossil [21] and are significantly higher than DOE and other targets. Incorporating CCS systems can reduce GHG emissions significantly but also require more energy and water inputs than non-CCS pathways [11]. Past studies also show the variability in impacts associated with upstream electricity consumption. Most LCA studies model electricity sources as different scenarios (e.g., grid average, wind, solar), which is especially important for electrolysis due to its high electricity consumption [21, 17]. However, studies often consider a site-specific renewable electricity source and thus are challenging to generalize and compare.

The review of past work found limited water consumption data and use of water as an LCA metric in assessing hydrogen production systems. Given the reliance of hydrogen production on ultrapure, deionized water and global freshwater scarcity, this is a significant gap that has begun to gain emphasis [22, 23, 24, 25]. Given a likely reliance on renewable energy use, geographic

plant dependence must go hand in hand with water consumption data, as it is a determining factor in which hydrogen technologies can be implemented, and more importantly, where they may best be located.

Thus, we perform detailed LCA studies of eleven pathways, fossil and non-fossil, by creating models based on literature sources and publicly available data. Impact results are summarized for GWP and water consumption. The LCA models created are inclusive of treatment processes needed to achieve desired process water quality, use expected technology paths, and build on a published framework that analyzed a smaller set of pathways for GHG and cost impacts [11].

Data and Methodology

The goal of this study is to model eleven hydrogen production pathways, both commercially ready and advanced technologies, and understand their environmental impact from a life cycle perspective in terms of GWP, water consumption, and other impacts. Given rising water scarcity in the U.S. and globally, water consumption is an important impact assessment metric that is often overlooked. The audience of this study is presumed to be decision makers in the energy domain interested in the viability of hydrogen production from an environmental perspective.

Further, we aim to understand the importance of water treatment (to meet the water purity standards as an input for each production technology) in life cycle results for GWP and water consumption. The inclusion of water treatment to meet purity standards before input into a process has been neglected in the system boundaries of previous studies on hydrogen production. This ignores the impact of producing ultrapure water as a feedstock in electrolysis pathways, as well as treated water needed in other pathways, leading to a gap in effects from modelled water consumption. Given the potential role of hydrogen in the global energy transition towards low-carbon solutions, treatment steps of water for hydrogen production must be considered moving forward.

This study was conducted in accordance with ISO 14040 and ISO 14044 [6, 7]. The scope of this LCA includes eleven distinct hydrogen production pathways. The pathways are SMR without CCS, SMR with CCS, ATR with CCS, coal gasification without CCS, coal gasification with CCS, coal and biomass co-gasification with CCS, biomass gasification without CCS, biomass gasification with CCS, methane pyrolysis, PEM electrolysis, and solid oxide electrolysis.

The functional unit is 1 kg of hydrogen, >99.90 vol-%, 925 psig. The study is considered cradle-to-gate, as the system boundary includes the upstream supply chain of necessary energy inputs (natural gas, coal, grid electricity, diesel, biomass), upstream material requirements, and the water treatment train, as well as the downstream sequestration of captured carbon in a saline aquifer, where applicable. The full generalized system boundary is shown in Figure 1, and a closer look at the water treatment train is provided in Figure 2. Technology-specific system boundary diagrams are included in the Appendix. The boundary does not include construction of the hydrogen production facility as this impact was deemed negligible over the expected lifetime of the plant, in line with various other past studies of large-scale energy production facilities [26, 27]. A potential exception to this statement is construction of an electrolysis facility that produces hydrogen with renewable electricity. However, a 2004 NREL report suggests that electrolyzer construction contributes less than 5% to total life cycle GWP [14]. With advances in electrolyzer efficiency and materials since then, the contribution of electrolyzer construction may

be even lower. Given this, this paper excludes facility construction for renewable electrolysis cases to maintain a consistent system boundary.

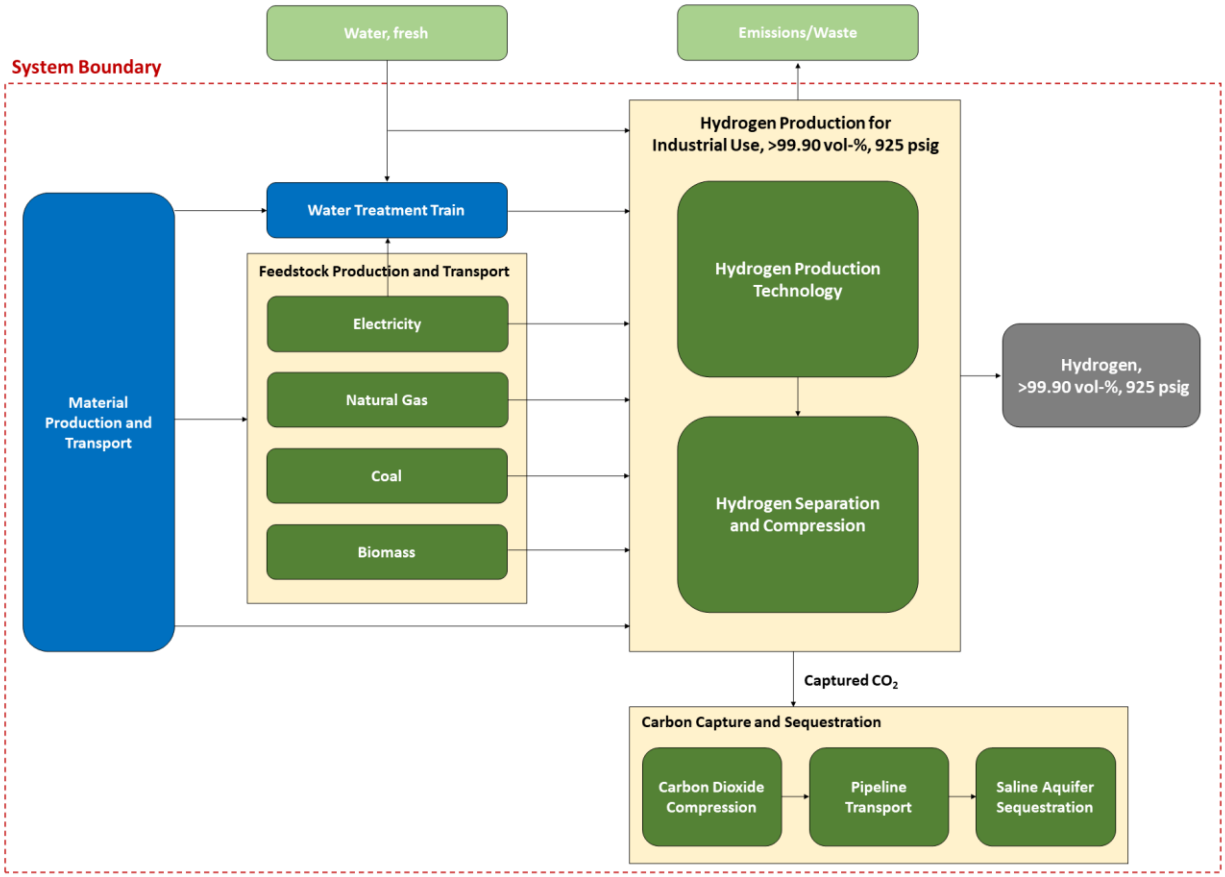

Figure 1. Generalized system boundary diagram for hydrogen production technologies

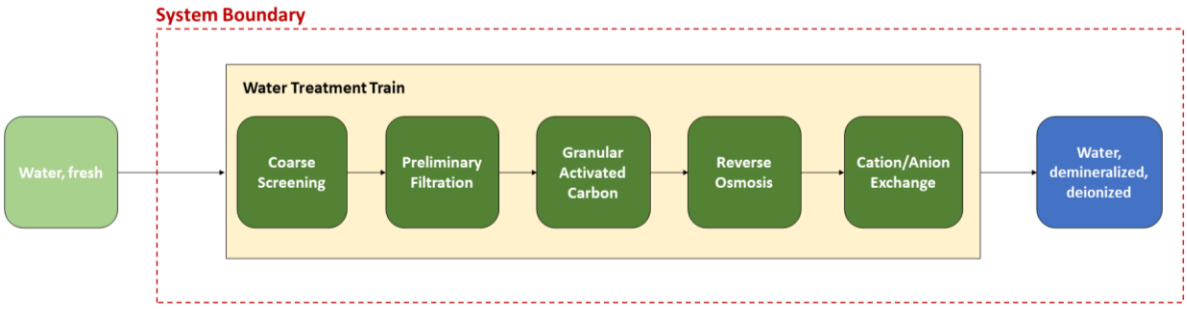

Figure 2. Diagram of water treatment train

For coal and biomass co-gasification with CCS, excess electricity is generated and sold back to the electricity grid. To consider this co-product, the system is expanded, and the co-product is displaced with U.S. average electricity. A similar system expansion and displacement method was used for traditional SMR, which generates excess steam. No other hydrogen production technologies in this study generate a coproduct.

The hydrogen production technologies were modeled Using openLCA version 1.11 with various assumptions and publicly available data, including:

- Upstream electricity generation was modeled with 2016 data from the U.S. Electricity Life Cycle Inventory (eLCI) [28]. Electricity was modeled using the consumption mix at-user. Renewable electricity profiles for 100% solar and 100% wind were also calculated from this dataset using a weighted average of U.S. production regions.
- Upstream natural gas production was modeled with 2017 data from past NETL natural gas baseline reports [29, 30]. The system boundary includes natural gas extraction through transmission, and the hydrogen production facility is modeled as a large-scale end user. The low case is represented by Alaska Offshore gas, and the high case is represented by San Juan Conventional gas.
- Upstream coal production leveraging modeling and default assumptions from the 2018 NETL Supercritical Pulverized Coal (SCPC) Power Plant study [26]. The Illinois #6 coal required in the coal gasification process is represented by the Illinois underground bituminous coal in the SCPC report. Coal mine methane emissions were assumed to be 0.0086 kg CH_4/kg coal processed at mine. Coal transport from mine to gasification facility assumes U.S. average distances of 3.8 miles by truck, 35.1 miles by barge, 42.1 miles by lake/ocean vessel, and 577 miles by train.
- Upstream production of Southern Yellow Pine (SYP) aligns with modeling in a 2013 NETL study with the Connecticut Center for Advanced Technology (CCAT) [31]. Modeling of hybrid poplar biomass agrees with the 2021 Bio-Energy with Carbon Capture and Storage (BECCS) Baseline [32]. The biomass loss rate during harvesting was assumed to be 5%, where the lost biomass decomposes on the forest floor. The transport distance to the gasification facility was assumed to be 34 miles. Nitrogen and phosphorous fertilizer profiles follow National Renewable Energy Laboratory (NREL) USLCI data [33, 34], and the potash fertilizer profile was sourced from a 2018 Chen et al. article [35].
- The water treatment train uses data from U.S. Environmental Protection Agency (EPA) Drinking Water Treatment Technology Unit Cost Models for granular activated carbon, reverse osmosis, and cation/anion exchange treatment processes [36]. This source provides information on unit costs, required materials, and energy demands for the various steps in the train. Pretreatment steps of coarse screening and preliminary filtration were included before the granular activated carbon process to remove larger suspended solids that would reduce the lifetime of the filter, but these first two treatment steps were modeled as 1:1 water input/output without any loss in water volume. In reality, these two steps would have slight water loss and material inputs, but these elements were not modeled due to a lack of specific process data. For the remaining treatment steps, these elements were modeled according to EPA data, and the full treatment train resulted in a 1 kg demineralized, deionized water output from a 1.24 kg freshwater input. This is largely driven by the reject stream from reverse osmosis being sent to an evaporation pond. Based on the water purity requirements of reforming in literature [37], thermochemical hydrogen production pathways are assumed to require feed water of ASTM and ISO Type II purity [38, 39]. Because water purity requirements may vary based on the catalyst used in the process, this Type II conclusion is a conservative assumption. Type II is the minimum water purity required for electrolysis pathways, but Type I is recommended for

optimal performance [40, 41]. A second pass through reverse osmosis before water is fed into the electrolysis system is used as a high-bound to represent a liberal estimate of additional energy requirements and water loss that may arise from an ultrafiltration step.

- Sequestration of captured carbon dioxide in a saline aquifer follows the modeling and assumptions outlined in a 2013 NETL Gate-to-Grave study [42]. A pipeline transportation distance of 100 mi with no change in elevation is assumed.
- Process data for SMR, SMR with CCS, ATR with CCS, CG, CG with CCS, and coal and biomass co-gasification with CCS follows modeling in the 2022 NETL Hydrogen Baseline report [11]. Process data for biomass gasification is found in a 2005 NREL report, with the CCS case assuming a 90% carbon capture rate using data from a 2022 NETL report [43, 44]. Process data for methane pyrolysis is sourced from a 2021 Riley et al. article [45]. PEM and SOEC process data is sourced from a 2018 Bareiß et al. paper and 2019 Daneshpour and Mehrpooya article, respectively [46, 47]. A summary of key process data used in this study is included in Table 1.

Table 1. Summary of process inputs for hydrogen production technologies (per kg H_2) [11, 43, 44, 45, 46, 47]
SMR (steam methane reforming); ATR (autothermal reforming); CG (coal gasification); BG/CG (biomass and coal co-gasification); BG (biomass gasification); MP (methane pyrolysis); PEM (proton exchange membrane); SOEC (solid oxide electrolysis cell); CCS (carbon capture and storage); NG (natural gas); SYP (southern yellow pine)

Type	Thermochemical									Electrolysis	
	Reforming			Gasification					Pyrolysis		
Conversion Pathway	SMR	SMR w/ CCS	ATR w/ CCS	CG	CG w/ CCS	BG/CG w/ CCS	BG	BG w/ CCS	MP	PEM	SOEC
Feedstock	NG	NG	NG	Coal	Coal	Coal, SYP	Hybrid Poplar	Hybrid Poplar	Methane	Electricity	Electricity
Natural gas (kg)	3.53	3.75	3.53	-	-	-	0.262	0.265	4.50	-	1.08
Coal (kg)	-	-	-	7.71	7.71	5.41	-	-	-	-	-
Biomass (kg)	-	-	-	-	-	4.16	25.8	25.8	-	-	-
Electricity (kWh)	0.629	2.03	4.07	0.909	1.42	-	0.901	3.01	1.39	55.0	42.9
Process Water (kg)	13.3	1.56	3.55	1.92	1.94	2.63	6.49	6.49	-	8.94	8.96
Cooling Water (kg)	3.16	29.0	38.3	24.3	27.8	39.3	7.83	14.1	1.48	3.20	2.50
Air (kg)	25.5	29.5	25.5	41.8	36.9	50.9	51.2	51.2	9.30	-	-
Catalyst (kg)	-	-	-	-	-	-	-	-	0.0846	-	-

Table 1 distinguishes between process water and cooling water for each hydrogen production technology. In this context, process water refers to the input required to be treated to the ASTM and ISO Type II purity standard [38, 39]. For reforming and gasification technologies, this includes the steam required for the thermochemical reaction. For electrolysis technologies, this includes feedstock water that is electrolyzed to separate out hydrogen and oxygen. Cooling water refers to the water recirculating through the process's cooling system, which runs through the water-gas shift reactor and heat recovery systems, to name a few examples. For cases with CCS, the small volume of water required for the MDEA scrubbers is also included in the category of cooling water as a specific purity standard is not required.

