CARBONMODEL.COM
REFERENCE AND USER GUIDE

SYZYGY PLASMONICS INC.
3250 South Sam Houston Tollway East, Houston, Texas, USA

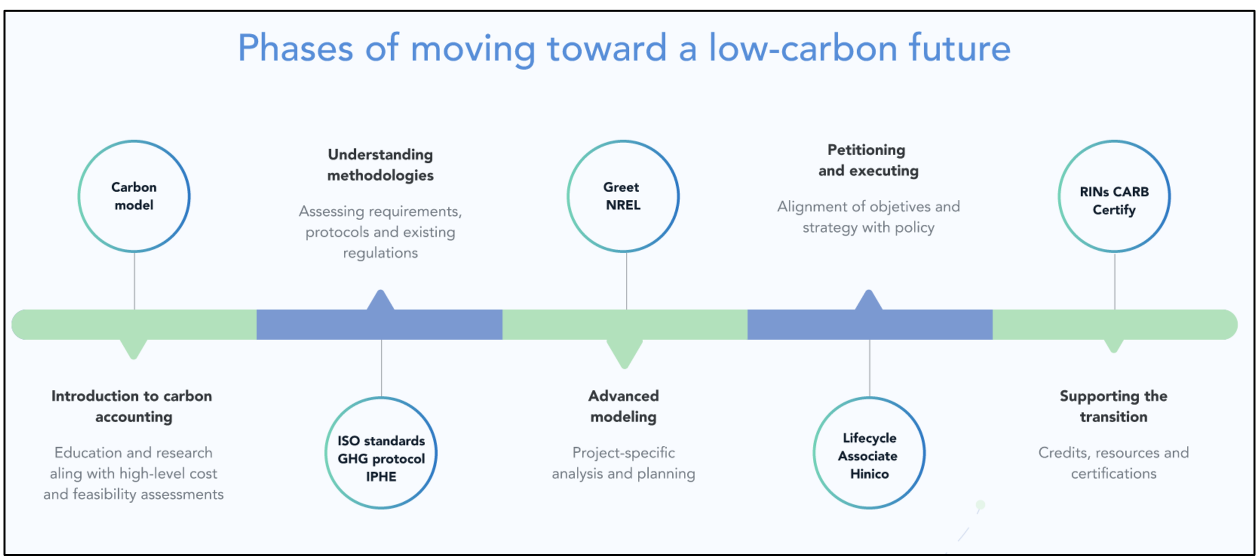
Table of Contents

CarbonModel.com Introduction

CarbonModel.com is an opensource software that gives analysts the ability to easily model specific cost and carbon intensity (CI) scenarios quicker than other cost and CI calculators and with more granularity than the simplistic implied scenarios of color. This model considers stoichiometric data, system efficiencies, and lifecycle carbon intensities of feedstocks to inform the carbon intensity of hydrogen production while providing a flexible, user-friendly interface to perform sensitivity analyses and case-by-case comparisons. Currently, the model focuses on hydrogen production; in the future, additional modules calculating the levelized cost and carbon intensity of additional energy transition chemicals such as ammonia, methanol, and sustainable aviation fuel will be added.

The process, feedstock, cost, and emissions inputs to this model are based on the best available public data and are meant to be used for comparison purposes only. In particular, the carbon intensities of electricity are based on figures provided by the International Panel on Climate Change in their 5th Assessment Report. The outputs should not be relied upon to guarantee actual costs or carbon emissions from specific real-world projects.

This model is meant to provide an intuitive and user-friendly tool for project developers, operators, policy makers, and other interested parties to conduct flexible and accurate analysis for cost and CI that can be the basis for further research into the economics, scale, and pace of deployment of energy transition technologies. We envision a CarbonModel.com analysis as the first step in a journey to deploying a project that will involve input and analysis from additional parties such as national standard-setting bodies, advanced modeling tools, and regulators.



Process Overview

Hydrogen Production

Photocatalytic Steam Methane Reforming (P-SMR) – Proprietary process pioneered by Syzygy that uses electricity in the form of light from LEDs to catalyze the reforming of methane to hydrogen and carbon dioxide. This process can be modeled as a single reforming process where the outputs are carbon dioxide and hydrogen, or a carbon capture enabled process where additional capex and opex inputs are estimated to capture process carbon emissions resulting in low-CI hydrogen.

$$CH_4 + 2H_20 \longrightarrow 4H_2 + CO_2$$

Photocatalytic Decomposition of Ammonia (P-DA) – Proprietary zero-carbon process pioneered by Syzygy that uses electricity to decompose ammonia into gaseous hydrogen and nitrogen. This process emits zero carbon dioxide. However, carbon intensities of feedstock ammonia and electricity contribute to the life-cycle carbon intensity per kilogram of hydrogen produced.

$$2NH_3 \longrightarrow N_2 + 3H_2$$

Steam Methane Reforming (SMR) – Traditional methane reforming process involving the decomposition of methane in the presence of a catalyst at high temperature and pressure to produce hydrogen and carbon dioxide. Carbon dioxide is produced both from the combustion of natural gas to provide heat to the reaction and from the conversion of methane to carbon dioxide and hydrogen. This process can be modeled to include carbon capture and storage.

