Environmental Life-Cycle Analysis of Hydrogen Technology Pathways in the United States

Supporting Information

This information provided here describes the simulation parameters used in this study to carry out the life cycle analysis (LCA) for each hydrogen production technology in R&D GREET 2023. We also include compression and transmission information for gaseous and liquid hydrogen transportation, distribution, and storage. A lower heating value basis is used for all energy calculations.

1. Hydrogen Production

1.1 Steam Methane Reforming

The data for steam methane reforming (SMR) used in R&D GREET was obtained from a 2022 study conducted by the National Energy Technology Laboratory (NETL) (Lewis et al. 2022). NETL determined these parameters by developing an ASPEN model based on a hypothetical industrial scale SMR plant. These parameters can be found in Table S1. In the scenario with no CCS, we assumed that excess steam is valorized. However, if CCS is required, then that steam will be used in the CCS process and cannot be valorized for credit.

Table S1: Parameters for natural gas and electricity consumed, and co-products for SMR in R&D GREET per mmBtu of hydrogen produced (Lewis et al. 2022).

Parameters (per kg H_2)	**Without CCS**	**With CCS**
Inputs		
Natural Gas as Feed (mmBtu)	0.11	0.11
Natural Gas as Fuel (mmBtu)	0.05	0.06
Electricity Consumption (kWh)	0.13	1.5
Co-Product		
Steam (mmBtu)	0.02	0

1.2 Autothermal Reforming

Like the data for SMR, the parameters for autothermal reforming (ATR) were also obtained from an ASPEN model developed by NETL (Lewis et al. 2022). However, only data for the scenario with CCS was available, as shown in Table S2.

Table S2: Natural gas and electricity consumed for ATR in R&D GREET per mmBtu of hydrogen produced (Lewis et al. 2022).

Parameters (per kg H_2)	**With CCS**
Natural Gas as Feed (mmBtu)	0.16
Natural Gas as Fuel (mmBtu)	0
Electricity Consumption (kWh)	3.6

1.3 Methane Pyrolysis

Operation data for methane pyrolysis was obtained from communication with Monolith Inc and can be found in Table S3. Methane pyrolysis uses a plasma arc to generate heat needed to decompose methane in an uncatalyzed reaction. As the plasma arc has a high electricity demand, electricity and natural gas (as feedstock) comprise most of the inputs for hydrogen production. In addition, there is a third undisclosed input that is essential for the methane pyrolysis process. After further discussion with Monolith, we accounted for carbon in the undisclosed input and used diesel as a surrogate to account for upstream emissions associated with supplying the undisclosed input. The hydrogen co-products from the methane pyrolysis process are carbon black, coke, and steam.

Table S3: Process inputs and co-products for hydrogen production via methane pyrolysis.

Parameters (per kg H_2)	
Inputs	
Natural gas (mmBtu)	0.20
Electricity (kWh)	37.3
Other Input (Diesel) (mmBtu)	0.05
Co-products	
Carbon Black (kg)	3.5
Coke (kg)	0.11

Steam (mmBtu)	0.03

As carbon black is primarily used as an additive for tires and dyes (i.e., not for its energy value), we used mass allocation to distribute the emissions between each of the co-product after using displacement method for steam export credit. The allocation factors used for this calculation are shown in Table S4.

Table S4: Allocation factors (AF) based on mass in methane pyrolysis process

Products	Normalized Output (per kg H_2)	Mass Allocation Factor
H_2	1.0	21.83%
Carbon Black	3.5	75.75%
Coke	0.11	2.42%

1.4 Coal Gasification

Table S5 shows the feedstock and energy consumption for coal gasification in R&D GREET. These values were obtained from an ASPEN simulation performed by NETL (Lewis et al. 2022).