In this analysis, the life cycle impact assessment (LCIA) methodology used for the GWP modeling is the Intergovernmental Panel on Climate Change (IPCC) Sixth Assessment Report (AR6) method GWP values with a 100-year time horizon [48]. Water consumption was

calculated as a difference between water withdrawal and water discharge. Only blue water (sourced from surface or ground) was considered; thus, rainwater consumed during biomass cultivation was excluded.

The life cycle inventory (LCI) produced for each technology incorporates data from a variety of sources and consequently, from a variety of temporal periods, geographic locations, and technology readiness levels. A data quality index (DQI) is thus assigned to each technology, documented in Table S-9.

Results

The results of the modeling are separated into consistently defined life cycle stages for each of eleven pathways. Process emissions refer to those occurring directly, or on site, at the hydrogen production facility. The water treatment train represents the upstream processes needed to supply water at the needed purity. Normalized on a per kilogram of H_2 basis, GWP results are shown in Figure 3. Error bars represent the high and low ranges of estimates within the model, arising from a Monte Carlo simulation. This uncertainty is sourced from varying regional parameters in upstream electricity, natural gas, coal, and biomass models.

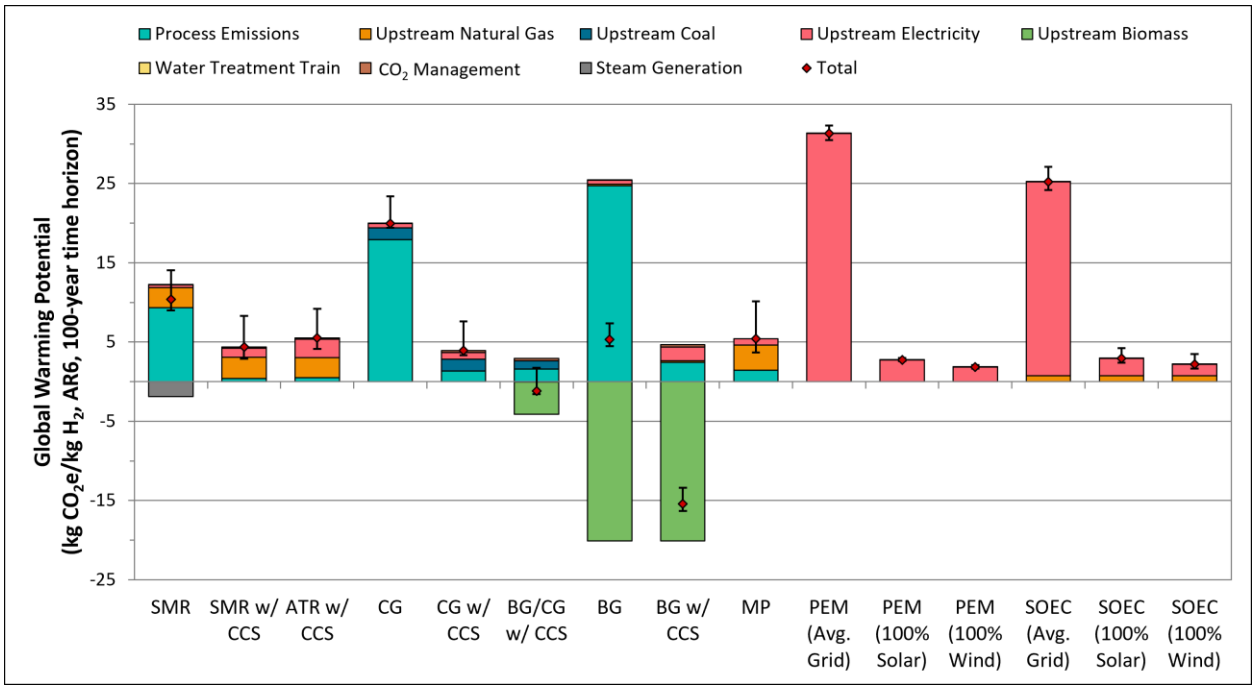

Figure 3. Life cycle global warming potential results for eleven hydrogen production pathways
SMR (steam methane reforming); ATR (autothermal reforming); CG (coal gasification); BG/CG (biomass and coal co-gasification); BG (biomass gasification); MP (methane pyrolysis); PEM (proton exchange membrane); SOEC (solid oxide electrolysis cell); CCS (carbon capture and storage)

Figure 3 shows that for fossil-based technologies, life cycle emissions range from 3.9 kg CO_2e/kg H_2 for coal gasification with CCS to 20 kg CO_2e/kg H_2 for coal gasification without CCS. For the biomass-based pathways, the GWP values range from -15 kg CO_2e/kg H_2 for biomass gasification with CCS to 5.3 kg CO_2e/kg H_2 for biomass gasification without CCS. The biomass pathways benefit from carbon 'credits' associated with biogenic storage of CO_2 from the atmosphere during growth, leading to net emissions that are negative to slightly positive.

Given the high electricity demand of electrolysis and the highly variable GWP impacts of electricity sources, three scenarios are modeled for each electrolysis pathway. For electrolysis using U.S. average grid electricity, GWP results are 31 kg CO_2e/kg H_2 for PEM and 25 kg CO_2e/kg H_2 for SOEC, the highest across all pathways. However, when using renewable electricity-based pathways, GWP ranges from 2-3 kg CO_2e/kg H_2 for PEM and SOEC, which are 90% lower than the grid average scenarios and lower than all non-biomass pathways.

For non-biomass pathways in general, the greater the energy needs for the given process, the larger the associated GWP values for the process itself. Considering the electrolysis pathways, SOEC and PEM rely heavily on the decarbonization of grid electricity to achieve lower GWP. For traditional fossil-based pathways, process emissions account for most emissions. Technologies operating using CCS systems to remove stack emissions achieve a lower GWP value, but at the cost of increased energy and water consumption. As a result, any further reduction in GWP values for fossil-based pathways would rely heavily on parallel reduction of upstream emissions.

Figure 4, Figure 5, and Figure 6 summarize the results of the life cycle water use modeling for fossil-based, biomass-based, and electrolysis pathways, respectively. All technologies have process water treated to Type II purity. The error bars are largest for the coal and biomass scenarios, as the upstream data contains a wide range of water consumption values highly dependent on region. This regional variability in water consumption is not seen for upstream electricity and natural gas.

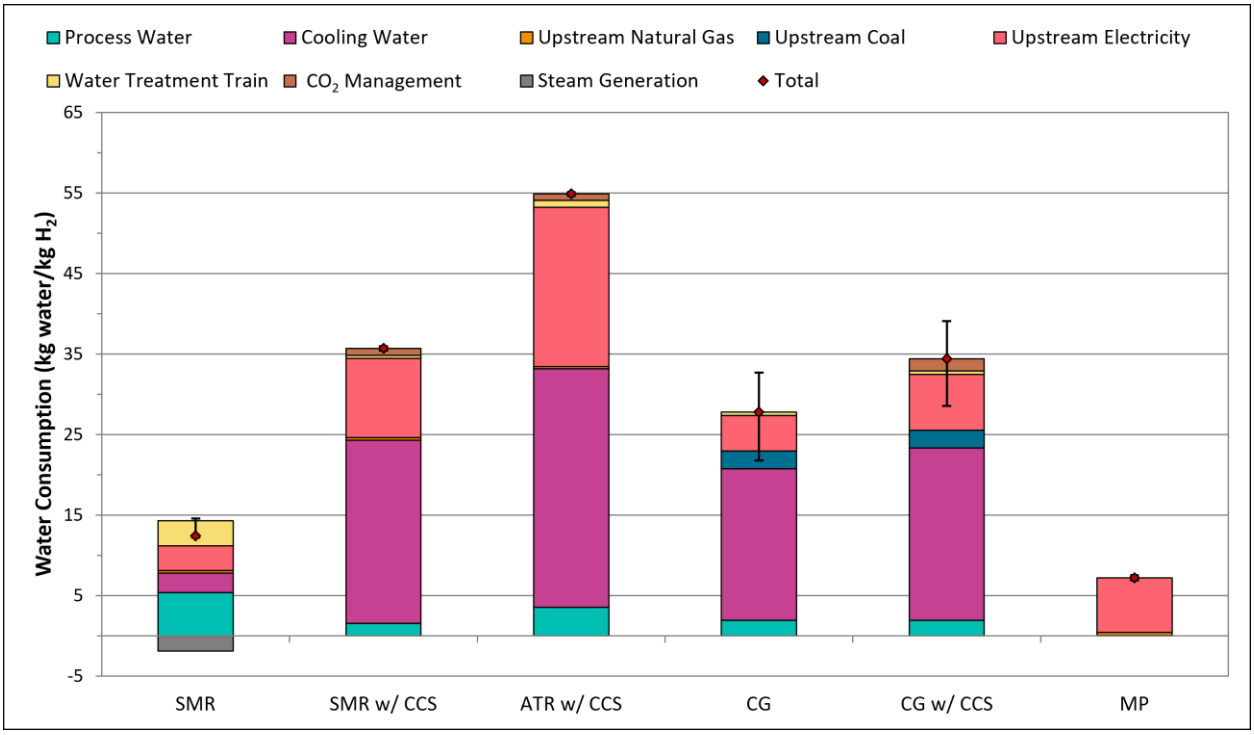

Figure 4. Life cycle water consumption results for fossil-based hydrogen production pathways
SMR (steam methane reforming); ATR (autothermal reforming); CG (coal gasification); MP (methane pyrolysis); CCS (carbon capture and storage)

All fossil pathways without a biomass co-feed result in water consumption less than 55 kg water/kg H_2. Methane pyrolysis is the lowest at only 7.2 kg water/kg H_2. Although cooling water circulates in a closed-loop system, a makeup water stream is required to offset drift losses,

blowdown losses, and evaporative losses from the cooling tower. This makeup water stream corresponds to cooling water consumption in these pathways. Water treatment train consumption is directly linked to process water input, leading to interesting water consumption results. The lower process water requirement in SMR with CCS stems from the additional water recovered from the flue gas via the post-combustion capture system, which offsets process water and water treatment requirements. Conversely, SMR with CCS has almost an order of magnitude higher cooling water consumption than SMR without CCS due to the significant additional cooling duty required for CCS, which includes two CO_2 capture systems.

Differences in process water and cooling water are apparent between SMR without CCS and SMR with CCS. The lower process water requirement in SMR with CCS is due to the additional water recovered from the flue gas via the post-combustion CO_2 capture system, a system that is not present in a process without CCS, which offsets the total process water needed. The additional water recovered consequently reduces the water treatment train impact for SMR with CCS as well. Conversely, the SMR with CCS process sees a much higher cooling water consumption than SMR without CCS. This is due to the significant cooling duty required for both the pre- and post-combustion CO_2 capture systems (75% of the total cooling load) as well as other cooling duties associated with CO_2 purification and compression [11].

The cooling water consumption difference due to CCS notably varies between gasification and reforming cases. This is driven by the need for sulfur removal in the coal and biomass gasification scenarios [11]. Gasification cases without CCS include a MDEA-based acid gas removal (AGR) system, while gasification cases with CCS use a dual-stage Selexol AGR system that captures both sulfur and pre-combustion CO_2. For SMR without CCS, however, no AGR system is required. This is in contrast to SMR with CCS, which includes two AGR systems: a MDEA-based system for pre-combustion capture and a CANSOLV system for post-combustion capture, adding significant cooling demands. When comparing cooling water consumption between without CCS and with CCS scenarios, the gasification cases see a lower relative increase as an AGR system is included in both with and without CCS cases. On the other hand, the transition from zero AGR systems in SMR without CCS to two AGR systems in SMR with CCS results in a more drastic increase from without CCS to with CCS.

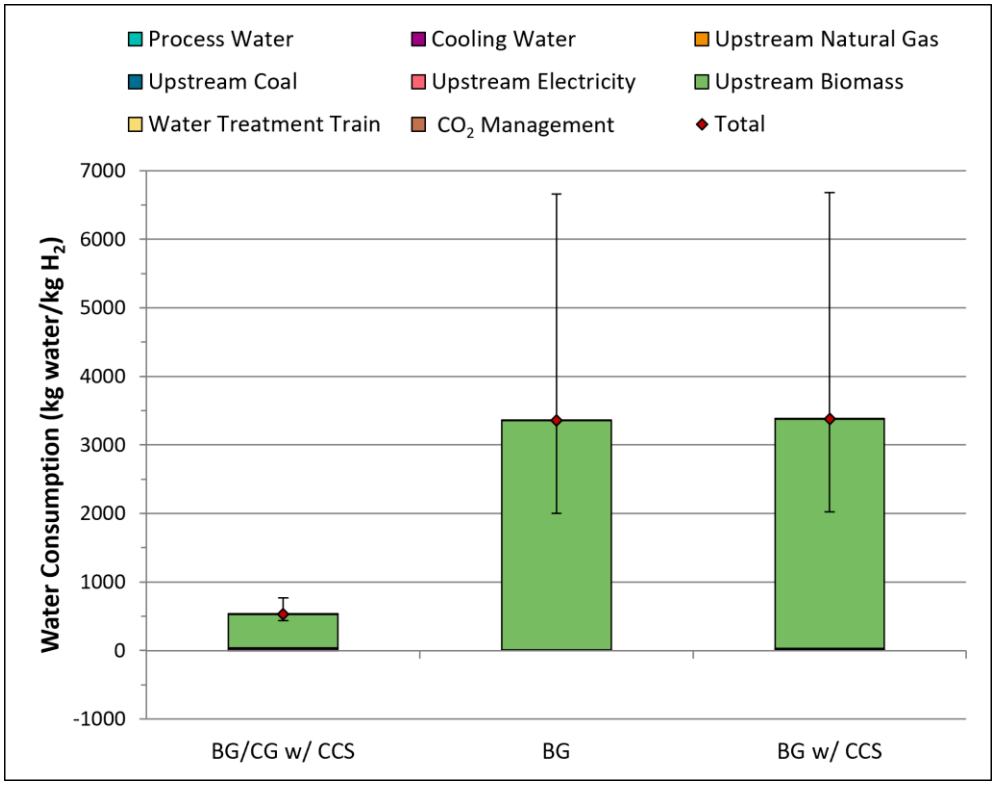

Figure 5. Life cycle water consumption results for biomass-based hydrogen production pathways
BG (biomass gasification); BG/CG (biomass and coal co-gasification); CCS (carbon capture and storage)

For the biomass-based pathways shown in Figure 5, biomass gasification with CCS consumed the most water at 3,380 kg water/kg H_2. Biomass and coal co-gasification yielded the lowest water consumption with 532 kg water/kg H_2 consumed. Water consumption for the biomass-based pathways is dominated by water demand of biomass cultivation. Regional differences in average yield and a fixed irrigation requirement per unit area cause the water consumption during cultivation to vary widely, thus accounting for the significant uncertainty displayed in Figure 5. Note that these results exclude naturally occurring rainfall. Including rainwater would further increase water consumption in the biomass pathways.