Heat from natural gas combustion results in additional CO_2 emissions

$$CH_4 + 2H_20 \longrightarrow 4H_2 + CO_2$$

Autothermal Reforming (ATR) – Emerging competitor with steam methane reforming for low-carbon hydrogen production. In autothermal reforming, pure oxygen is introduced into the reaction chamber where methane is oxidized to provide reaction energy. This oxidation provides the energy to perform the catalytic reforming process to convert the remaining feedstock methane into hydrogen and carbon dioxide. In this process, additional electricity is required for an air separation unit (ASU) to produce the necessary oxygen. However, the additional operating expenses and capex from ASU is offset by lower carbon capture capex compared to steam methane reforming.

$$CH_4 + O_2 + H_2O \longrightarrow 3H_2 + CO_2$$

Electrolysis – Electrochemical process that utilizes electricity to split water into hydrogen and oxygen. Emissions intensity is based solely on the electricity source for this process.

$$H_2O \longrightarrow H_2 + \tfrac{1}{2}O_2$$

Methane Pyrolysis – High temperature decomposition of methane into hydrogen and solid carbon. This process has no carbon emissions from combustion or from the conversion of methane into hydrogen. However, emissions from the procurement of methane and electricity contribute to the lifecycle emissions intensity of methane pyrolysis.

$$CH4 \longrightarrow 2H_2 + C$$

Thermal Ammonia Splitting – High temperature decomposition of ammonia into hydrogen and nitrogen. This technology is prevalent for small scales at low energy efficiencies (30-50%). Larger scale ammonia decomposition plants are conceptual only with new technologies emerging. Future plant designs anticipate using ammonia as a fuel and a feedstock (similar to SMR and ATR) where the fuel will be burned to produce zero-process-emission heat to crack ammonia into nitrogen and hydrogen.

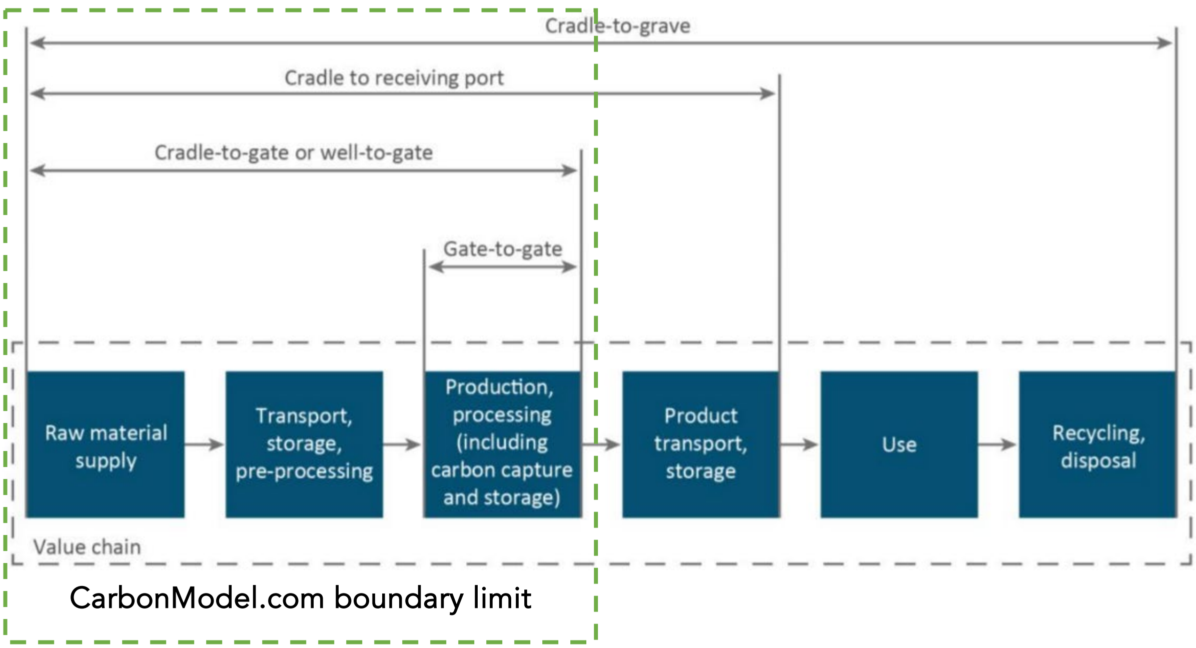
Heat from ammonia combustion results in no additional CO_2 emissions

$$2NH_3 \longrightarrow N_2 + 3H_2$$

Boundary Limit and Functional Unit

Boundary Limit

Carbonmodel.com sets the boundary limit for analysis from cradle to plant gate. Our carbon intensities and cost calculations include all emissions and costs associated with producing one functional unit of product. For hydrogen that is one kg of fuel-cell grade hydrogen at 20 bar. Any additional infrastructure costs or carbon emissions for compression, liquefaction, or conversion to LOHC/ammonia for transport would need to be accounted for downstream.