Table S5: Input parameters for coal gasification in R&D GREET per mmBtu of hydrogen produced

Parameters (per mmBtu H_2)	Without CCS	With CCS
Coal (mmBtu)	0.19	0.19
Electricity Consumption (kWh)	0.53	1.0

1.5 Biomass Gasification

The feedstock and energy consumption required for the gasification of poplar biomass are shown in Table S6. These values are based on the H2A model developed by National Renewable Energy Laboratory (NREL) that are currently used in the R&D GREET model (Mann and Steward 2018). The values for CCS were calculated based on the assumption that the energy required for CCS is 357 kWh/ton of carbon captured.

Table S6: Input data for biomass gasification in R&D GREET per mmBtu of hydrogen produced

Parameters (per mmBtu H_2)	**Without CCS**	**With CCS**
Biomass (mmBtu)	0.25	0.25
Natural Gas (mmBtu)	0.006	0.006
Electricity Consumption (kWh)	0.44	3.0

1.6 By-product of Chlor-alkali

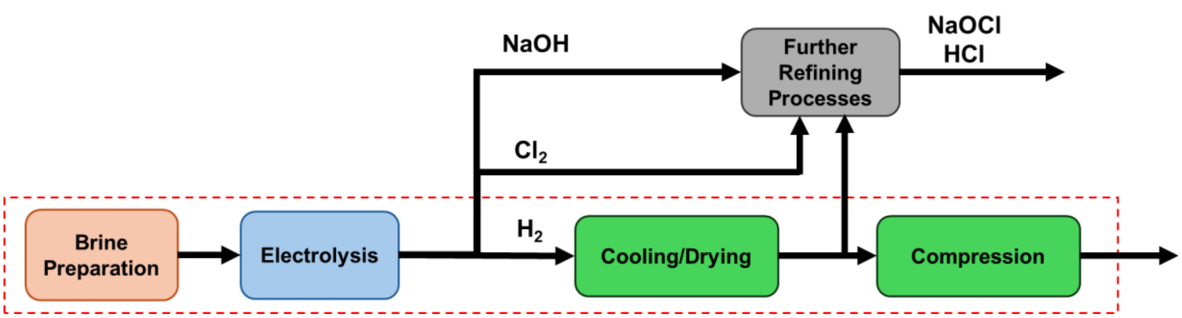

Figure S1: System boundary diagram for chlor-alkali pathway for hydrogen production.

This process refers to the electrolysis of a sodium or potassium chloride brine solution, from which chlorine, sodium hydroxide, and hydrogen are the primary products. In our study, we focused on the use of sodium chloride brine, and limited the system boundary to the hydrogen production and refinement processes. Data for this study is shown in Table S7 and was obtained from the Chemical Database Reporting (CDR) database for production, Greenhouse Gas Reporting Program (GHGRP) for on-site fuel use, and EIA-923 forms from industry for electricity use.

Table S7: Mass allocated parameters for hydrogen production for the chlor-alkali process.

Parameters (per kg H_2)	
Natural Gas (Btu)	496
Brine (kg)	1.7

Electricity (kWh)	2.9

1.7 NGL Cracking by-product

Hydrogen production from steam cracking of NGL (natural gas liquid) cracking involves purifying hydrogen from produced tail gas and substitute the energy lost with an equivalent amount of natural gas. Therefore, the CI for hydrogen production is dependent on the upstream emissions from obtaining the natural gas, the combustion emissions of the natural gas, and the electricity required to purify the hydrogen. All these information can be found in Table S8

Table S8: Simulation data for the quantity of natural gas and electricity required for hydrogen production as a by-product of NGL cracking

Parameters (per kg H_2)	
Natural Gas Substitute (mmBtu)	0.11
Electricity Consumption (kWh)	0.5

1.8 Electrolysis

The electricity and thermal energy consumption for low and high temperature electrolysis were obtained from studies published by the Department of Energy Hydrogen and Fuel Cells Program Record (Peterson et al. 2020a; Peterson et al. 2020b). These values can be found in Table S9 below.