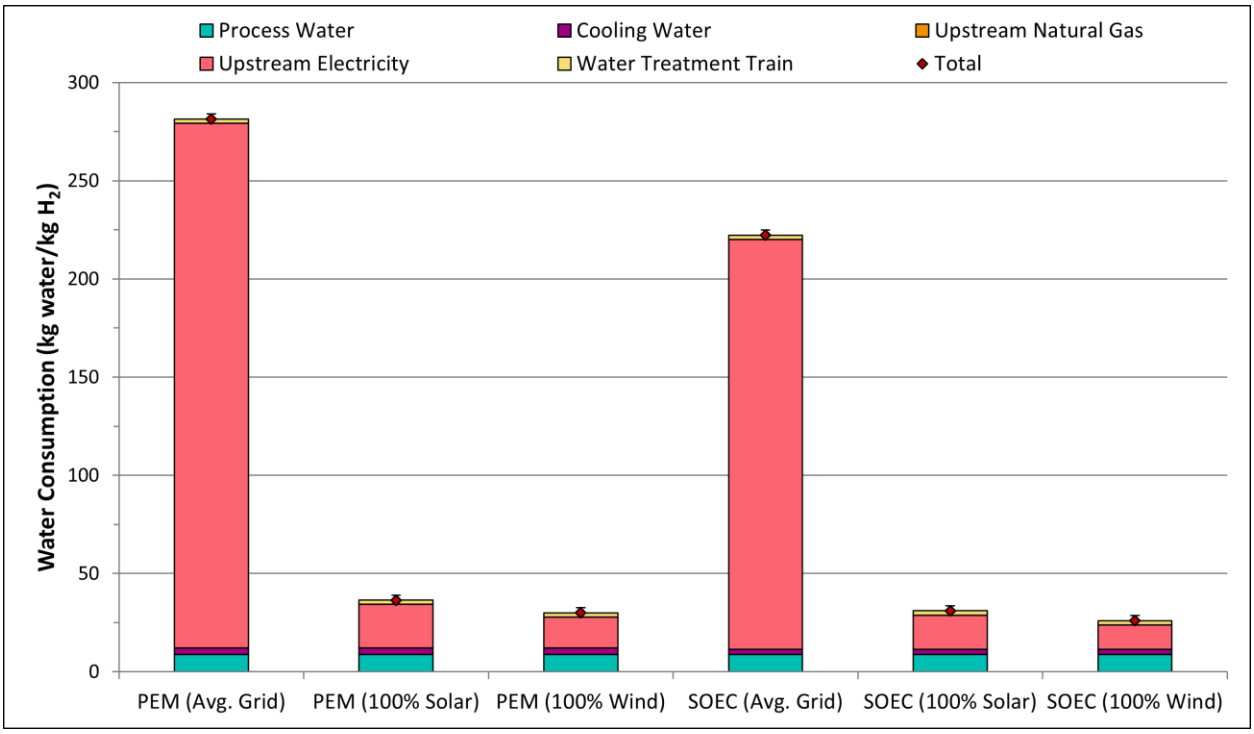

Figure 6. Life cycle water consumption for electrolysis pathways including renewable electricity scenarios
PEM (proton exchange membrane); SOEC (solid oxide electrolysis cell)

For electrolysis pathways shown in Figure 6, scenarios using U.S. average grid electricity result in a water consumption of 280 kg water/kg H_2 for PEM and 220 kg water/kg H_2 for SOEC. The use of renewable electricity, however, greatly decreases water consumption, approximately a 87% reduction for the 100% solar case and 89% reduction for the 100% wind case.

Overall, including the impact of the water treatment train increases the water consumption for each pathway by only 1% on average, but is much larger (10%) for SMR without CCS. For the electrolysis-based pathways, this value is proportionately higher than the thermochemical pathways since water is considered the primary feedstock for hydrogen production. The water treatment train's water consumption value will proportionately contribute a greater percentage to overall consumption when renewable electricity is used, more accurately depicting its impact on overall consumption.

Total water consumption is more impacted by cooling water than process water for traditional gasification and reforming pathways, whereas the opposite is true for electrochemical pathways. For biomass-based cases, upstream biomass cultivation is by far the largest contributor to total water consumption. In cases where process water contributes significantly to total water consumption, the upstream water treatment train is also a notable contributor. This is most apparent in traditional SMR and the electrochemical pathways fueled by renewable electricity.

To aid decision making, GWP and water consumption results can be plotted against each other to visualize tradeoffs, as shown in Figure 7. The water consumption y-axis is expressed on a logarithmic scale. Electrolysis technologies powered by wind electricity minimize joint GWP and water consumption results, followed closely by electrolysis powered by solar electricity. Fossil-based hydrogen production using CCS performs much better than their non-CCS counterparts from a GWP perspective, but with a slightly higher water consumption.

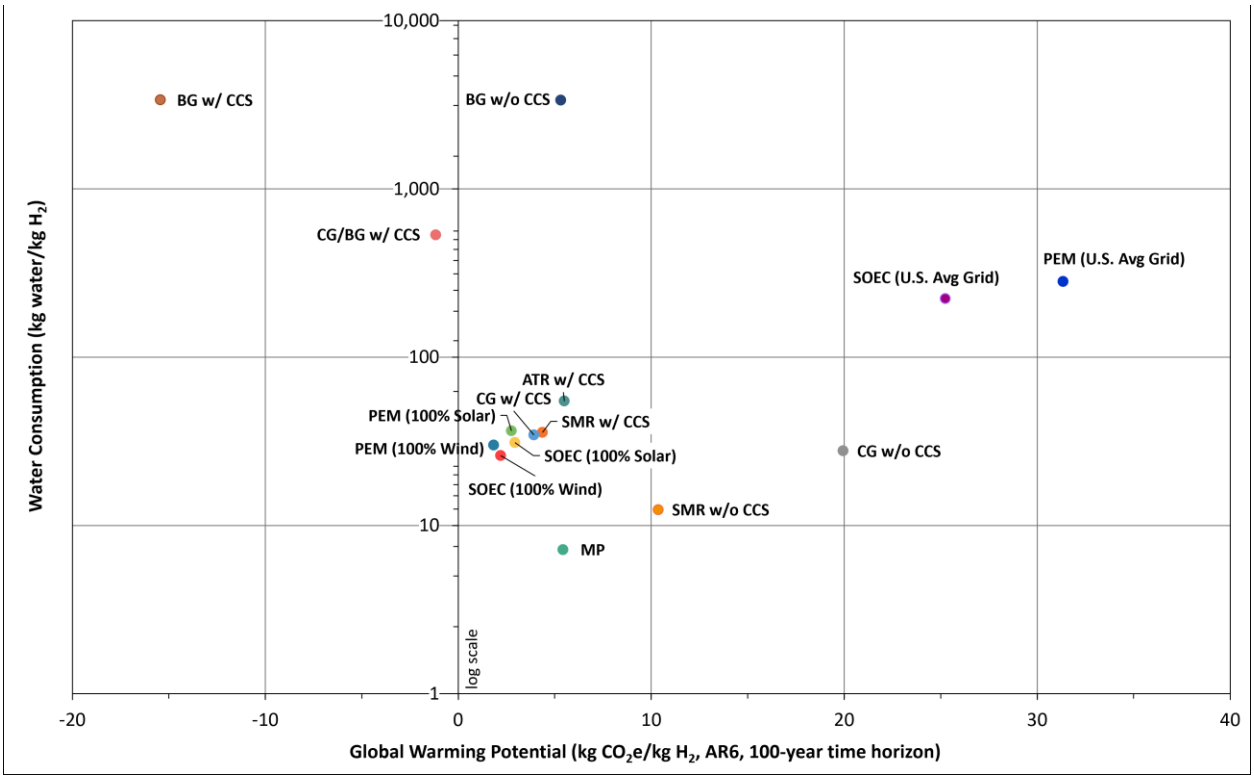

Figure 7. Tradeoff analysis of water consumption versus GWP results for hydrogen production technologies
SMR (steam methane reforming); ATR (autothermal reforming); CG (coal gasification); BG/CG (biomass and coal co-gasification); BG (biomass gasification); MP (methane pyrolysis); PEM (proton exchange membrane); SOEC (solid oxide electrolysis cell); CCS (carbon capture and storage)

The results from biomass production pathways highlight a key tradeoff between decarbonization goals and water scarcity concerns. The findings indicate that biomass pathways have in general the lowest GWP values; however, these technologies have the highest water consumption of the technologies examined, one to three orders of magnitude higher than the non-biomass pathways.

Though less technologically ready, methane pyrolysis is competitive with many of the low-GWP pathways and is estimated to have the lowest water consumption among fossil-based production methods. Electrolysis appears as a pathway of promise for both low carbon and low water production, but only when sourced from renewable electricity, which is the main determinant of its impact. As a result, life cycle environmental performance of electrolysis is highly sensitive to changes in the electricity grid.

Discussion

Overall, the results of this study compare favorably to GWP results in previous literature. Gate-to-gate GWP results for the subset of common pathways agree with the 2011 NETL baseline [8]. Life-cycle GWP results for common pathways also align with the recent 2022 NETL baseline [11]. This paper reports a GWP for SMR of 10.4 kg CO_2e/kg H_2, a result that is similar to the 10.6 kg CO_2e/kg H_2 reported by Susmozas et al. [49] but slightly lower than the 11.4 kg CO_2e/kg H_2 reported by Valente et al., 11.9 kg CO_2e/kg H_2 reported by Çetinkaya et al., and 11.8 kg CO_2e/kg H_2 reported by Spath and Mann [21, 13, 15]. This can be explained by this paper's displacement of a steam co-product; without this displacement, the GWP result would equal 12.4 kg CO_2e/kg H_2 [11]. Comparison of results for biomass-based pathways show more variability.

This paper reports a GWP of 5.3 kg CO_2e/kg H_2 for biomass gasification, while Mehmeti et al. reports 2.7 kg CO_2e/kg H_2, Kalinci et al. reports 8.5 kg CO_2e/kg H_2, Susmozas et al. reports 0.41 kg CO_2e/kg H_2, and Acar and Dincer report 8.2 kg CO_2e/kg H_2 [20, 50, 49, 51]. This is unsurprising, as GWP results for biomass gasification are highly sensitive to the carbon content of the biomass feedstock and gasification efficiency.

Electrolysis results generally show closer agreement. For wind-based electrolysis, this paper reports a GWP of 1.8 kg CO_2e/kg H_2 for PEM and 2.2 kg CO_2e/kg H_2 for SOEC, which agrees with a range of 0.68 to 2.2 kg CO_2e/kg H_2 defined by literature [52, 13, 21, 16, 20, 14]. Similarly, for solar-based electrolysis, this paper's results of 2.8 kg CO_2e/kg H_2 for PEM and 2.9 kg CO_2e/kg H_2 for SOEC are similar to the GWP of 2 kg CO_2e/kg H_2 reported by Ozbilen et al., 2.4 kg CO_2e/kg H_2 reported by Cetinkaya et al, and 3.1 kg CO_2e/kg H_2 reported by Olabi et al., though lower than the 5.0 kg CO_2e/kg H_2 reported by Palmer et al. and higher than the 0.94 kg CO_2e/kg H_2 reported by Sadeghi and Ghandehariun [16, 13, 52, 17, 53]. In terms of water consumption, a comparison with results reported by Mehmeti et al. would first require harmonization to reconcile impact assessment differences.

Electrolysis pathways are highly sensitive to the electricity source and result in a low GWP only when paired with renewable energy. The use of renewable electricity does not have the same impact on fossil-based pathways as electricity is not the primary feedstock. **Error! Reference source not found.** and **Error! Reference source not found.** show GWP results for all hydrogen production technologies using 100% solar and 100% wind electricity, respectively. This applies to all cases except biomass and coal co-gasification with CCS, as electricity is generated internally with a steam turbine. Excess electricity generated is sold back to the grid, and thus the negative electricity impact is not subject to the renewable energy scenarios.