Functional Unit

Hydrogen: CarbonModel.com's functional unit for the Hydrogen module is 1 kg of fuel cell grade hydrogen (99.999% purity) at 20 bar pressure. This purity and pressure are a close representation of the conditions at the outlet of a PSA unit or electrolyzer.

Calculation Engine Overview

System Cost

System cost consists of hydrogen production plant costs and any additional CO_2 capex costs. Plant costs are driven by modeled plant size and capacity costs (given in $/kg/d or $/kw for electrolyzers). CO_2 capex costs depend on the emissions related to plant processes (defined as stoichiometric CO_2 emissions from CH_4 combustion and conversion to Hydrogen – there are no process emissions for P-DA, Electrolysis, Methane Pyrolysis, or Thermal Ammonia Splitting).

Ex: SMR w/ CCUS

	Hydrogen System Capex	
A	Capacity kg/d	1,000
B	Capacity Cost $/kg/d	$1,000
C	(A)*(B) = (C)	$1,000,000
	CO_2 Capex	
D	Methane Input (mmbtu/kg H_2)	.18
E	Emissions from CH_4 conversion (kg CO_2 / mmbtu CH_4)	53.08
F	Total CO_2 Emitted (Tons / year) = (A)*365*(D)*(E)/1,000	~3,500
G	CO_2 Capture %	90%
H	Total CO_2 Capacity Required (tons per year) (F)*(1-G) = (H)	3,150
I	CO_2 Capex Costs ($ / ton / year)	$250
J	(H)*(I) = (J)	$787,500

Total Costs = C+J = $1,787,500. However, our engine rounds outputs to the nearest $10,000 for simplicity, so the output shown would be $1,790,000. If CO_2 capture percentage were set to zero, the system cost would be $1,000,000 reflecting the hydrogen capex only.

Product CI

Product CI is a simple calculation where we take the required inputs per kg of H_2 and multiply by the chosen reference point to get feedstock emissions and add any process emissions (net of CO_2) capture.

Ex: P-SMR with CCUS (90% CCUS; CNG In-State: 6.33kgCO_2e/MMBtu; Solar PV: 48 gCO_2e/kwh)

Process Emissions	
Methane Input (MMBtu / kg H_2) (A)	.115
CO_2 from conversion (kg CO_2 / MMBtu CH_4) (B)	53.08
CO_2 Capture % (C)	90%
Emissions (kg/kg H_2) = (A)*(B)*(1-C) = (D)	0.61

Methane Feedstock Emissions	
Methane Input (MMBtu / kg H_2) (E)	.115
Feedstock cradle-to-gate emissions (kg CO_2e/MMBtu) (F)	6.33
CH_4 Feed Emissions (kg/kg H_2) = (E)*(F) = (G)	0.73

Electricity Feedstock Emissions	
Electricity Input (kwh / kg H_2) (H)	15
Feedstock cradle-to-grave emissions (kgCO_2e/kwh) (I)	0.048
Electricity Emissions (kg/kg H_2) = (H)*(I) = (J)	0.72

Total carbon intensity for this configuration would be D+G+J = 2.06 kg CO_2e / kg H_2

