

Supplemental Information

Advanced Pathways for Hydrogen Production: A collective view from a technical experts meeting

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SI Figure S1: Emerging definition of bio-hydrogen (bioH₂).

SI Figure S2: Detailed process flow diagram (PFD) showing 50 MT/day BioH₂ production from solid food waste (SFW) through integrated dark fermentation and microbial electrolysis cell.

SI Table S1. Summary of MEC internal resistance and corresponding parameters.

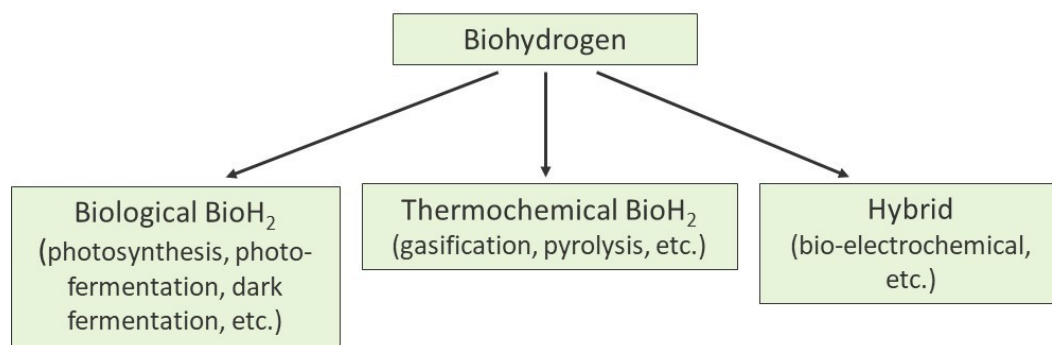
SI Table S2. Data and assumptions for figure 5.

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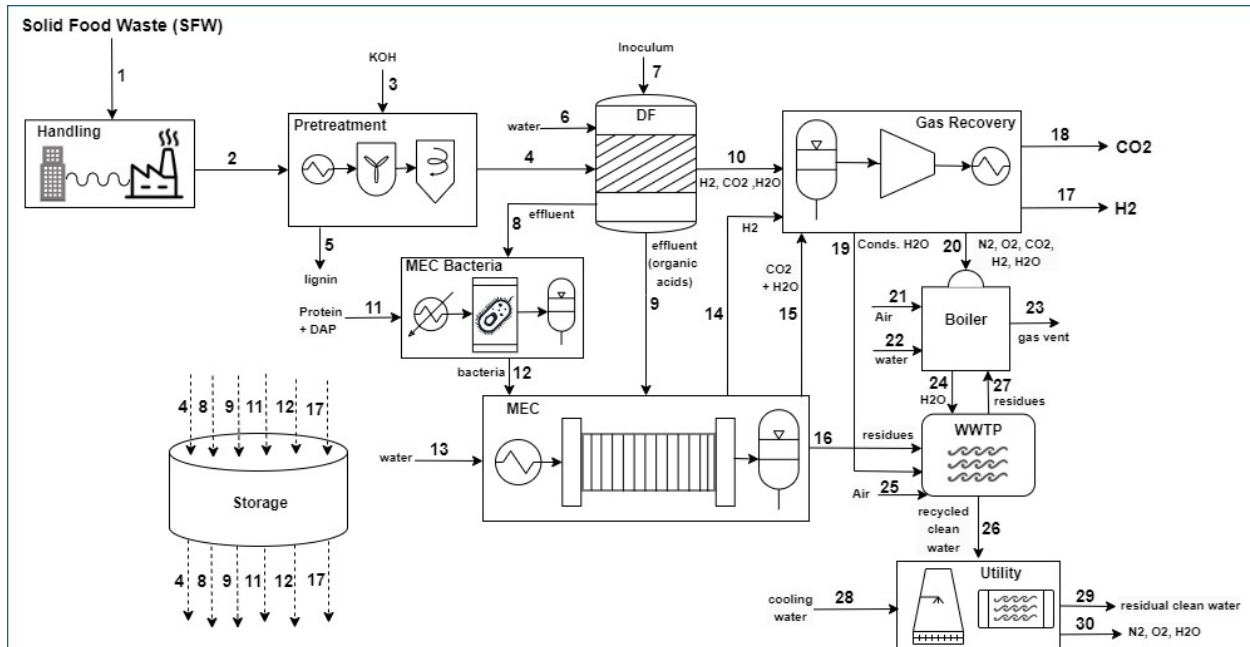
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SI Table S6. Material usage per $MW_{Radiation}$ and costs in 2024 USD.