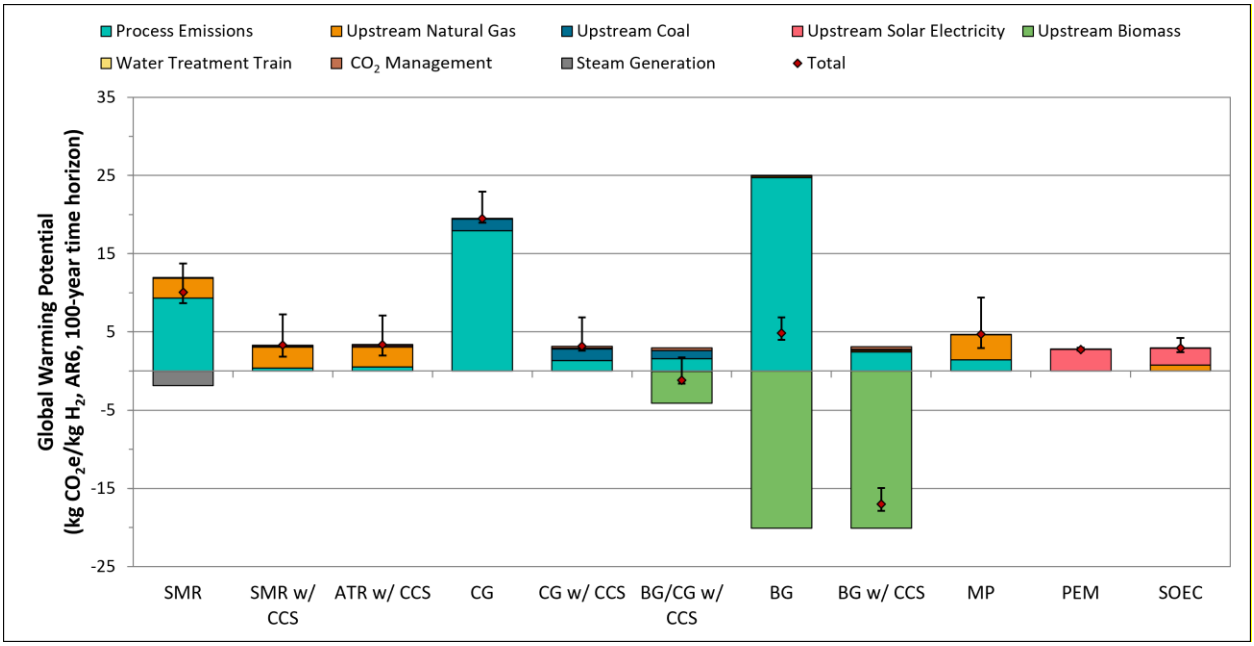

Figure 8. Life cycle global warming potential results for eleven hydrogen production pathways with solar electricity

SMR (steam methane reforming); ATR (autothermal reforming); CG (coal gasification); BG/CG (biomass and coal co-gasification); BG (biomass gasification); MP (methane pyrolysis); PEM (proton exchange membrane); SOEC (solid oxide electrolysis cell); CCS (carbon capture and storage)

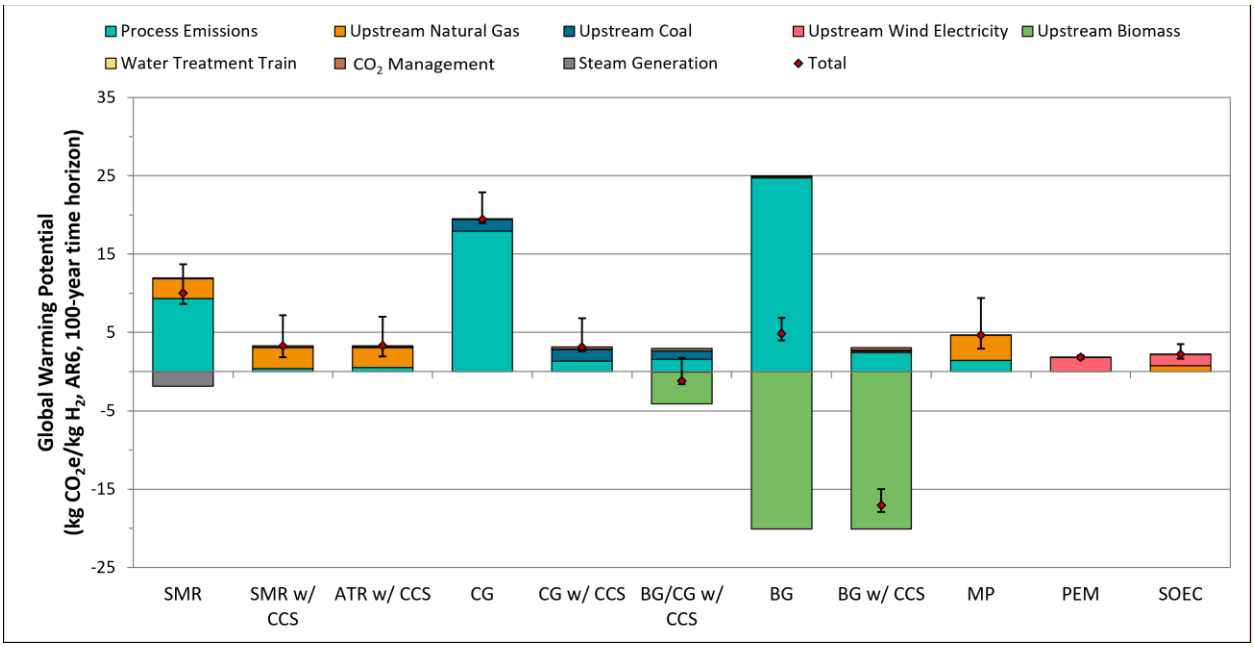

Figure 9. Life cycle global warming potential results for eleven hydrogen production pathways with wind electricity

SMR (steam methane reforming); ATR (autothermal reforming); CG (coal gasification); BG/CG (biomass and coal co-gasification); BG (biomass gasification); MP (methane pyrolysis); PEM (proton exchange membrane); SOEC (solid oxide electrolysis cell); CCS (carbon capture and storage)

When using renewable electricity, scenarios with CCS show a greater decrease in GWP than their non-CCS counterparts as compared to grid electricity results. In both renewable electricity scenarios, SMR decreased by 3%, SMR with CCS decreased by 24%, ATR with CCS decreased by 39%, CG decreased by 2%, CG with CCS decreased by 10%, BG decreased by 9%, BG with CCS decreased by 10%, and methane pyrolysis decreased by 13%, on average.

Given the sensitivity of electrolysis scenarios to electricity source, it is valuable to understand the renewable electricity contribution required for their GWP to be lower than that of fossil-based pathways. Using EIA U.S. average grid projections through 2050, the GWP results for electrolysis can be compared against SMR and CG, as seen in **Error! Reference source not found.** [54].

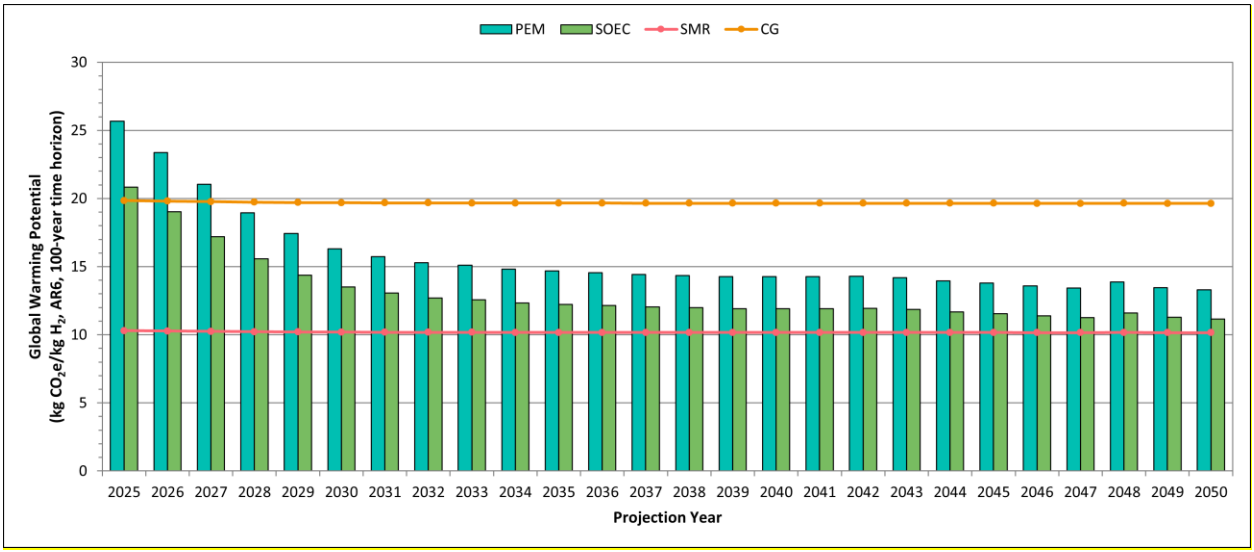

Figure 10. Life cycle global warming potential results for hydrogen production scenarios with U.S. average grid electricity projected through 2050

SMR (steam methane reforming); CG (coal gasification); (proton exchange membrane); SOEC (solid oxide electrolysis cell)

SOEC reaches a lower GWP than CG in 2026, with a breakeven renewable electricity contribution of 33%. PEM reaches a lower GWP than CG in 2028, with a breakeven renewable electricity contribution of 42%. Through 2050, however, neither PEM nor SOEC with average grid electricity overtakes SMR. Projecting beyond 2050, with the assumption that a linear increase in renewable electricity corresponds with a linear decrease in the average grid's GWP, SOEC reaches a lower GWP than SMR in 2065 with a breakeven renewable electricity contribution of 67%, and PEM reaches a lower GWP than SMR in 2089 with a breakeven renewable electricity contribution of 78%. While true for U.S. average grid electricity, these breakeven years vary widely by North American Electric Reliability Corporation (NERC) region. Within the Western Electricity Coordinating Council (WECC) region, for example, SOEC reaches a lower GWP than SMR in 2029, and PEM reaches a lower GWP than SMR in 2038. However, this does not account for the sale of renewable energy certificates (RECs). A residual grid mix must be calculated to accurately characterize grid electricity, but this cannot be done through projections.

Conclusion

Previous research into hydrogen production excluded consideration of upstream water treatment. Detailed modeling of water treatment to purity for use in hydrogen production was a novel aspect of this work, but was focused on the most common treatment processes, and on GWP and water consumption impacts. The water treatment train generally contributed less than 1% in terms of the GWP for a pathway. Including water purification is more important, however, when its impact on total water consumption (and potentially, the need for even higher purity levels) is considered. Contributions to total water consumption from losses in the water treatment train range from less than 1% for biomass pathways to around 10% for traditional SMR. As emerging hydrogen production technologies reach commercial readiness, a deeper look at process requirements, especially for water, will be key to accurately represent life cycle impacts.

The results from biomass production pathways highlight a key tradeoff between GWP reduction and water consumption for energy crops. The findings indicate that biomass gasification without and with CCS generate some of the lowest GWP of all other pathways, with values of 5.3 kg CO_2e/kg H_2 and -15 kg CO_2e/kg H_2, respectively. However, these technologies have the highest water consumption of the technologies examined, with 3,360 kg water/kg H_2 consumed for biomass gasification without CCS and 3,380 kg water/kg H_2 consumed for biomass gasification with CCS. For the traditional fossil-based technologies, GWP values ranged from 3.9 kg CO_2e/kg H_2 to 20 kg CO_2e/kg H_2, and water consumption values ranged from 7.2 kg water/kg H_2 to 55 kg water/kg H_2. Additionally, it should be noted that the impact of electrolysis technologies is strongly related to upstream electricity generation, as the electricity contributions to both the GWP and water consumption primarily determines the overall impact of these technologies. As a result, their life cycle environmental performance is highly sensitive to changes in the electricity grid.

Strategic facility siting will play a meaningful role in the environmental impact of large-scale hydrogen production. These results could be regionalized to better consider the needs of each technology and could incorporate specific fossil fuel, electricity, or biomass supply profiles. As such, the viability of an individual hydrogen production technology can be evaluated based on the priorities of the location, cost, GWP, water consumption, access to feedstock, and other factors. Regionalized water stress impact could be considered with methods like AWARE-US [55] or following a hydrogen-specific methodology framework [22]. Future work may also include exploring how water purity requirements are impacted by different catalysts, incorporating additional treatment processes, and expanding the scope to include influent water of other starting quality such as wastewater or saline water.

Finally, these results can support emerging efforts that exist to standardize the measurement of life cycle impacts of hydrogen deliveries around the world and to create market-based standards to help compare specific suppliers in terms of various impacts (especially GHG). These include the Open Hydrogen Initiative [56] and European CertifHy efforts [57].

While the presence of a water treatment train within the system boundary contributes little to the total life cycle water consumption for most hydrogen production technologies considered, its impact can still be seen in technologies that require large inputs of high purity water. As emerging hydrogen production technologies reach commercial readiness, a meaningful look at process requirements will be key to accurately represent life cycle impacts.

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Validation: MSH, HSM

Formal analysis: MSH

Investigation: MSH, HSM

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Writing – review & editing: MSH, HSM, EG, MJ, TJS

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Supervision: TJS, EG, MJ

Project administration: TJS, MJ

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Supplementary Text

Figure 1 provides a generalized system boundary diagram for the model, but the processes included within the boundary for each hydrogen production technology is slightly different. Figure S-1 to Figure S-11 display system boundary diagrams by technology, including a simplified block-flow diagram of the hydrogen production facility. The figures show major equipment and flows and do not represent a complete material balance.