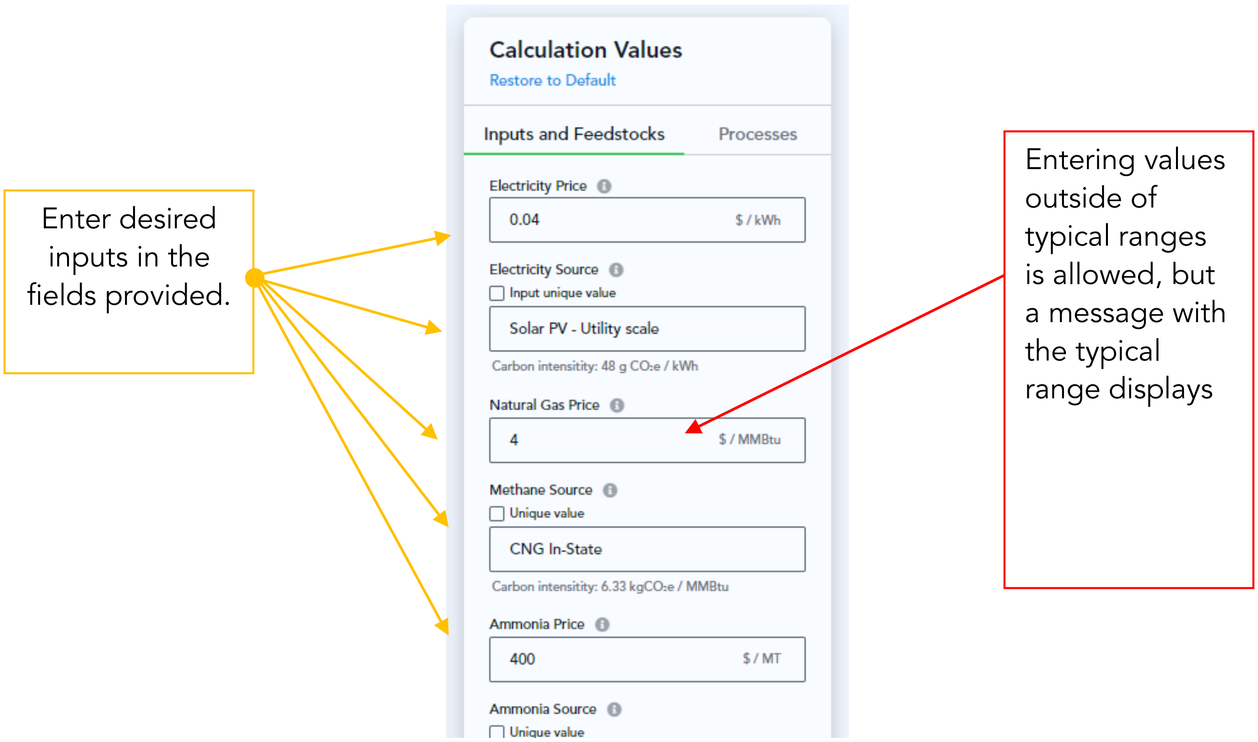
System Parameters

System parameters consist of **generic inputs** applied to each process such as the price / source of inputs, system utilization / size, useful life, and discount rate as well as **process specific inputs** unique to each process such as system capex, feedstock consumption and carbon capture percentage.

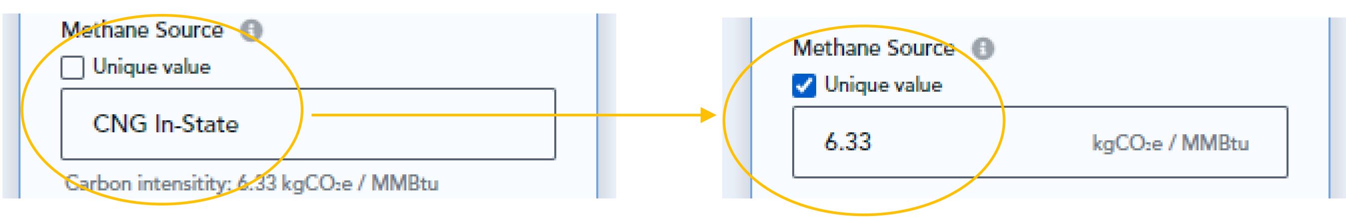
Adjust input values under the **Calculation Values** tab on the right of the screen.

Toggle between generic **Inputs and Feedstocks** or unique chemical **Processes** by selecting the preferred sub-tab.

Select the desired inputs in the **Calculation Values** tab. If an input is outside the range typically observed in practice, a message displays that includes the typical range.



Feedstock intensity inputs include all emissions from well to plant gate including any embodied emissions related to extraction, processing and transport, and fugitive emissions. The input selections are based on reference points from publicly available data. We have included a toggle for users to input their own carbon intensities if desired.



Keeping **Unique value** unchecked results in using a reference point, while checking the box enables a unique input.