SI Figure S1: Emerging definition of bio-hydrogen (bioH₂).

This emerging definition of bioH₂ encompasses a broader scope and contrasts earlier literature which limited the term bioH₂ to H₂ produced biologically by microorganisms. Biological bioH₂ generally refers to hydrogen production catalyzed by microbes, which include hydrogen produced from splitting water molecules through light-driven reactions by photosynthetic organisms as well as fermentative conversion of biogenic/organic and waste materials to hydrogen without any light input. Thermochemical bioH₂ generally refers to hydrogen produced from organic biomass through means of gasification, pyrolysis, etc. Bio H₂ also includes hydrogen produced from organic substances through a combination of fermentation, electrochemical, or other approaches.



SI Figure S2: Process flow diagram (PFD) showing 50 MT/day BioH₂ production from solid food waste (SFW) through integrated dark fermentation (DF) and microbial electrolysis cell (MEC).

Figure S2 shows the process flow diagrams of 50 MT/day bioH₂ production process using solid food waste as a feedstock. Below is a description of the various process units:

- Handling: feedstock handling and transportation to pretreatment unit.
- Pretreatment: grinding and treating SFW with KOH to enhance the feedstock-to-H₂ yield. The insoluble food waste content is separated and disposed of.
- Dark fermentation (DF) and gas recovery: fermentation of the treated waste in the absence of O₂ to generate H₂, CO₂, organic acids, and other by-products, such as ethanol. The gaseous product from DF is fed to the gas recovery unit for separating CO₂ and H₂ using a Selexol unit and pressure swing adsorption (PSA).
- Microbial electrolysis cell (MEC): bacteria produced from the effluents from DF as well as protein and diammonium phosphate (DAP) are fed to MEC. The organic acids in DF effluent are utilized by microorganisms at the anode of MEC to generate electrons and protons at a low voltage. The electrons go to the cathode side and reduce protons to produce H₂. The MEC effluent and remaining impurities are fed to the Wastewater treatment plant (WWTP).
- Boiler, Wastewater treatment and utility: The boiler generates steam and onsite electricity via the combustion of waste from DF and MEC. WWTP treats wastewater before its discharge to the environment, while a portion of the treated water is recirculated to meet process water requirements. The utility unit includes a cooling tower and supply of the treated water from WWTP for process requirements.
- Storage: stores process chemicals.

SI Table S1. Summary of MEC internal resistance and corresponding parameters

Conditions	Previous MEC	MEC Compact
Solution & Membrane: R_{Ω} ($m\Omega m^2$)	14	0.9
Anode: R_{An} ($m\Omega m^2$)	16	1.4
Cathode: R_{Cat} ($m\Omega m^2$)	22	5.3
Total: R_{int} (Ωm^2)	52	7.6

Conditions	28 mL	85 L -active area
Electrode spacing (cm)	1.3	1.3
Solution cond. (mS/cm)	1.2	1.5
Solution: R_{Ω} ($m\Omega m^2$)	118	87
Anode: R_{An} ($m\Omega m^2$)	71	238 (3x)
Cathode: R_{Cat} ($m\Omega m^2$)	66	555 (8x)
Total: R_{int} ($m\Omega m^2$)	255	880
Power (mW/m^2)	304	101

SI Table S2. Data and assumptions for figure 5.