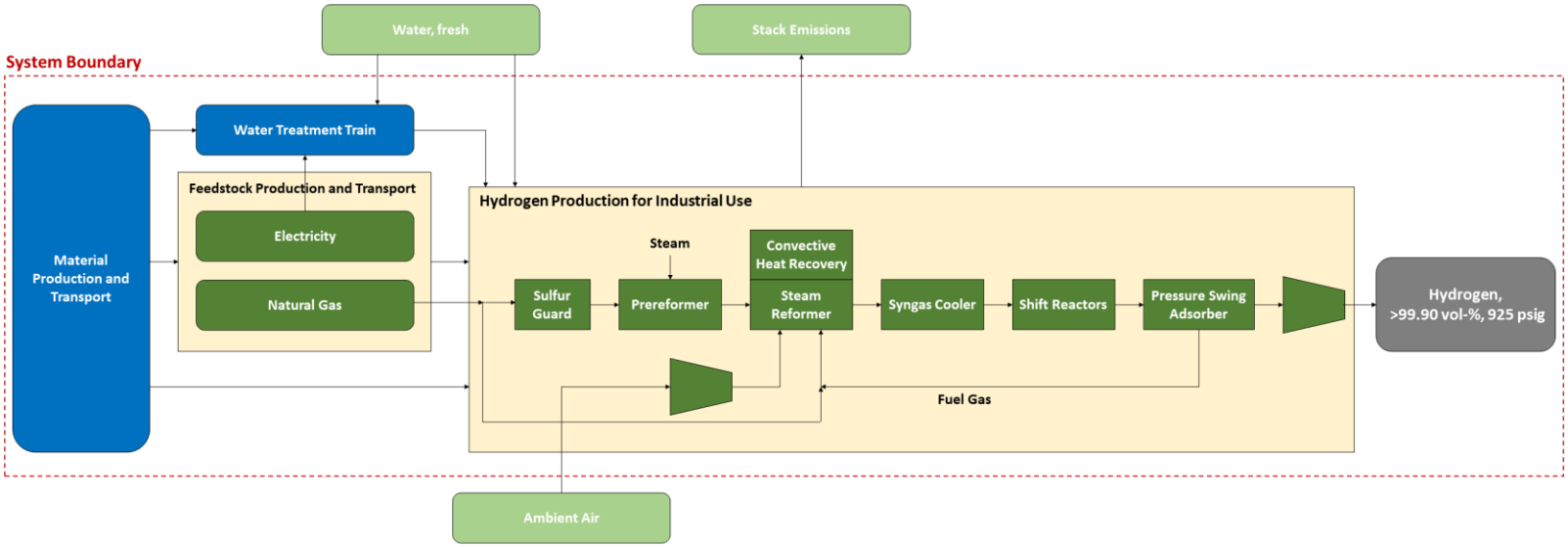

Figure S-1. System boundary diagram for steam methane reforming scenario [11]

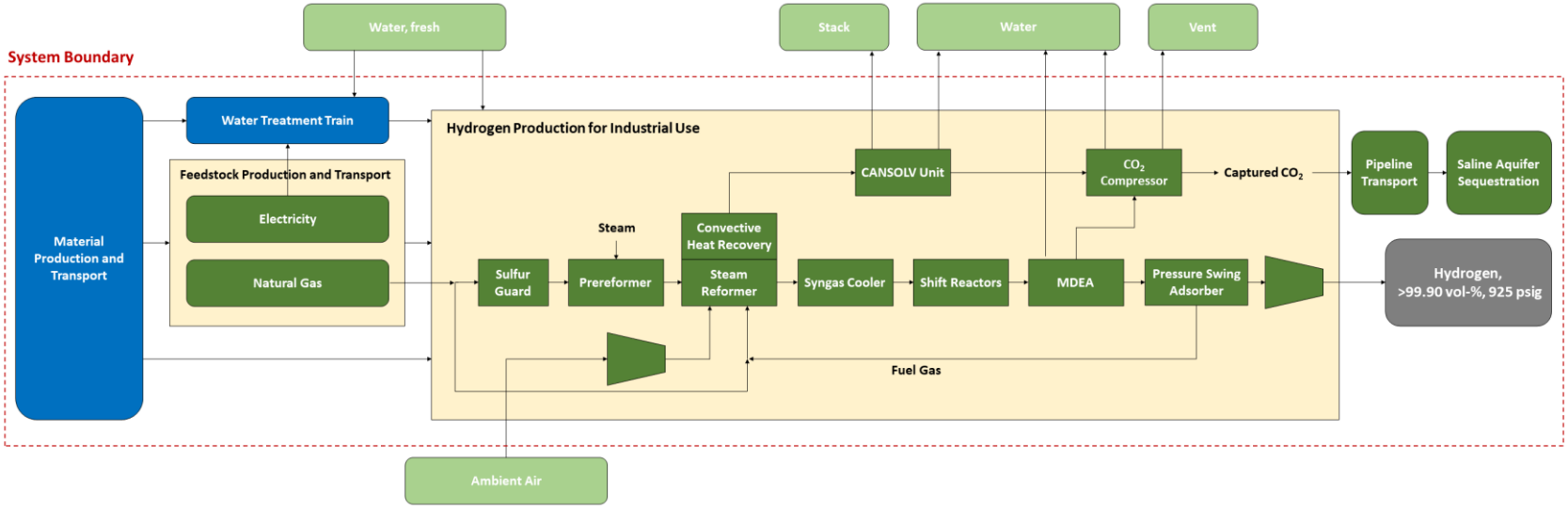

Figure S-2. System boundary diagram for steam methane reforming with CCS scenario [11]

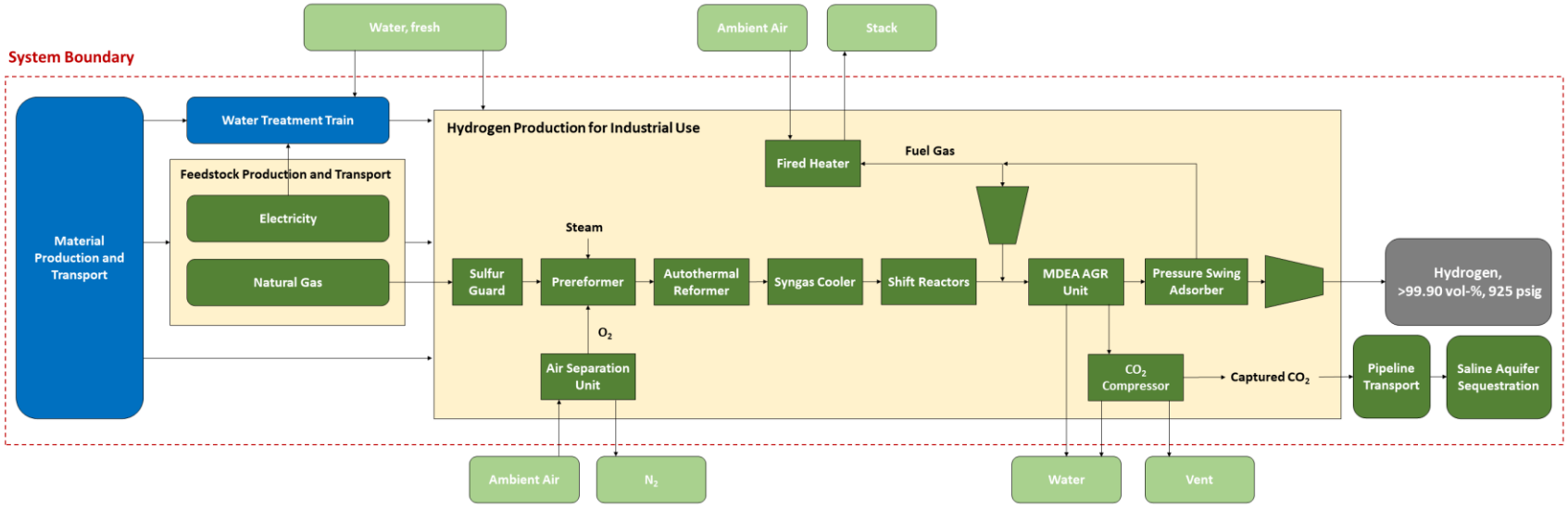

Figure S-3. System boundary diagram for autothermal reforming with CCS scenario [11]

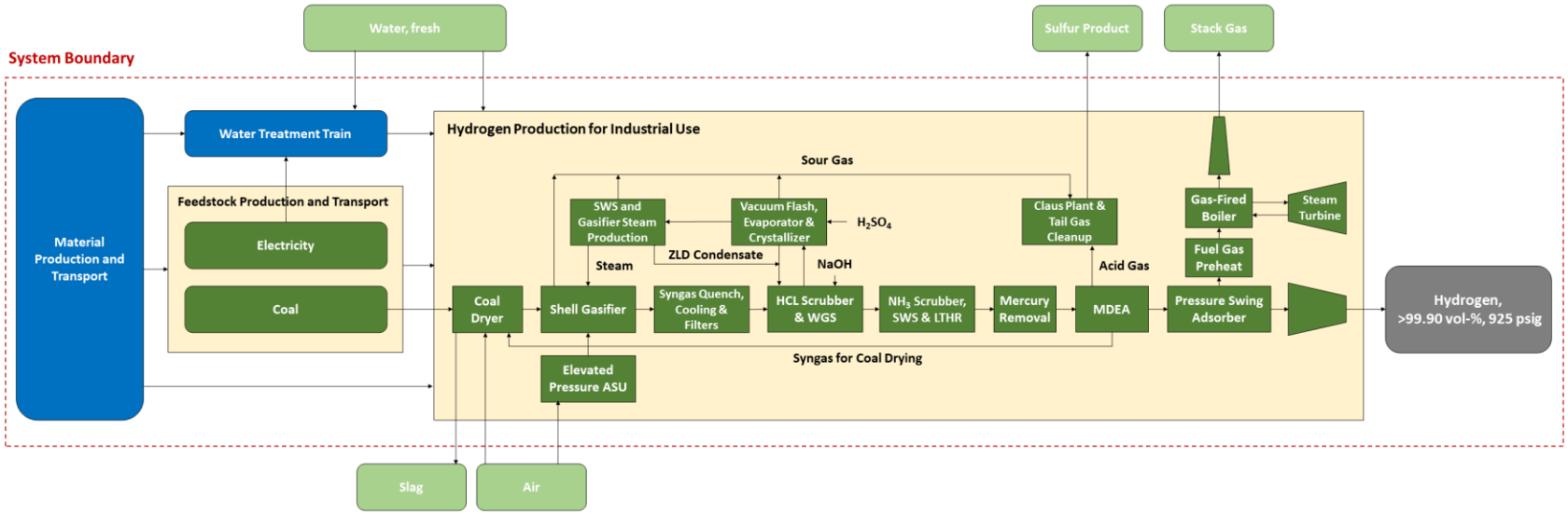

Figure S-4. System boundary diagram for coal gasification scenario [11]

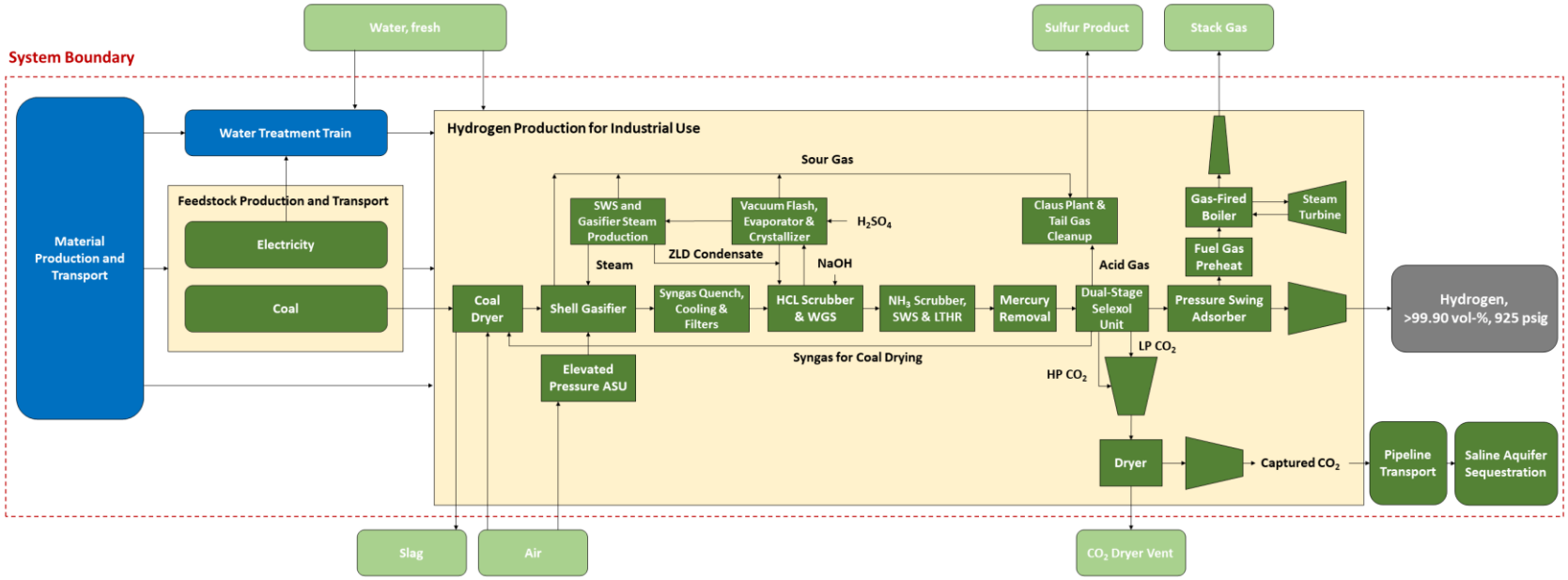

Figure S-5. System boundary diagram for coal gasification with CCS scenario [11]

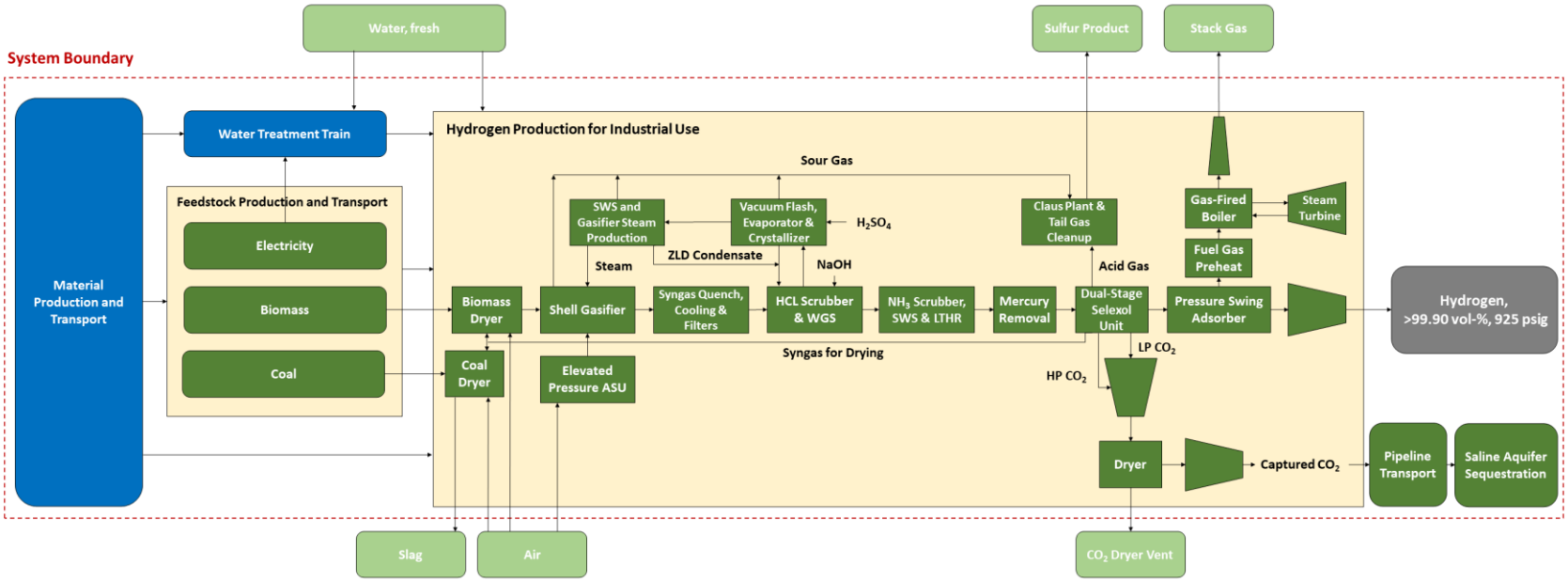

Figure S-6. System boundary diagram for biomass and coal co-gasification with CCS scenario [11]