Table S9: Electricity and thermal energy consumption by low and high temperature electrolysis from Peterson et al. 2020a and Peterson et al. 2020b.

Parameters (per kg H_2)	**Low Temperature Electrolysis**	**High Temperature Electrolysis**
Electricity Consumption (kWh)	55.5	39.8
Thermal Energy (mmBtu)	0	0.023

2. Hydrogen Transportation, Storage, and Liquefaction

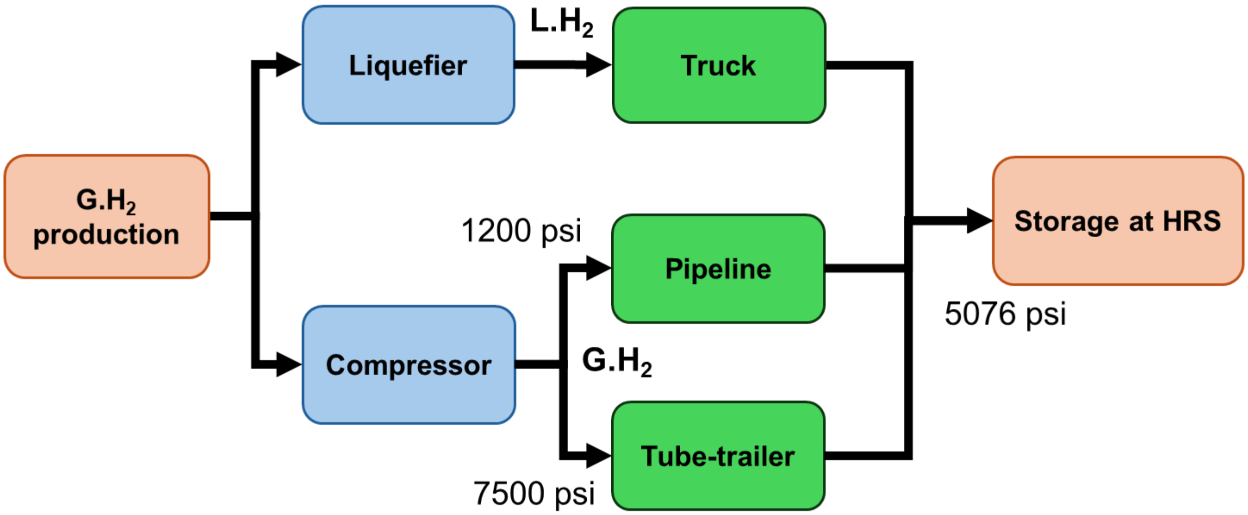

Figure S2: Diagram of hydrogen transportation and distribution in R&D GREET. HRS refers to the hydrogen refueling station.

For transportation of gaseous hydrogen, we assumed that it would either be liquefied, or compressed before being transported to the hydrogen refueling station (HRS). The liquefaction and compressor steps are assumed to be co-located with the hydrogen production facility. For gaseous hydrogen transportation via tube-trailer, we assume that it will be first compressed from the production pressure of 300 psi to 7500 psi for tube-trailer loading. For pipeline transportation, it will instead be compressed to 1200 psi. The hydrogen will then be dispensed to the storage tank at the hydrogen refueling station (HRS) to be stored at 5076 psi. The inlet temperature for the compressors is assumed to be 21°C for all cases. As for the liquefaction step, the pump at the HRS is assumed to consume 0.3 kWh/kg H_2.

3. Grid Carbon Intensity

Table S9 shows the carbon intensity of each electricity source used in this study. HICC (Hawaiian Islands Coordinating Council) is one of ten NERC (North American Electric Reliability Corporation) designated regions of electricity production. The final carbon intensity is calculated based on the shares of each type of electricity production from the EIA (Energy Information Administration)'s 2023 Annual Energy Outlook (AEO).

Table S10: Carbon intensity of electricity sources used in this study. These values were determined using R&D GREET 2023.