Figure 5						
Top						
Panel Based						
Assumptions						
Case	-	1	2	3	4	5
Label	-	10 MTD Plant	-> 2030 Perf.	-> 100 MTD Plant	-> 2040 Perf.	-> 500 MTD Plant
Concept	-	Base Case	2030 Technology	Commercial -Scale Deployment	2040 Technology	Large-Scale Deployment
Plant Capacity (Average over Lifetime)	MTD	10	10	100	100	500
Systems per Plant	# / plant	1	1	3	3	5
Solar to Hydrogen (STH) Efficiency (BOL)	%	5.5%	10.0%	10.0%	25.0%	25.0%
Catalyst Lifetime	year	5	5	5	10	10
Housing Lifetime	year	10	10	10	20	20
Performance Degradation	% / 1000 hr	5.0%	2.5%	2.5%	1.2%	1.2%
Performance Degradation	% / year	8.8%	4.4%	4.4%	2.0%	2.0%
Average Reactor STH	%	4.3%	8.9%	8.9%	22.5%	22.5%
Reactor Cost	\$/reactor	300	300	300	300	300
Refurbishment Cost	\$/reactor	100	100	100	100	100
Levelized Cost of Hydrogen						
Capital Costs - Direct Costs	2020 \$ / kg H2	\$1.18	\$0.65	\$0.59	\$0.32	\$0.28
Capital Costs - Indirect Costs	2020 \$ / kg H2	\$0.45	\$0.28	\$0.15	\$0.09	\$0.06
Capital Costs - Land	2020 \$ / kg H2	\$0.52	\$0.22	\$0.19	\$0.05	\$0.06
Capital Costs - Yearly Unplanned Replacements	2020 \$ / kg H2	\$0.15	\$0.09	\$0.07	\$0.04	\$0.03
Capital Costs - Specified Replacements	2020 \$ / kg H2	\$2.07	\$1.00	\$1.00	\$0.14	\$0.14
Fixed Operating Costs - Labor	2020 \$ / kg H2	\$0.43	\$0.46	\$0.08	\$0.14	\$0.04

Fixed Operating Costs - Property Tax and Insurance	2020 \$ / kg H2	\$0.69	\$0.38	\$0.31	\$0.16	\$0.13
Fixed Operating Costs - Material Costs for Maintenance and Repairs	2020 \$ / kg H2	\$0.59	\$0.33	\$0.30	\$0.17	\$0.14
Utilities - Electricity	2020 \$ / kg H2	\$0.09	\$0.09	\$0.08	\$0.08	\$0.07
Utilities - Water	2020 \$ / kg H2	\$0.01	\$0.01	\$0.01	\$0.01	\$0.01
Decommissioning Costs	2020 \$ / kg H2	\$0.01	\$0.01	\$0.01	\$0.00	\$0.00
Total	2020 \$ / kg H2	\$6.18	\$3.52	\$2.78	\$1.21	\$0.97
Figure 5						
Bottom						
Particle Based						
Assumptions						
Case	-	1	2	3	4	5
Label	-	10 MTD Plant	-> 2030 Perf.	-> 100 MTD Plant	-> 2040 Perf.	-> 500 MTD Plant
Concept	-	Base Case	2030 Technology	Commercial -Scale Deployment	2040 Technology	Large-Scale Deployment
Plant Capacity (Average over Lifetime)	MTD	10	10	100	100	500
Systems per Plant	# / plant	1	1	3	3	5
Solar to Hydrogen (STH) Efficiency (BOL)	%	1.0%	5.0%	5.0%	10.0%	10.0%
Catalyst Lifetime	year	1	2	2	5	5
Housing Lifetime	year	10	10	10	20	20
Performance Degradation	% / 1000 hr	5.0%	2.5%	2.5%	1.2%	1.2%
Performance Degradation	% / year	8.8%	4.4%	4.4%	2.0%	2.0%
Average Reactor STH	%	1.0%	4.8%	4.8%	9.5%	9.5%
Reactor Cost	\$/reactor	50	50	50	50	50
Refurbishment Cost	\$/reactor	-	-	-	-	-

H2A Output - Detailed						
Capital Costs - Direct Costs	2020 \$ / kg H2	\$ 2.10	\$0.56	\$0.50	\$0.33	\$0.29
Capital Costs - Indirect Costs	2020 \$ / kg H2	\$1.01	\$0.30	\$0.16	\$0.10	\$0.07
Capital Costs - Land	2020 \$ / kg H2	\$2.34	\$0.41	\$0.35	\$0.13	\$0.13
Capital Costs - Yearly Unplanned Replacements	2020 \$ / kg H2	\$0.29	\$0.08	\$0.06	\$0.04	\$0.03
Capital Costs - Specified Replacements	2020 \$ / kg H2	\$3.50	\$0.53	\$0.53	\$0.08	\$0.08
Fixed Operating Costs - Labor	2020 \$ / kg H2	\$0.43	\$0.46	\$0.08	\$0.14	\$0.04
Fixed Operating Costs - Property Tax and Insurance	2020 \$ / kg H2	\$1.56	\$0.39	\$0.31	\$0.18	\$0.16
Fixed Operating Costs - Material Costs for Maintenance and Repairs	2020 \$ / kg H2	\$0.88	\$0.25	\$0.22	\$0.15	\$0.13
Utilities - Electricity	2020 \$ / kg H2	\$0.09	\$0.09	\$0.08	\$0.08	\$0.07
Utilities - Water	2020 \$ / kg H2	\$0.01	\$0.01	\$0.01	\$0.01	\$0.01
Decommissioning Costs	2020 \$ / kg H2	\$0.02	\$0.01	\$0.00	\$0.00	\$0.00
Total	2020 \$ / kg H2	\$12.23	\$3.08	\$2.32	\$1.24	\$1.02

SI Table S3. Data and assumptions for figure 7.