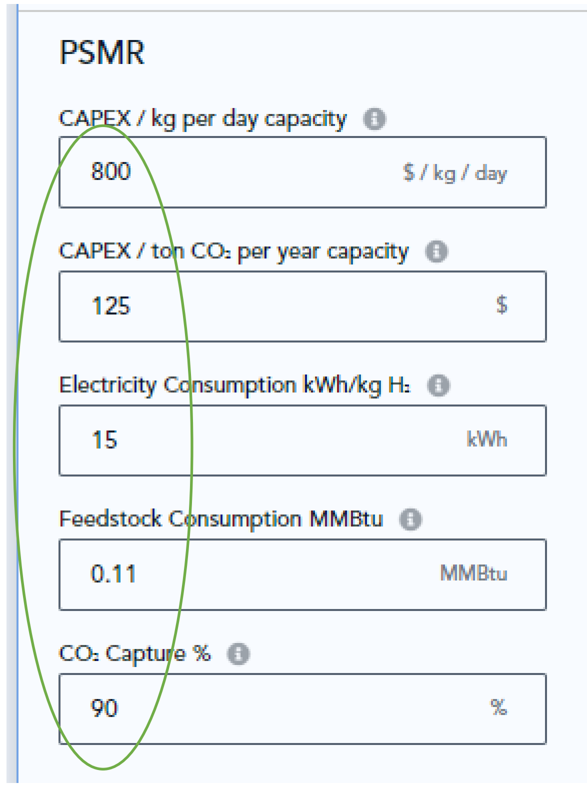
Generic Inputs

Input	Description	Unit	Typical Range
Electricity Price	price of electricity	$ / kwh	$0.03 - $0.20
Electricity Source	Electricity source and resulting carbon intensity	$kgCO_2e/kwh$	N/A
Natural Gas Price	Price of natural gas (city gate)	$ / mmbtu	$2.50 - $15.00
Natural Gas Source	Natural gas source and resulting carbon intensity	$kgCO_2e/mmbtu$	N/A
Ammonia Price	Price of ammonia	$ / ton	$ 300 - $1,000
Ammonia Source	Choice of source of ammonia and resulting carbon intensity	$kgCO_2e$ / kg NH_3	N/A
Water Price	Price of water	$/gallon	$0.01 - $0.10
Carbon Tax	Tax on uncaptured process carbon emissions	$/ton CO_2 emitted	$0 - $250
System Utilization	% Of year that system is producing hydrogen	%	25% - 99%
System Size	Nameplate production capacity	kg H_2/day	100 – 200,000
Depreciation Time	Useful life of system – used to calculate capex costs per kilogram using equivalent annual cost method	Years	7 - 30
Discount rate	Weighted average cost of capital – used to calculate capex costs per kilogram H2 using equivalent annual cost method	%	4% - 20%
CCUS Cost per ton	Opex costs to store carbon dioxide	$ / ton CO_2e	$30 – $200
O&M RateTransmission Form Factor	Yearly O&M to operate the hydrogen production systemCarbon intensity to transport hydrogen from the plant site to end user. "None" assumes on-site hydrogen production	% Of plant capexkgCO_2e / kg H_2	3% - 8%
O&M Rate	Yearly O&M to operate the hydrogen production system	% Of plant capex	3% - 8%

Process Specific Inputs

Select process specific inputs such as system capex, additional CCUS capex, and feedstock required to produce 1kg H_2 in this pane. These parameters are set to default values for convenience. Enter unique values as desired.

Use the default values or update them as needed.



Unique Input Default Values

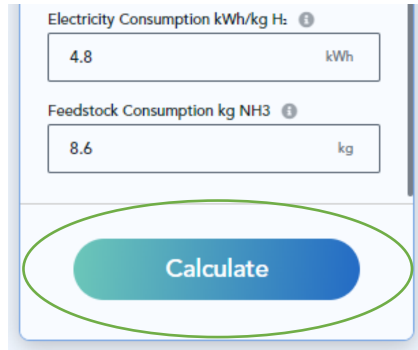
Process	Input	Unit	Default Value	Description
P-SMR	Capex	$/kg H_2/d	$800	$800 is Syzygy's internal view of full system costs at mature commercial operations
	CO_2 Capex	$/ton CO_2/year	$125	Syzygy's no-combustion process results in an ultra-pure CO_2 off gas stream that can be easily captured; therefore, $125/ton cost is the same as ATR (ATR also produces an easily captured CO_2 stream and is ~75% cheaper than SMR)
	Electricity	Kwh / kg H_2	15	Estimates for electricity consumption for a fully optimized and developed system
	Methane	Mmbtu / kg H_2	.11	Stoichiometric requirement per kg of H_2 produced
	CO_2 Capture %	%	90	Current MDEA based technologies can reach upwards of 90% CO_2 captured

Process	Input	Unit	Default Value	Description
P-DA	Capex	$/kg H_2/d	$1000	$1,000 is Syzygy's internal view of full system costs at mature commercial operations
	Electricity	Kwh / kg H_2	10	Estimates for electricity consumption for a fully optimized and developed system
	Ammonia	Kg NH_3 / kg H_2	5.7	Stoichiometric requirement per kg of H_2 produced
SMR w/ CCUS	Capex	$/kg H_2/d	$1,000	$1000 is the median price for a large-scale installation
	CO_2 Capex	$/ton CO_2/year	$300	CCUS costs for large-scale SMR installations observed in literature
	Electricity	Kwh / kg H_2	1	electricity consumption based off public literature
	Methane	Mmbtu / kg H_2	.18	Fuel and feedstock inputs of methane for SMR
	CO_2 Capture %	%	90	Current MDEA based technologies can reach upwards of 90% CO_2 captured
Auto Thermal Reforming w/ CCUS	Capex	$/kg H_2/d	$1,250	$1,250 is the median price for a large-scale installation
	CO_2 Capex	$/ton CO_2/year	$125	CCUS costs for large-scale ATR installations pulled from literature
	Electricity	Kwh / kg H_2	3.6	electricity consumption based off public literature
	Methane	Mmbtu / kg H_2	.20	Fuel and feedstock inputs of methane for ATR
	CO_2 Capture %	%	90	Current pre-combustion-based technologies can reach upwards of 99% CO_2 captured; 90% is default to provide same basis as SMR w/ CCUS
Electrolysis	Capex	$/kwh	$700	Represents current costs for mature alkaline technology
	Electricity	Kwh / kg H_2	50	Electricity cost for best-in-class alkaline technology
	Water	Gallon / kg H_2	2.4	Approximately 9kg/H_2O per kg H_2 produced
Methane Pyrolysis	Capex	$/kg H_2/d	$2,200	Estimated capacity cost for commercial plant
	Electricity	Kwh/ kg H_2	11	Estimated electricity consumption
	Feedstock	Mmbtu / kg H_2	.22	Stoichiometric feedstock requirement
Thermal Ammonia Splitting	Capex	$/kg H_2/d	$1000	Estimates for long term, large-scale installation costs which are projected to be like SMR w/out CCUS costs
	Electricity	Kwh / kg H_2	4.8	Electricity consumption based off public literature
	Ammonia	Kg NH_3 / kg H_2	8.6	Stoichiometric requirement per kg of H_2 produced plus additional ~2.9kg NH_3 required as a fuel