Electricity Source	**Carbon Intensity (gCO_2e/kWh)**
Hawaiian (HICC)	866.5
United States average grid mix	439.5

Nuclear	2.8
Renewables (wind, solar, hydro)	0

4. Bill of Materials for embodied emission calculation

The bill of materials used to calculate the embodied emissions for a steam methane reforming (SMR) plant can be found in Table S11. This assumes that the SMR plant has a capacity of 18.5 mmscf/day and would have a lifespan of 35 years (Wang et al. 2012).

Table S11: Bill of Materials for the construction of a steam methane reforming plant assumed to have a lifetime of 35 years with a production capacity of 18.5 mmscf/day (Wang et al. 2012).

Construction Materials (per kg H_2)	**Steam Methane Reforming**
Steel (kg)	0.0003
Stainless Steel (kg)	0.0001
Concrete (kg)	0.001

Table S12 shows the bill of materials for the construction of clean electricity infrastructure that was used in this study to calculate the CapEx embodied emissions from electricity (Gan et al. 2024). Others refer to construction materials that did not fit into the other categories such as sand and other chemicals required during construction. Table S13 shows the materials required to construct the facilities, pipelines, and chemicals required for natural gas and coal extraction. Finally, table S14 shows the materials required to construct the farming equipment necessary to cultivate the poplar needed for biomass gasification. These equipment were assumed to have a lifespan of 10 years and that the farm has an acreage of 545.8 acres producing a yield of 1.2 tons of biomass per acre at a collection rate of 30%.

Table S12: Bill of materials for the construction of various renewable and nuclear electricity infrastructure (Gan et al. 2024)

Construction Materials (MT/TWh)	**Nuclear LWR**	**Hydro**	**Wind**	**Solar PV**
Aluminum	0	0	71	1004

Cement	0	0	0	0
Concrete	502	32592	7903	202
Copper	2	0	80	304
Glass	0	0	0	1382
Iron	0	0	192	1
Lead	0	0	0	0
Plastic	0	3197	152	430
Silicon	0	0	0	91
Steel	101	461	2081	1615
Others	0	21893	53	45

Table S13: Materials required to construct necessary infrastructure to extract natural gas and coal.

Materials (kg/mmBtu)	**Natural Gas Extraction**	**Coal Mining**	**Petroleum Drilling**
Cement	0.09	0	0.002
Steel	0.32	0.008	0.34
Gilsonite	0.006	0	0.0004
Bentonite	0.02	0	0.0005
Soda Ash	0.0004	0	0
Gelex	0.00001	0	0
Polypac	0.0006	0	0.00001
Xanthum Gum	0.0003	0	0
Water	5.3	0	2.4

Rubber	0	0.00002	0
Concrete	0	0.002	0
Asphalt	0	1.7	0

Table S14: Materials required to construct the needed farming equipment to produce poplar for gasification. The farming equipment has a lifespan of 10 years.

Materials* **(per dry MT per year)**	
Steel (MT)	0.13
Tires (MT)	0.03

*Emissions from assembling the equipment were 15 kgCO_2e/dry MT-year.

The embodied emissions for the solid oxide electrolyzer cell (SOEC) and proton exchange membrane (PEM) electrolyzers can be calculated using the materials for construction found in Table S15. We assumed that the electrolyzer BOP (balance of plant) would have a lifespan of 20 years while the stack has a lifespan of 4 and 7 years for SOEC and PEM respectively. The stacks were also assumed to operate at a capacity factor of 90 and 97% for SOEC and PEM respectively.

Table S15: Materials required to construct the stack and BOP for SOEC and PEM electrolyzers (Iyer et al. 2024).