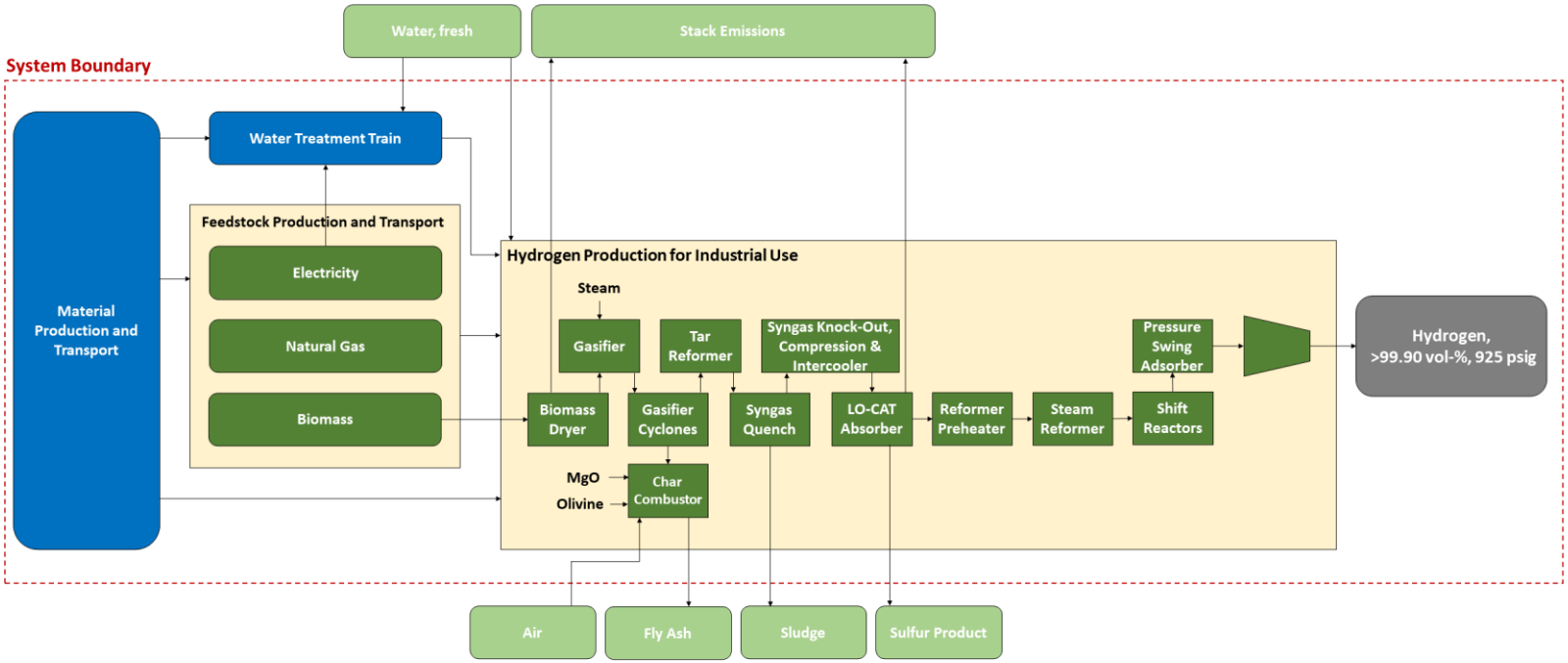

Figure S-7. System boundary diagram for biomass gasification scenario [43]

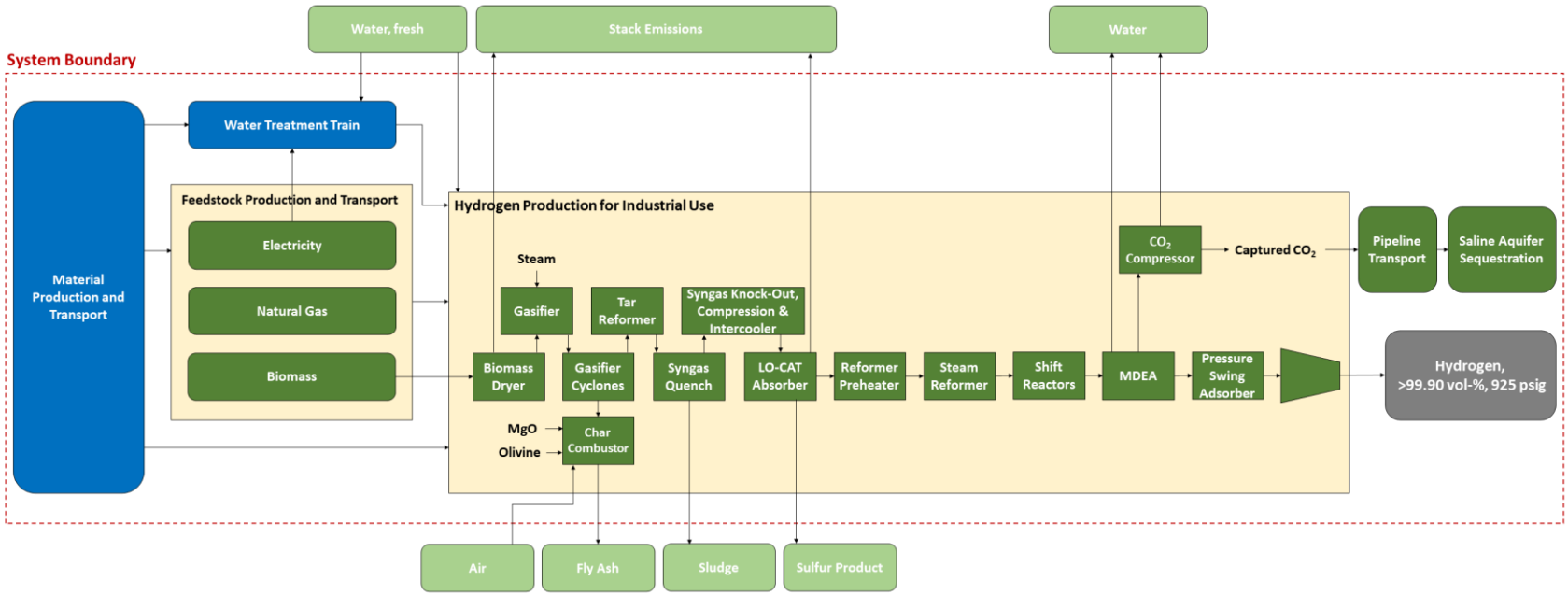

Figure S-8. System boundary diagram for biomass gasification with CCS scenario [43, 44]

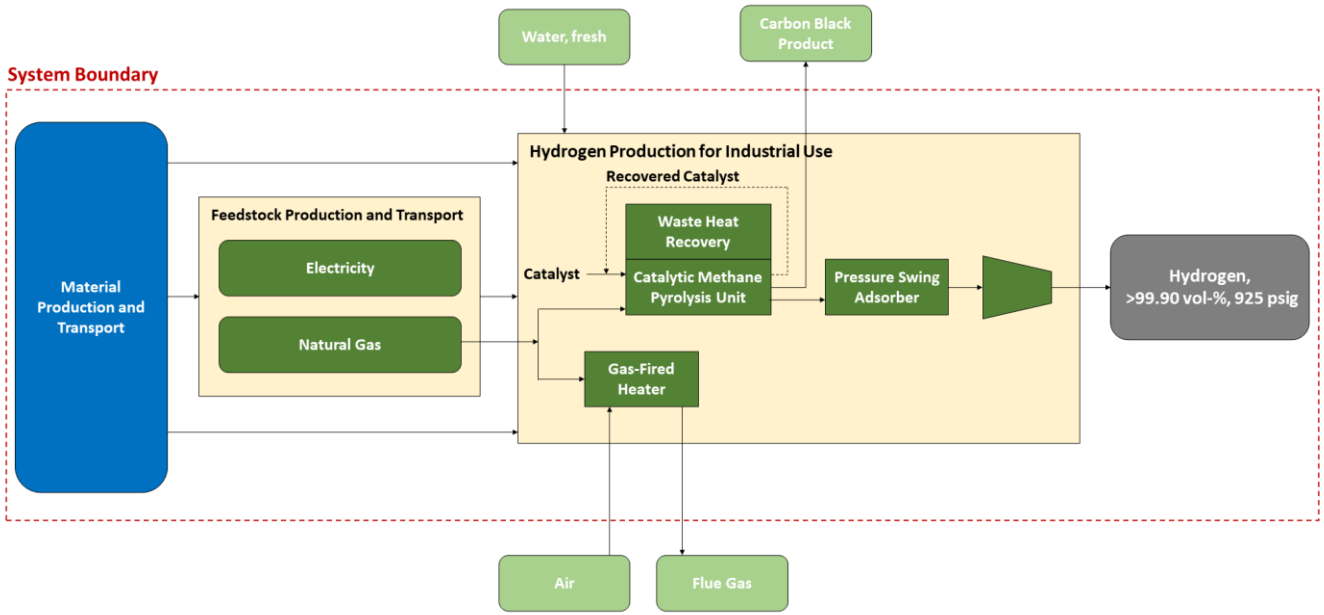

Figure S-9. System boundary diagram for methane pyrolysis scenario [45]

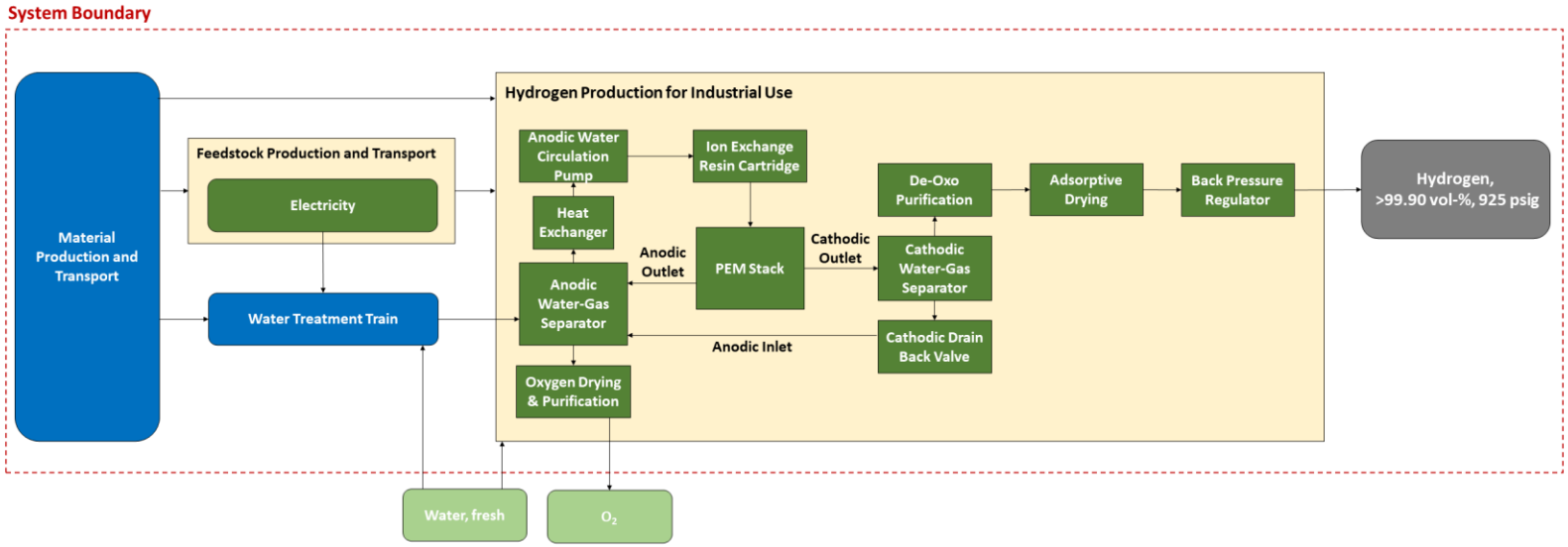

Figure S-10. System boundary diagram for PEM electrolysis scenario [46]

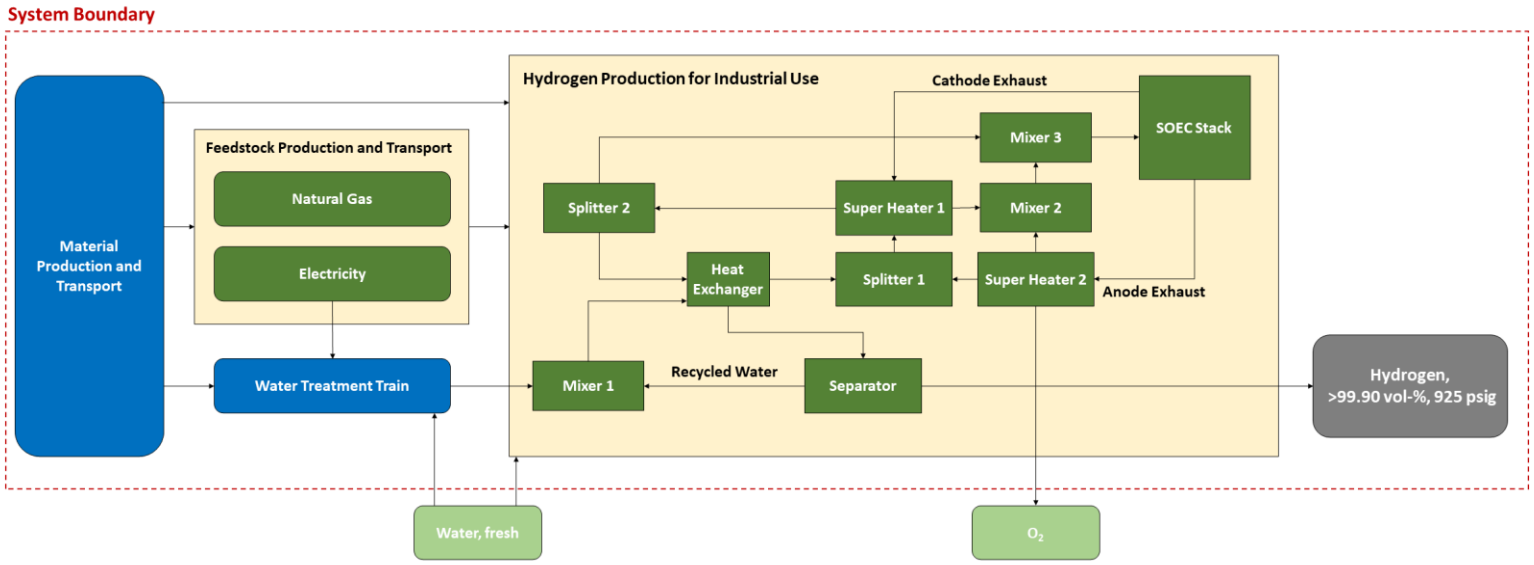

Figure S-11. System boundary diagram for solid oxide electrolysis scenario [47]

Life cycle analysis (LCA) is a methodology for assessing environmental impacts of a defined product, known as the functional unit, across its life cycle. Each stage of the life cycle is broken into unit processes, which are then linked together by intermediate flows, creating a product system. A generalized product system is shown in Figure S-12.