Calculation and Output Comparison

After the inputs are selected, click **Calculate** to calculate the net cost in $ per kg H_2 produced and carbon emissions in kg CO_2e per kg H_2 produced.

Click **Calculate** after selecting parameters to see the results.



Production data is displayed in table and graph format. Selecting the column header at the top of the data table will update the chart below to reflect the selected column. Users may also download a CSV file of the data by selecting the **Download Data** button.

Download data for further analysis by selecting **Download Data**

The selected column is highlighted.

Select which parameter to display using this row

Production Data | Filter | Download Data | Levelized Cost of Hydrogen | Carbon Footprint

Processes	Levelized Cost of Hydrogen ($ / kg H_2)	Carbon Footprint (kg CO_2e / kg H_2)
Photocatalytic Steam Methane Reforming (PSMR)	$1.85	2.00 kg
Photocatalytic Decomposition of Ammonia (PDA)	$3.15	1.03 kg
Steam Methane Reforming with CCUS (SMR)	$2.20	2.14 kg
Electrolysis	$2.73	2.40 kg
Methane Pyrolysis	$2.36	1.92 kg
Auto-thermal Reforming w/CCUS (ATR)	$2.33	2.50 kg
Thermal Ammonia Splitting (TAS)	$4.10	1.06 kg

Additional Outputs

Access additional analysis tools by scrolling to the bottom of the page and selecting one of the available buttons.

Scenario Analysis

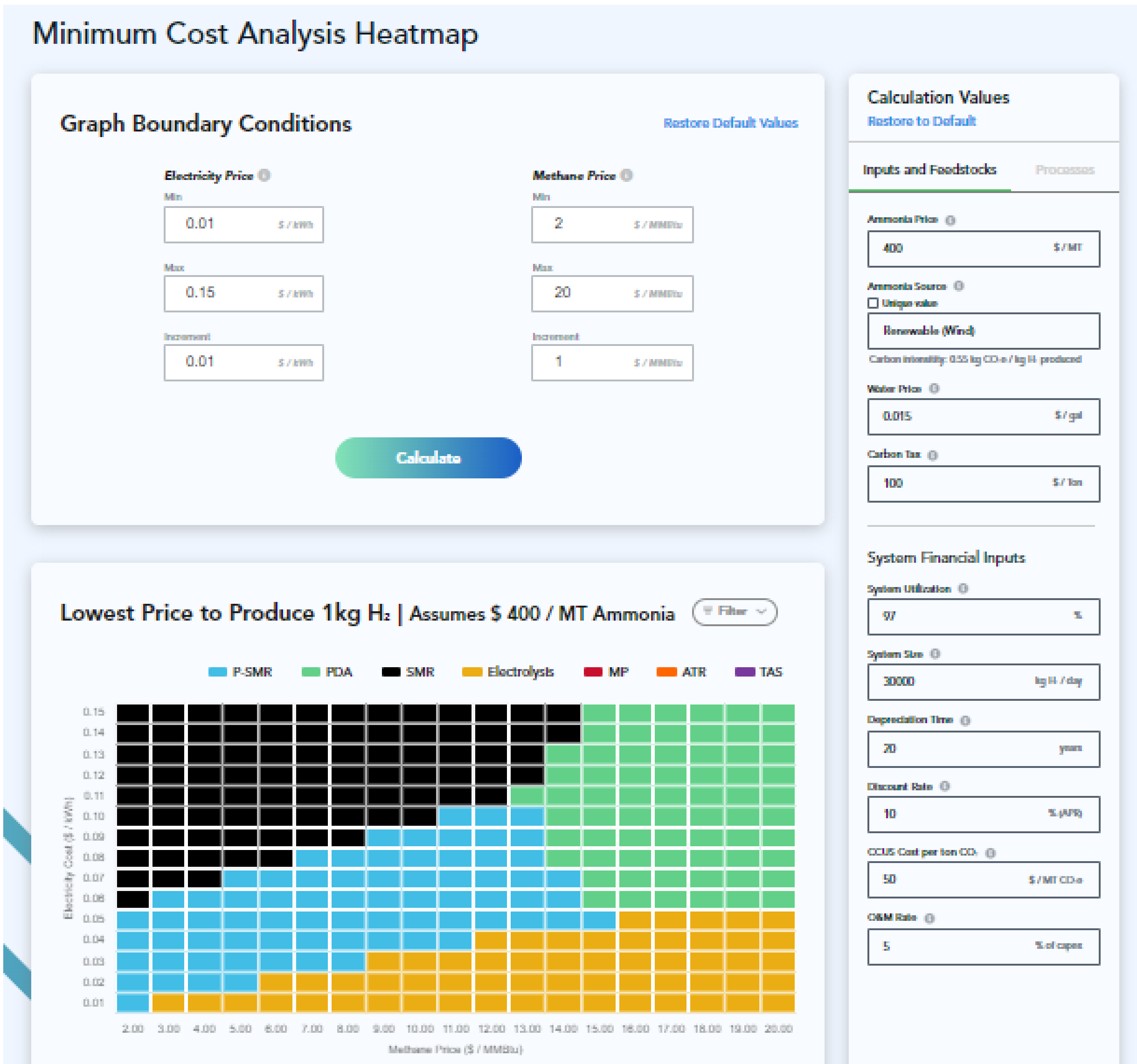
The **Scenario Analysis** button displays a page that enables you to compare multiple scenarios. This is particularly useful for understanding sensitivities, boundaries, and high-level outcomes as variables change (feedstock price, capex, input consumption etc.).