Figure 7a						
Levelized Cost (\$/kg)						
	Discharge/ Tipping Fee Credits	Capital Costs	Decommissioning Costs	Fixed O & M	Other Variable Costs	Taxes
CW US mix CCS	-5.6	5.5	0	2.2	3.4	0.22
CW RE CCS	-6.3	5.5	0	2.2	3.4	0.21
SFW US mix CCS	-11.3	5.5	0	2.2	3.4	0.22
SFW RE CCS	-2.9	6.4	0	2.5	3.0	0.19

Figure 7b						
Well-to-Gate Emissions (kgCO2e/kgH2)						
	CCS	Onsite Electricity	Nutrients	KOH(PT)	DAP	CSL
CW US mix CCS	-10.9	9.5	2.3	0	0	0
CW RE CCS	-10.9	0	2.3	0	0	0
SFW US mix CCS	-10.9	11.3	0	2.9	0	0
SFW RE CCS	-10.9	0	0	2.9	0	0
NG SMR	9.3					
NG SMR CCS	3.2					
PEM US Mix	26					

SI Table S4. Data and assumptions for figure 8.

Currently achieved		12.4	0
Membrane price	\$500 to \$300/m ²	11.5	0.890681016
	\$300 to \$100/m ²	10.6	0.890681016
Electrode price	\$200 to \$100/m ²	9.7	0.890184694
	\$100 to \$50/m ²	9.3	0.445092347
MEC current density	66 to 300 A/m ²	7.5	1.771371412
	300 to 500 A/m ²	7.3	0.199348563
Electricity price	¢7 to ¢3.5/kWh	6.4	0.916271221
Corn stover price	\$96 to \$48/tonne	5.6	0.799088674
Potential tipping and discharge fees obtained from solid food waste (SFW) & cheese wastewater (CW)	Tipping fees \$0.03/kg SFW	1.7	3.876124422
	Discharge fees \$0.06/kg CW	-0.8	2.5

SI Table S5. Data and assumptions for figure 12.

Cost Category	Unit	Baseline Variable	Target Variable	Waterfall Energy Cost (\$ per metric ton)	Waterfall Conversion Capital (\$ per metric ton)	Total Levelized Cost of H2 (\$ per metric ton)
Baseline Costs	\$ per metric ton			5070.6	1528.7	6599.3
material	\$ per MW_radiation	189,300	125,000	3348.3	1528.7	4877.0
multiple_radiation	-	5	2	1339.3	1528.7	2868.0
discount rate	% per year	9%	7%	1170.4	1343.2	2513.6
lifetime	years	25	30	1115.2	1282.6	2397.8
fixed OpEx_radiation	% per year	2.50%	1.50%	1009.6	1282.6	2292.2
energy utilization	MWh_radiation per metric ton	100	80	807.7	1282.6	2090.3
material intensity_conversion	metric ton per cubic meter	2	1.5	807.7	962	1769.7
material cost_conversion	\$ per metric ton	5000	2500	807.7	481	1288.7
multiple_conversion	-	6	4	807.7	320.7	1128.4
deltaDelta per atom	mole H2 per mole atom MOx per cycle	0.01	0.015	807.7	213.8	1021.5
cycles per hour	per hour	6	8	807.7	160.3	968.0
active fraction	-	0.17	0.2	807.7	136.3	944.0
capacity factor_conversion	hours per year	2000	2200	807.7	123.9	931.6
fixed OpEx_conversion	% per year	3%	2%	807.7	112.7	920.4

TCH Technoeconomic Considerations and Cost Drivers

Thermochemical hydrogen (TCH) systems present a promising long-term pathway for clean hydrogen production, particularly in regions with abundant high-temperature renewable or nuclear heat. A robust technoeconomic analysis (TEA) framework is essential to guide developments and benchmark TCH alongside electrolysis and other emerging pathways. Recent TEA studies have identified several key cost drivers and performance parameters that determine the levelized cost of hydrogen (LCOH₂):