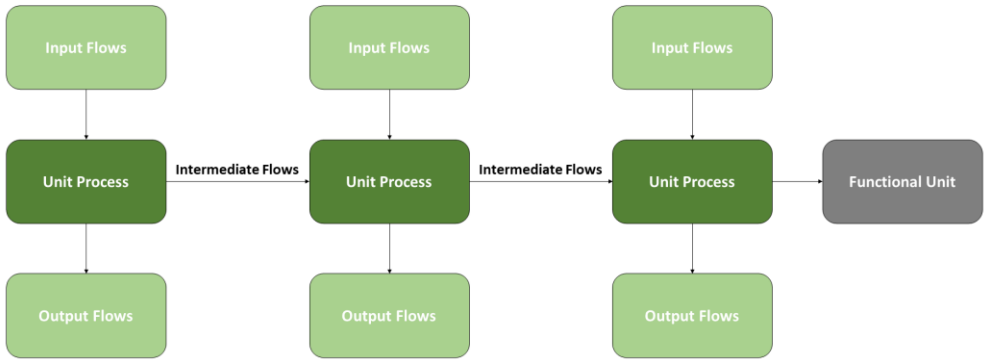

Figure S-12. Example of connected unit processes in a product system [6]

The aggregation of input and output flows within a defined system boundary culminates in a life cycle inventory. This inventory can then be used to calculate environmental impacts for a given impact assessment method, as seen in Equation S-1.

Equation S-1

$$\begin{bmatrix} m_1 \\ m_2 \\ m_3 \\ \cdots \\ m_n \end{bmatrix} \cdot [c_1 \quad c_2 \quad c_3 \quad \ldots \quad c_n] = Impact\ Result$$

where:

m = mass of inventory flow
c = characterization factor

Global warming potential results for the hydrogen technologies are detailed in tabular form in Table S-1. Note that additional significant figures are shown here to highlight the often-small differences in the total, low, and high result values. Inclusion of these additional digits should not imply more confidence in the underlying results.

Table S-1. Life cycle GWP results for all hydrogen production scenarios (IPCC AR6, 100-yr) (kg CO_2e/kg H_2)

Technology	SMR	SMR w/ CCS	ATR w/ CCS	CG	CG w/ CCS	BG/CG w/ CCS	BG	BG w/ CCS	MP	PEM U.S. Avg	PEM Solar	PEM Wind	SOEC U.S. Avg	SOEC Solar	SOEC Wind
Process Emissions	9.35	0.380	0.514	17.9	1.35	1.59	24.7	2.45	1.42	-	-	-	-	-	-
Natural Gas Emissions	2.53	2.69	2.53	-	-	-	0.188	0.190	3.22	-	-	-	0.771	0.771	0.771
Coal Emissions	-	-	-	1.50	1.50	1.06	-	-	-	-	-	-	-	-	-
Biomass Emissions	-	-	-	-	-	-4.06	-20.1	-20.1	-	-	-	-	-	-	-
Electricity Emissions	0.358	1.15	2.32	0.518	0.811	-0.0515	0.513	1.71	0.791	31.3	2.76	1.82	24.5	2.15	1.43
Water Treatment Train Emissions	0.0091	0.0011	0.0024	0.0013	0.0013	0.0018	0.0446	0.0446	-	0.00614	0.00614	0.00614	0.00616	0.00616	0.00616
CO_2 Management Emissions	-	0.150	0.138	-	0.260	0.296	-	0.328	-	-	-	-	-	-	-
Steam Generation	-1.87	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total	10.4	4.37	5.50	20.0	3.92	-1.16	5.31	-15.4	5.43	31.3	2.76	1.83	25.2	2.93	2.20
Low (5^{th} Percentile)	8.98	2.90	4.11	19.4	3.34	-1.60	4.47	-16.3	3.68	30.5	2.60	1.64	24.2	2.40	1.66
High (95^{th} Percentile)	14.1	8.30	9.21	23.4	7.59	1.76	7.33	-13.4	10.1	32.3	3.00	2.09	27.1	4.24	3.50

The high and low values represent the 5th and 95th percentile results from a Monte Carlo simulation with 5,000 iterations performed in openLCA. This uncertainty is derived from several parameters included in the underlying models for natural gas, coal, biomass, and electricity listed above. Many parameters in the upstream natural gas model are stochastically defined, and regional variability is also accounted for in the high and low results values. The upstream coal model is similarly parameterized, though GWP results are largely driven by the coal mine methane assumption. The upstream electricity model incorporates a lognormal uncertainty distribution for select air emissions, which are derived from variation in emissions factors reported in facility data. The upstream biomass model includes triangular distributions for key parameters, like biomass yield and fertilization rates, to account for regional variations.

GWP results can also be presented in terms of energy content. Assuming a higher heating value (HHV) of 59,970 Btu/lb for the produced hydrogen product, results are shown in Table S-2 and Table S-3.

Table S-2. Life cycle GWP results for all hydrogen production scenarios (IPCC AR6, 100-yr) (kg CO_2e/kg H_2)

Technology	SMR	SMR w/ CCS	ATR w/ CCS	CG	CG w/ CCS	BG/CG w/ CCS	BG	BG w/ CCS	MP	PEM U.S. Avg	PEM Solar	PEM Wind	SOEC U.S. Avg	SOEC Solar	SOEC Wind
Process Emissions	70.7	2.87	3.89	136	10.2	12.0	187	18.5	10.7	-	-	-	-	-	-
Natural Gas Emissions	19.1	20.3	19.1	-	-	-	1.42	1.43	24.4	-	-	-	5.83	5.83	5.83
Coal Emissions	-	-	-	11.3	11.3	8.01	-	-	-	-	-	-	-	-	-
Biomass Emissions	-	-	-	-	-	-30.7	-152	-152	-	-	-	-	-	-	-
Electricity Emissions	2.71	8.73	17.5	3.92	6.13	-0.389	3.89	13.0	5.99	237	20.8	13.8	185	16.3	10.8
Water Treatment Train Emissions	0.0691	0.0081	0.0185	0.0100	0.0101	0.0137	0.0337	0.0337	-	0.0464	0.0464	0.0464	0.0466	0.0466	0.0466
CO_2 Management Emissions	-	1.13	1.05	-	1.97	2.24	-	2.48	-	-	-	-	-	-	-
Steam Generation	-14.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total	78.4	33.1	41.6	151	29.6	-8.77	40.2	-117	41.1	237	20.9	13.8	191	22.2	16.7
Low (5th Percentile)	67.9	22.0	31.1	147	25.3	-12.1	33.8	-123	27.8	230	19.6	12.4	183	18.2	12.5
High (95th Percentile)	106	62.8	69.7	177	57.4	13.3	55.4	-101	76.7	245	22.7	15.8	205	32.1	26.5

Table S-3. Life cycle GWP results for all hydrogen production scenarios (IPCC AR6, 100-yr) (kg CO_2e/MJ H_2)

Technology	SMR	SMR w/ CCS	ATR w/ CCS	CG	CG w/ CCS	BG/CG w/ CCS	BG	BG w/ CCS	MP	PEM U.S. Avg	PEM Solar	PEM Wind	SOEC U.S. Avg	SOEC Solar	SOEC Wind
Process Emissions	6.70E-2	2.72E-3	3.69E-3	1.29E-1	9.66E-3	1.14E-2	1.77E-1	1.76E-2	1.02E-2	-	-	-	-	-	-
Natural Gas Emissions	1.81E-2	1.93E-2	1.81E-2	-	-	-	1.35E-3	1.36E-3	2.31E-2	-	-	-	5.53E-3	5.53E-3	5.53E-3
Coal Emissions	-	-	-	1.07E-2	1.07E-2	7.60E-3	-	-	-	-	-	-	-	-	-
Biomass Emissions	-	-	-	-	-	-2.91E-2	-1.44E-1	-1.44E-1	-	-	-	-	-	-	-
Electricity Emissions	2.57E-3	8.28E-3	1.66E-2	3.71E-3	5.81E-3	-3.69E-4	3.68E-3	1.23E-2	5.67E-3	2.25E-1	1.98E-2	1.31E-2	1.75E-1	1.54E-2	1.02E-2

Water Treatment Train Emissions	6.55E-5	7.67E-6	1.75E-5	9.46E-6	9.53E-6	1.30E-5	3.20E-5	3.20E-5	-	4.40E-5	4.40E-5	4.40E-5	4.42E-5	4.42E-5	4.42E-5
CO_2 Management Emissions	-	1.07E-3	9.92E-4	-	1.86E-3	2.12E-3	-	2.35E-3	-	-	-	-	-	-	-
Steam Generation	-1.34E-2	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total	7.43E-2	3.13E-2	3.94E-2	1.43E-1	2.81E-2	-8.31E-3	3.81E-2	-1.11E-1	3.89E-2	2.25E-1	1.98E-2	1.31E-2	1.81E-1	2.10E-2	1.58E-2
Low (5^{th} Percentile)	6.44E-2	2.28E-2	2.95E-2	1.39E-1	2.40E-2	-1.15E-2	3.21E-2	-1.17E-1	2.64E-2	2.18E-1	1.86E-2	1.17E-2	1.73E-1	1.72E-2	1.19E-2
High (95^{th} Percentile)	1.01E-1	5.95E-2	6.60E-2	1.68E-1	5.44E-2	1.26E-2	5.26E-2	-9.59E-2	7.27E-2	2.32E-1	2.15E-2	1.50E-2	1.94E-1	3.04E-2	2.51E-2

Similarly, water consumption results are detailed in Table S-4, and in imperial units in Table S-5.

Table S-4. Life cycle water consumption results for all hydrogen productions scenarios (kg water/kg H_2)

Technology	SMR	SMR w/ CCS	ATR w/ CCS	CG	CG w/ CCS	BG/CG w/ CCS	BG	BG w/ CCS	MP	PEM U.S. Avg	PEM Solar	PEM Wind	SOEC U.S. Avg	SOEC Solar	SOEC Wind
Process Water	5.33	1.56	3.55	1.92	1.94	2.63	0.992	0.992	-	8.94	8.94	8.94	8.94	8.94	8.94
Cooling Water	2.44	22.7	29.6	18.8	21.4	30.3	6.49	12.7	0.029	3.20	3.20	3.20	2.50	2.50	2.50
Natural Gas Consumption	0.314	0.334	0.314	-	-	-	0.0224	0.0226	0.401	-	-	-	0.0965	0.0965	0.0965
Coal Consumption	-	-	-	2.20	2.20	1.69	-	-	-	-	-	-	-	-	-
Biomass Consumption	-	-	-	-	-	495	3346	3346	-	-	-	-	-	-	-
Electricity Consumption	3.05	9.84	19.8	4.41	6.91	-0.439	4.38	14.6	6.75	267	22.2	15.7	209	17.3	12.3
Water Treatment Train Consumption	3.17	0.373	0.847	0.458	0.463	0.629	1.55	1.55	-	2.13	2.13	2.13	2.17	2.17	2.17
CO_2 Management Consumption	-	0.865	0.799	-	1.50	1.82	-	2.01	-	-	-	-	-	-	-
Steam Generation	-1.90	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total	12.4	35.7	54.9	27.8	34.4	532	3359	3378	7.18	281	36.4	30.0	222	31.0	26.0
Low (5^{th} Percentile)	12.2	35.4	54.6	21.8	28.5	436	2004	2023	6.86	281	36.4	30.0	222	30.9	25.9
High (95^{th} Percentile)	14.5	36.0	55.1	32.7	39.1	771	6664	6682	7.51	284	39.0	32.5	225	33.6	28.6

Table S-5. Life cycle water consumption results for all hydrogen production scenarios (gal water/lb H_2)

Technology	SMR	SMR w/ CCS	ATR w/ CCS	CG	CG w/ CCS	BG/CG w/ CCS	BG	BG w/ CCS	MP	PEM U.S. Avg	PEM Solar	PEM Wind	SOEC U.S. Avg	SOEC Solar	SOEC Wind
Process Water	0.629	0.184	0.418	0.226	0.228	0.310	0.117	0.117	-	1.05	1.05	1.05	1.05	1.05	1.05
Cooling Water	0.287	2.68	3.49	2.22	2.52	3.58	0.765	1.50	0.0034	0.377	0.377	0.377	0.295	0.295	0.295
Natural Gas Consumption	0.0371	0.0394	0.0371	-	-	-	0.0026	0.0027	0.0473	-	-	-	0.0114	0.0114	0.0114
Coal Consumption	-	-	-	0.259	0.259	0.199	-	-	-	-	-	-	-	-	-
Biomass Consumption	-	-	-	-	-	58.4	395	395	-	-	-	-	-	-	-
Electricity Consumption	0.360	1.16	2.33	0.521	0.815	-0.0518	0.516	1.72	0.796	31.5	2.62	1.85	24.6	2.04	1.45

Water Treatment Train Consumption	0.374	0.0440	0.0999	0.0540	0.0546	0.0741	0.183	0.183	-	0.252	0.252	0.252	0.256	0.256	0.256
CO_2 Management Consumption	-	0.102	0.0942	-	0.177	0.214	-	0.238	-	-	-	-	-	-	-
Steam Generation	-0.224	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total	1.46	4.21	6.47	3.28	4.06	62.7	396	398	0.846	33.2	4.30	3.53	26.2	3.66	3.06
Low (5th Percentile)	1.44	4.18	6.44	2.57	3.36	51.4	236	239	0.809	33.2	4.30	3.53	26.2	3.65	3.05
High (95th Percentile)	1.72	4.24	6.50	3.85	4.61	90.9	786	788	0.886	33.5	4.59	3.83	26.5	3.96	3.37

The results can also be displayed in terms of percent contribution, as shown for GWP in Figure S-13.