Compare up to three scenarios and import data from the main calculator page, or start fresh for each scenario by clicking the **Add Data** button under each option. Results are shown at the bottom of the page and can be compared by option or process. "By option" will compare each process across the same scenario as the main page. "By process" compares the same process across different scenarios. This function enables you to determine the low cost and/or CI option among many processes and can be used to plot the journey of expected costs as technologies mature.

Minimum Cost Analysis

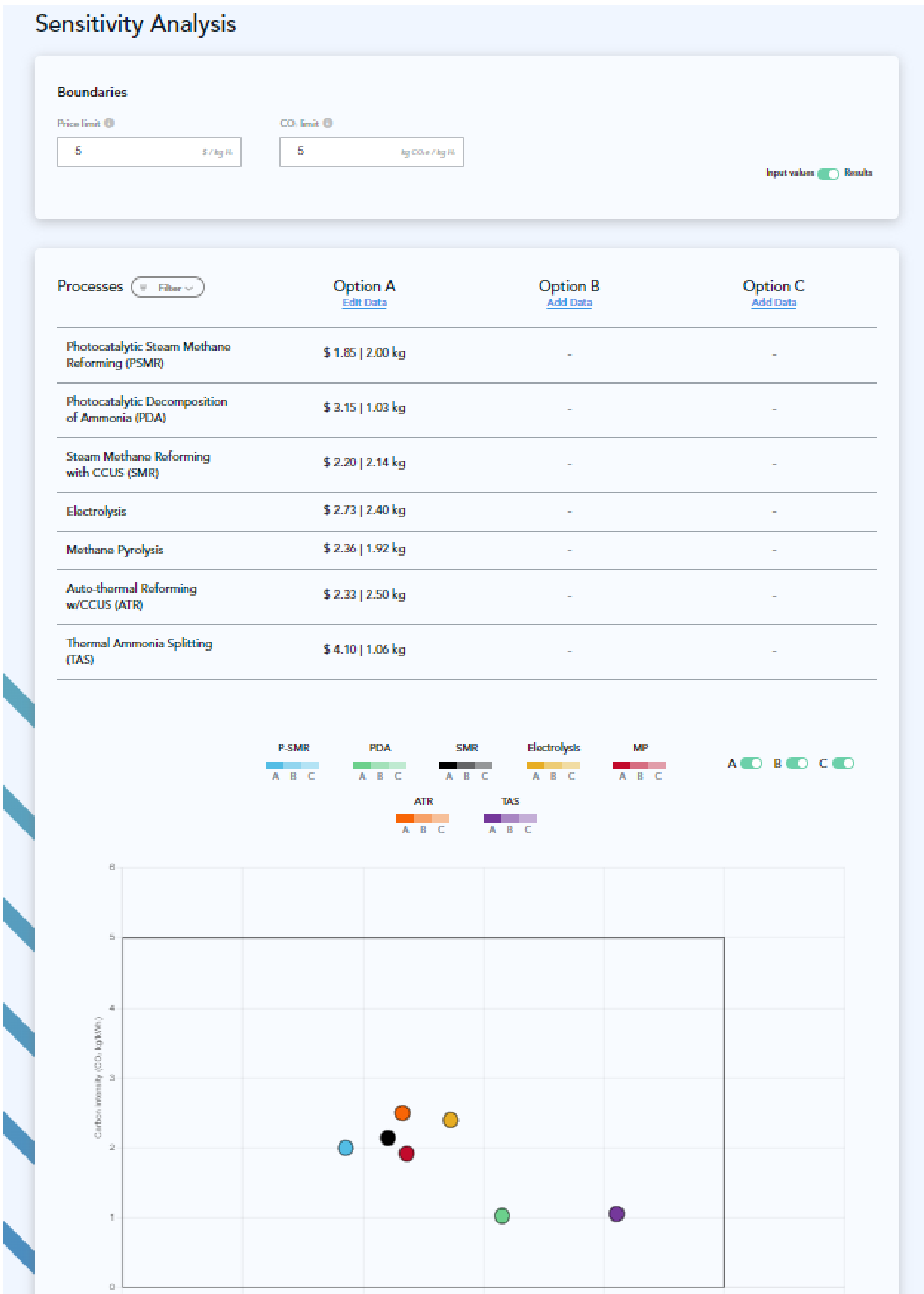
The **Minimum Cost Analysis** button displays a sensitivity analysis on major inputs methane and electricity. Enter default process-specific inputs and select which processes to compare to show a visual heatmap of the results. In addition to the typical inputs, you can also select boundary conditions for the chart and filter processes to evaluate only the technologies of interest.