- Redox Material Cost and Performance: Material degradation, material costs, redox capacity, and fast kinetics along with financial recovery factors significantly influence system cost, system longevity and replacement costs.
- Reactor Efficiency and Heat Management: High-temperature operation (>1500 °C) imposes strict demands on reactor design, materials, and insulation. Without efficient heat recuperation, solar-to-hydrogen conversion efficiencies remain low <6%, and energy consumption can exceed 150 kWh_{th} kg⁻¹ H₂. Achieving low energy utilization—on par with electrolysis—requires better thermal integration and good heat recovery.
- Capital Intensity and Scale: Capital expenditures are dominated by the receiver-reactor subsystem and heliostat field. Unlike electrolysis, TCH has no fuel cost if powered directly from concentrated solar and minimal O&M, but it must spread capital over fewer annual full-load hours unless capacity factors can improve through part load efficiency gains or thermal storage is achieved.
- System Configuration and Flexibility: The two-step nature of redox cycles allows for intrinsic separation of hydrogen and oxygen, avoiding downstream gas separation costs of H₂ from O₂. Furthermore, TCH systems can be coupled with gas storage to decouple hydrogen input to downstream processing from the solar input, enabling flexible operation without requiring thermal energy storage at extreme temperatures.
- Deployment Strategy: TCH may be most competitive when co-located with syngas- or hydrogen-based chemical production (e.g., ammonia, methanol, dimethyl ether, liquid (drop-in) hydrocarbons), where hydrogen is immediately consumed, and heat integration is feasible. These industrial synergies can improve overall process economics and energy utilization.

Levelized Cost of Solar Radiation Delivered (LCOSR)

The solar radiation delivery subsystem comprises only the heliostat field and the tower for a concentrating solar plant. To determine the Levelized Cost of Solar Radiation (LCOSR)

$$LCOSR = CAPEX (USD/MW_{Radiation}) \times \frac{\left(CRF \left(\frac{1}{yr} \right) + Fixed\ O\&M \left(\frac{1}{yr} \right) \right)}{Capacity\ Factor\ (hr/yr)}$$

Inputs

- CAPEX (heliostat + tower only): \$946,500 per MW_{radiation} delivered at the aperture of the receiver

- CRF: e.g., 10.2% (lifetime(n)=25 years @ discount rate (r)=9%) $CRF = \frac{r(1+r)^n}{(1+r)^n - 1}$
- Fixed O&M: 2.5% of CAPEX
- Capacity factor: 2,367 hours per year (or 27%)

Result: LCOSR=50.8 $USD/MWh_{Radiation}$ or 14.1 USD/GJ

Capacity Factor and DNI Filtering

Calculate the capacity factor at a given location from typical metrological year data and using a DNI threshold:

$$Capacity\ Factor = \frac{1}{DNI_{DP}} \sum_{j=1}^{8760} DNI_j \times H(DNI_j - DNI_{cutoff})$$

Inputs

- DNI_{DP} is the design point DNI, typically $\frac{1000\ W}{m^2}$
- $DNI_{cutoff} \approx 300-400\ W/m^2$ and $H(x) = 1$ if $x \geq 0$, 0 otherwise
- Material Intensity and CAPEX Breakdown

SI Table S6. Material usage per $MW_{Radiation}$ and costs in 2024 USD.

Material	Intensity (metric ton/ $MW_{Radiation}$)	Unit Cost (USD/metric ton)	Cost Contribution (USD/ $MW_{Radiation}$)
Steel	100	\$750	\$ 75,000
Aluminum	25	\$2100	\$ 52,500
Copper	3	\$8600	\$ 25,800
Glass	60	\$300	\$ 18,000
Concrete	150	\$120	\$ 18,000
Total	338	\$547	\$189,300

These material costs account for \$189,300/ $MW_{Radiation}$. The final installed CAPEX of \$946,500/ $MW_{Radiation}$ is reached through the additive contributions of fabrication, transport, installation, EPC, and contingency assuming that the material costs are 20% of total given the simplicity of this subsystem relative to a full concentrating solar plant, which is ~10-15% and comparable to PV at ~20-30%. Factoring in the materials also facilitates doing lifecycle analyses.