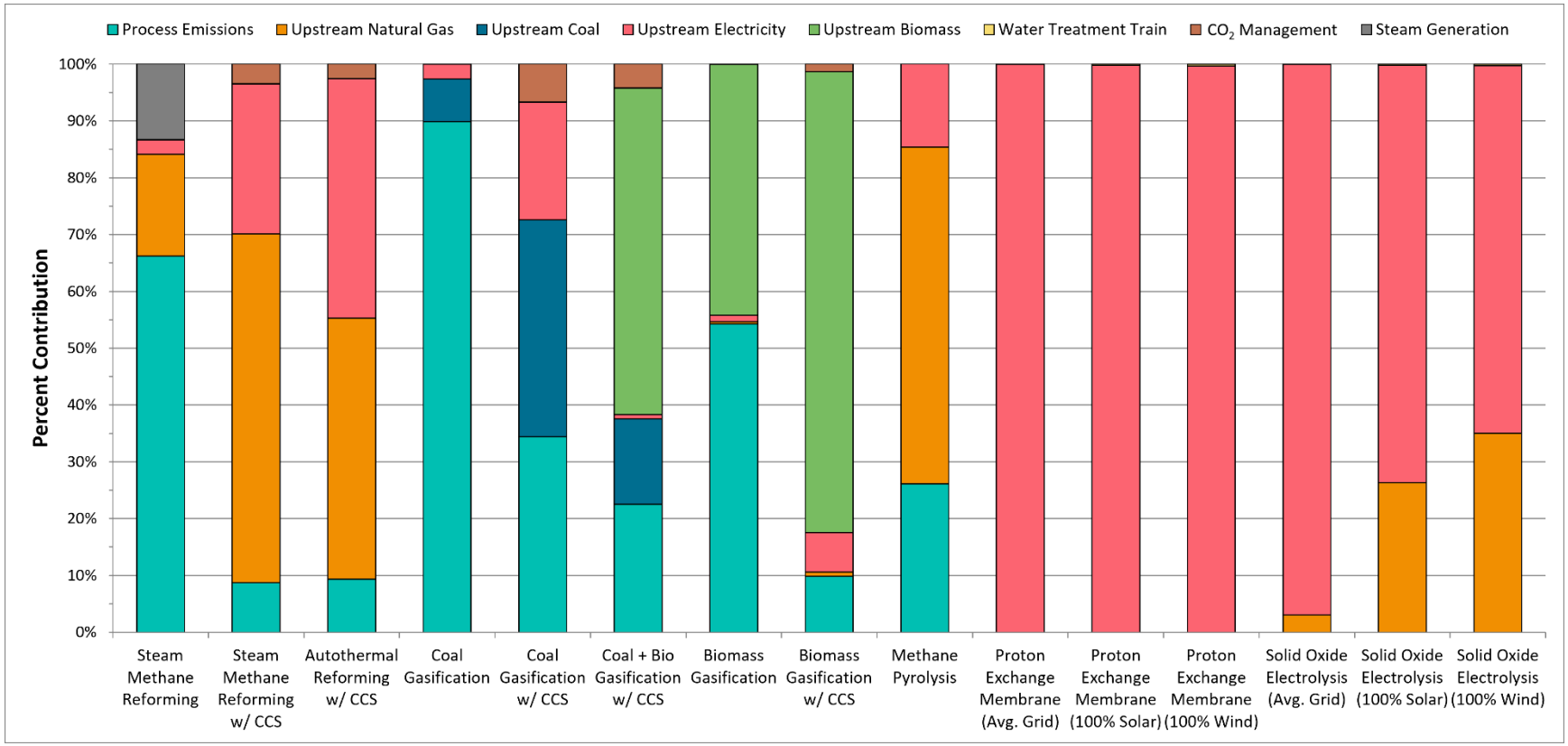

Figure S-13. GWP results by percent contribution

For the fossil-based cases, the process feedstock and stack emissions are the largest contributors to total GWP. In contrast, the highest contributor to GWP for the electrochemical hydrogen production technologies is electricity.

A similar percent contribution comparison for water consumption is shown in Figure S-14.

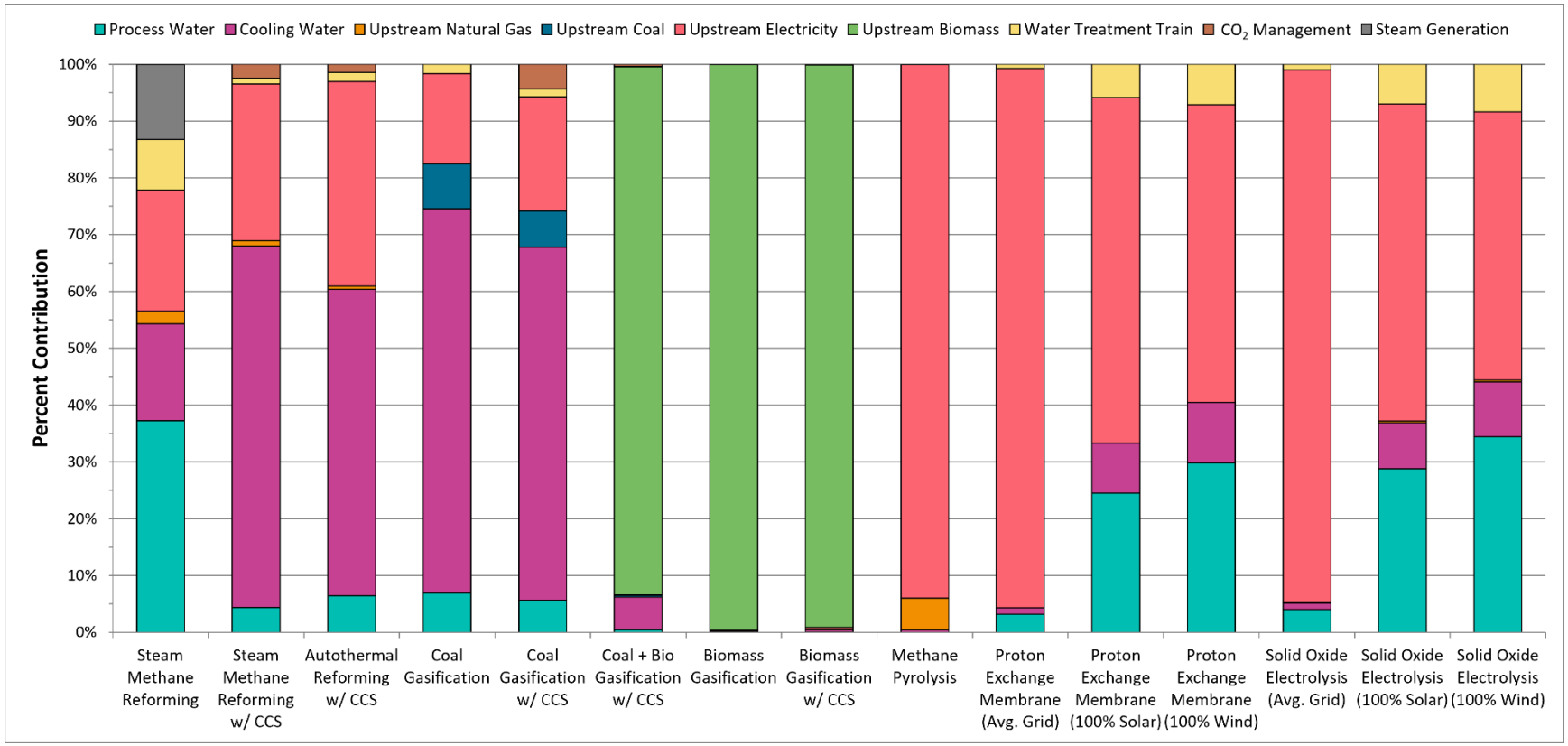

Figure S-14. Water consumption results by percent contribution

GWP results in this report are calculated using IPCC AR6 characterization factors, assuming a 100-year time horizon. This is just one of many assessment methods released in IPCC reports in recent years, and values are also available at a 20-year time horizon and with and without climate carbon feedback [58, 59]. Table S-6 shows results calculated for seven other GWP methods to demonstrate the sensitivity of results to various impact assessment methods. It is noted that the selection of a specific IPCC method does not qualitatively change the conclusions expressed in the manuscript.

Table S-6. GWP results for all technologies by IPCC scenario (kg CO_2e/kg H_2)

	Technology	SMR	SMR w/ CCS	ATR w/ CCS	CG	CG w/ CCS	BG/CG w/ CCS	BG	BG w/ CCS	MP	PEM U.S. Avg	PEM Solar	PEM Wind	SOEC U.S. Avg	SOEC Solar	SOEC Wind
100-yr	AR6	10.4	4.37	5.50	20.0	3.92	-1.16	5.31	-15.4	5.43	31.3	2.76	1.83	25.2	2.93	2.20
	AR5, with climate carbon feedback	10.6	4.66	5.79	20.1	4.07	-1.04	5.45	-15.2	5.77	31.7	2.80	1.86	25.6	3.04	2.30
	AR5, without climate carbon feedback	10.4	4.38	5.51	20.0	3.92	-1.16	5.30	-15.4	5.44	31.4	2.76	1.83	25.2	2.93	2.21
	AR4	10.2	4.18	5.30	19.8	3.80	-1.24	5.33	-15.4	5.20	31.1	2.74	1.81	25.0	2.86	2.14
20-yr	AR6	12.3	6.84	7.94	21.1	5.24	-0.226	5.91	-14.6	8.32	34.5	3.06	2.04	28.4	3.83	3.04
	AR5, with climate carbon feedback	12.4	7.00	8.11	21.2	5.33	-0.148	5.93	-14.6	8.51	34.8	3.08	2.05	28.6	3.89	3.09
	AR5, without climate carbon feedback	12.3	6.91	8.01	21.2	5.28	-0.185	5.90	-14.6	8.40	34.6	3.07	2.04	28.5	3.86	3.06
	AR4	11.9	6.38	7.48	20.9	4.98	-0.398	5.83	-14.7	7.78	33.9	3.00	2.00	27.8	3.66	2.88

DQI is assessed for each hydrogen production technology using EPA pedigree matrices [60]. Two DQI scores are assigned to each technology: one at the process level, which assesses process review and completeness, and one at the flow level, which considers flow reliability and representativeness. The matrices used to evaluate flow-level and process-level DQI are shown in **Error! Reference source not found.** and Table S-8, respectively.

Table S-7. Data quality pedigree matrix for flow indicators

Indicator		1	2	3	4	5 (default)
Flow reliability		Verified data based on measurements	Verified data based on a calculation **or** non-verified data based on measurements	Non-verified data based on a calculation	Documented estimate	Undocumented estimate
Flow Representativeness	**Temporal correlation**	Less than 3 years of difference	Less than 6 years of difference	Less than 10 years of difference	Less than 15 years of difference	Age of data unknown or more than 15 years
	Geographical correlation	Data from same resolution **and** same area of study	Within one level of resolution **and** a related area of study	Within two levels of resolution **and** a related area of study	Outside of two levels of resolution **but** a related area of study	From a different or unknown area of study
	Technological correlation	All technology categories are equivalent	**Three** of the technology categories are equivalent	**Two** of the technology categories are equivalent	**One** of the technology categories is equivalent	**None** of the technology categories are equivalent
	Data collection methods	Representative data from >80% of the relevant market, over an adequate period	Representative data from 60-79% of the relevant market, over an adequate period **or** representative data from >80% of the relevant market, over a shorter period of time	Representative data from 40-59% of the relevant market, over an adequate period **or** representative data from 60-79% of the relevant market, over a shorter period of time	Representative data from <40% of the relevant market, over an adequate period **or** representative data from 40-59% of the relevant market, over a shorter period of time	Unknown **or** data from a small number of sites and from shorter periods

Table S-8. Data quality pedigree matrix for process indicators [60]

Indicator	1	2	3	4	5 (default)
Process review	Documented reviews by a minimum of two types of third-party reviewers	Documented reviews by a minimum of two types of reviewers, with one being a third party	Documented review by a third-party reviewer	Documented review by an internal reviewer	No documented review
Process completeness	>80% of determined flows have been evaluated and given a value	60-79% of determined flows have been evaluated and given a value	40-59% of determined flows have been evaluated and given a value	<40% of determined flows have been evaluated and given a value	Process completeness not scored

Data quality was assessed for each technology, and the resulting DQIs are presented in Table S-9.

Table S-9. DQI scores for hydrogen production technologies

Technology	Flow Reliability	Temporal Correlation	Geographical Correlation	Technological Correlation	Data Collection Methods	Flow-Level DQI	Process Review	Process Completeness	Process-Level DQI
SMR	2	1	2	1	2	**2,1,2,1,2**	4	1	**4,1**
SMR w/ CCS	2	1	2	1	2	**2,1,2,1,2**	4	1	**4,1**
ATR w/ CCS	2	2	3	3	1	**2,2,3,3,1**	4	1	**4,1**
CG	2	2	1	2	1	**2,2,1,2,1**	4	1	**4,1**
CG w/ CCS	2	3	1	2	1	**2,3,1,2,1**	4	1	**4,1**
BG/CG w/ CCS	2	2	1	2	1	**2,2,1,2,1**	4	1	**4,1**
BG	2	5	1	2	3	**2,5,1,2,3**	4	1	**4,1**
BG w/ CCS	2	5	1	3	3	**2,5,1,3,3**	4	1	**4,1**
MP	2	4	3	3	3	**2,4,3,3,3**	4	1	**4,1**
PEM	2	3	1	3	3	**2,3,1,3,3**	4	2	**4,2**
SOEC	2	3	3	2	4	**2,3,3,2,4**	4	2	**4,2**