The output of this chart illustrates which process provides the minimum cost given the feedstock price scenario. Looking at the graphic below in the scenario for $10/mmbtu natural gas and $0.05/kwh electricity, Syzygy P-SMR is the low-cost option. By hovering over the colored tile, you can also see the actual cost for the low-cost and 2nd lowest cost option.



Sensitivity Analysis

The **Sensitivity Analysis** button focuses on feedstock prices. In this window, you can select boundary conditions for maximum price and CI, then change feedstock price and CI to arrive at the final levelized cost and carbon intensity. Changing inputs in options A, B, and C moves the bubbles on the chart to illustrate which technologies meet cost and carbon intensity preferences.



Appendix A: Methane and Electricity Emission Sources

A.1: Well-to-tank methane emissions [1]

	Carbon Intensity	
Methane Source	g CO2 / MJ	kg CO2 / mmbtu
Interstate CNG	10	10.6
Interstate LNG	25	26.4
CNG In-State	6	6.3
LNG In-state	16	16.9
LNG Max	75	79.1
RNG - Dairy Gas	-70	-73.9
Landfill Gas	-55	-58.0

A.2: IPCC estimates of emissions related to electricity production[2(figA.III.2)]

Options	Direct emissions	Infrastructure & supply chain emissions	Biogenic CO_2 emissions and albedo effect	Methane emissions	Lifecycle emissions (incl. albedo effect)
	Min/Median/Max	Typical values			Min/Median/Max
Currently Commercially Available Technologies					
Coal—PC	670/760/870	9.6	0	47	**740/820/910**
Gas—Combined Cycle	350/370/490	1.6	0	91	**410/490/650**
Biomass—cofiring	n.a. [ii]	–	–	–	**620/740/890** [iii]
Biomass—dedicated	n.a. [ii]	210	27	0	**130/230/420** [iv]
Geothermal	0	45	0	0	**6.0/38/79**
Hydropower	0	19	0	88	**1.0/24/2200**
Nuclear	0	18	0	0	**3.7/12/110**
Concentrated Solar Power	0	29	0	0	**8.8/27/63**
Solar PV—rooftop	0	42	0	0	**26/41/60**
Solar PV—utility	0	66	0	0	**18/48/180**
Wind onshore	0	15	0	0	**7.0/11/56**
Wind offshore	0	17	0	0	**8.0/12/35**
Pre-commercial Technologies					
CCS—Coal—Oxyfuel	14/76/110	17	0	67	**100/160/200**
CCS—Coal—PC	95/120/140	28	0	68	**190/220/250**
CCS—Coal—IGCC	100/120/150	9.9	0	62	**170/200/230**
CCS—Gas—Combined Cycle	30/57/98	8.9	0	110	**94/170/340**
Ocean	0	17	0	0	**5.6/17/28**

A.3: Estimates of well to tank emissions from ammonia

Assumes ~50kwh of renewable electricity needed to provide hydrogen and nitrogen feedstocks to produce ammonia that can then be decomposed into nitrogen and hydrogen. We will utilize the emissions table from IPCC to inform our emission intensities for wind onshore, solar-utility and biomass-dedicated green ammonia pathways. This results in roughly .09, .38, and 1.84 kg CO_2 / kg ammonia for wind, solar, and biomass procurement pathways, respectively.

Per ammoniaindustry.com, North American ammonia producers emit 2.13 kg CO_2 / kg ammonia while Chinese producers emit 4.43 kg CO_2 / kg ammonia.

1. Hagos DA, Ahlgren EO. Well-to-wheel assessment of natural gas vehicles and their fuel supply infrastructures – Perspectives on gas in transport in Denmark. *Transp Res Part Transp Environ*. 2018;65:14-35. doi:10.1016/j.trd.2018.07.018

2. Schlömer S, Hänsel G, de Jager D, Neelis M. IPCC - Technology-specific Cost and Performance Parameters. :28. https://www.ipcc.ch/site/assets/uploads/2018/02/ipcc_wg3_ar5_annex-iii.pdf