Levelized Hydrogen Conversion Cost (LCOHC)

This subsystem begins at the receiver/reactor aperture and includes everything to produce hydrogen given the energy input. Calculate LCOHC similarly to :

$$LCOHC_{CAPEX}(USD/metric\ ton\ H_2) = CAPEX(USD/MW_{H_2}) \times \frac{\left(CRF\left(\frac{1}{yr}\right) + Fixed\ O\&M\left(\frac{1}{yr}\right) \right)}{Capacity\ Factor\ (hr/yr)} \times \frac{32.7\ MWh_{H_2}}{metric\ ton\ H_2}$$

Here the hydrogen yield is based on Gibbs free energy. Other choices can be used as long as the definition of the CAPEX is consistent. Here we define:

$$Mass\ Energy\ Conversion\ (EC) = \frac{32.7\ MWh_{H_2}}{metric\ ton\ H_2}$$

Determine the energy cost using this conversion factor from delivered energy to H_2 using:

$$LCOHC_{ENERGY} = EUF \left(\frac{MWH}{metric\ ton\ H_2} \right) \times LCOSR$$

$$EUF = 100 \frac{MWH}{metric\ ton\ H_2}$$

Where EUF stands for energy utilization factor. Here we assume that $EUF = 100 \frac{MWH}{metric\ ton\ H_2}$ or ~41% from delivered radiation to hydrogen.

Result:
$$LCOHC_{ENERGY} = \frac{USD\ 5080}{metric\ ton\ H_2}$$

With these assumptions the cost of the energy is ~ \$5/kg H₂. Improving on this estimate would require either a lower levelized cost of heat and/or a lower energy utilization factor.

CAPEX for the Conversion Subsystem

$$CAPEX \left(\frac{USD}{MW_{H_2}} \right) = \frac{Material\ Intensity \left(\frac{metric\ ton}{m^3} \right) \times Material\ Cost \left(\frac{USD}{metric\ ton} \right)}{Power\ Density \left(\frac{MW_{H_2}}{m^3} \right)} \times multiplier$$

Here volume refers to that of the receiver/reactor, encompassing the reduction, solid-solid heat recuperation, and re-oxidation. However, the material intensity includes downstream heat exchangers and separations normalized to the receiver/reactor volume. Decomposing the cost

$$Power\ Density \left(\frac{MW_{H_2}}{m^3} \right) = \frac{\Delta\delta/N_A \times cycles/hour}{f_{Active}} \times \frac{Molar\ Energy\ Conversion \left(\frac{MWh}{mol_{H_2}} \right)}{Molar\ Atomic\ Volume \left(\frac{m^3}{mol_{Atoms}} \right)}$$

The higher the *Power Density*, the lower the cost. The *Power Density* scales linearly with $\Delta\delta/N_A$ and *cycles/hour* and inversely with the active solid fraction. The remaining terms involve a constant conversion factor and the molar volume per atom of active material. Like the molar heat capacity per atom, the molar volume per atom does not vary significantly and therefore can be estimated for most purposes.

Inputs

- Material Intensity: $2 \text{ metric ton} / m^3$
- Material Cost: $USD\ 5000 / \text{metric ton}$
- Multiplier: 6
- Power Density: $0.1 \text{ MW}_{H_2} / m^3$
- CRF: same as above 10.2%
- Fixed O&M: 3% of CAPEX

- Capacity factor: 2000 hours per year (or 22.8%)

$$\text{Result: CAPEX} = \text{USD } 600,000 / \text{MW}_{\text{H}_2}; \text{ LCOHC}_{\text{CAPEX}} = \text{USD } 1295 / \text{metric ton H}_2$$

Capacity Factor for H₂ Conversion Subsystem

Assuming no thermal storage, the hydrogen production subsystem operates synchronously with the energy delivery system. However, the capacity needs to reflect that the productivity is not linear with DNI, since the energy losses are essentially independent of DNI, dominated by re-radiation and convective losses. Hence, the efficiency is generally a decreasing function with DNI.

$$\text{Capacity Factor} = \left(\frac{1}{\varepsilon_{DP} \times \text{DNI}_{DP}} \right) \times \sum_{j=1}^{8760} [\varepsilon(\text{DNI}_j) \times \text{DNI}_j \times H(\text{DNI}_j - \text{DNI}_{\text{cutoff}})]$$

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