Construction Materials	**Stack (lbs per stack)**		**BOP (lbs per BOP)**	
	SOEC	**PEM**	**SOEC**	**PEM**
8 mol.% Yttria-stabilized Zirconia	1.031	0	0	0
3 mol.% Yttria-stabilized Zirconia	8.779	0	0	0
Nickel oxide	15.920	0	0	0
Gadolinia doped ceria	2.789	0	0	0
Lanthanum strontium cobalt ferrite	1.191	0	0	0

Mylar/PET/Polyester	0	44.774	0.065	0
Fe-24% Cr alloy	60.098	0	0	0
Polypropylene	0	17.741	0	0
Cobalt carbonate	0.229	0	0	0
Manganese carbonate	0.208	0	0	0
Glass powder	0.896	0	0	0
Ni-Cr-Fe alloy (Alloy 600)	28.528	0	368.883	3,307.858
Stainless steel	12.774	158.649	0	0
Alumina	0.441	0	5.498	17.547
Aluminum silicate fiber	1.680	0	0	0
SGL Carbon: GDL 34 BA (Non-Woven)	0	4.802	0	0
PTFE	0	2.908	0.003	0.000
Nafion	0	27.289	0	0
Iridium Powder	0	1.213	0	0
Pt/C Powder	0	0.661	0	0
CeO2 Additive	0	0.049	0	0
Titanium Powder	0	125.046	0	0
Adhesive Powder (Polyurethane)	0	0.573	0	0
Lubricant Powder (Zinc Stearate)	0	0.639	0	0
Vulcan XC-72	0	0.805	0	0
Titanium Grade 2	0	237.808	0	0

Pt Coating	0	0.280	0	0
Au Coating	0	0.029	0	0
Polyolefin Elastomer	0	2.831	0	0
HDPE	0	32.908	0.047	0.368
Copper	0	11.861	276.530	5,182.833

5. References

Gan Y.; Ng, C.; Elgowainy, A.; Marcinkoski, J. *Considering Embodied Greenhouse Emissions of Nuclear and Renewable Power Plants for Electrolytic Hydrogen and Its Use for Synthetic Ammonia, Methanol, Fischer−Tropsch Fuel Production*. Environmental Science and Technology, 2024 DOI: https://doi.org/10.1021/acs.est.3c06769.

Iyer, R.; Prosser J.; Kelly, J.; James, B.; Elgowainy, A. Life-cycle analysis of hydrogen production from water electrolyzers. *International Journal of Hydrogen Energy*, **2024**, 81, 1467-1478. DOI: https://doi.org/10.1016/j.ijhydene.2024.06.355.

Lewis, E.; McNaul, S.; Jamieson, M.; Henriksen, M.; Matthews, H. S.; Walsh, L.; Grove, J.; Shultz, T.; Timothy J. Skone, P. E.; Stevens, R. *Comparison of Commercial, State-of-the-Art, Fossil-Based Hydrogen Production Technologies;* United States, 2022. DOI: 10.2172/1862910.

Mann, M. K.; Steward, D. M. *Current Central Hydrogen from Biomass via Gasification and Catalytic Steam Reforming*; National Renewable Energy Laboratory, 2018. https://www.nrel.gov/hydrogen/assets/docs/current-central-biomass-gasification-v3-2018.xlsm

Peterson, D., Vickers, J., DeSantis, D, "Hydrogen Production Cost From High Temperature Electrolysis – 2020," DOE Hydrogen and Fuel Cells Program Record #20006, Department of Energy Office of Energy Efficiency and Renewable Energy, Washington DC, 2020a

Peterson, D., Vickers, J., DeSantis, D, "Hydrogen Production Cost From PEM Electrolysis - 2019," DOE Hydrogen and Fuel Cells Program Record #19009, Department of Energy Office of Energy Efficiency and Renewable Energy, Washington DC, 2020b

Wang, M.; Elgowainy, A.; Han, J.; Cai, H. *Life-Cycle Analysis of Vehicle and Fuel Systems with the GREET model*. Department of Energy Fuel Cell Technologies Program Annual Merit Review, 2012. https://www.hydrogen.energy.gov/library/annual-progress/annual_progress12/annual_progress12_analysis