

Supporting Information: Techno-Economic Evaluation of Palladium-Membrane Reactors for Industrial-Scale Methane Pyrolysis

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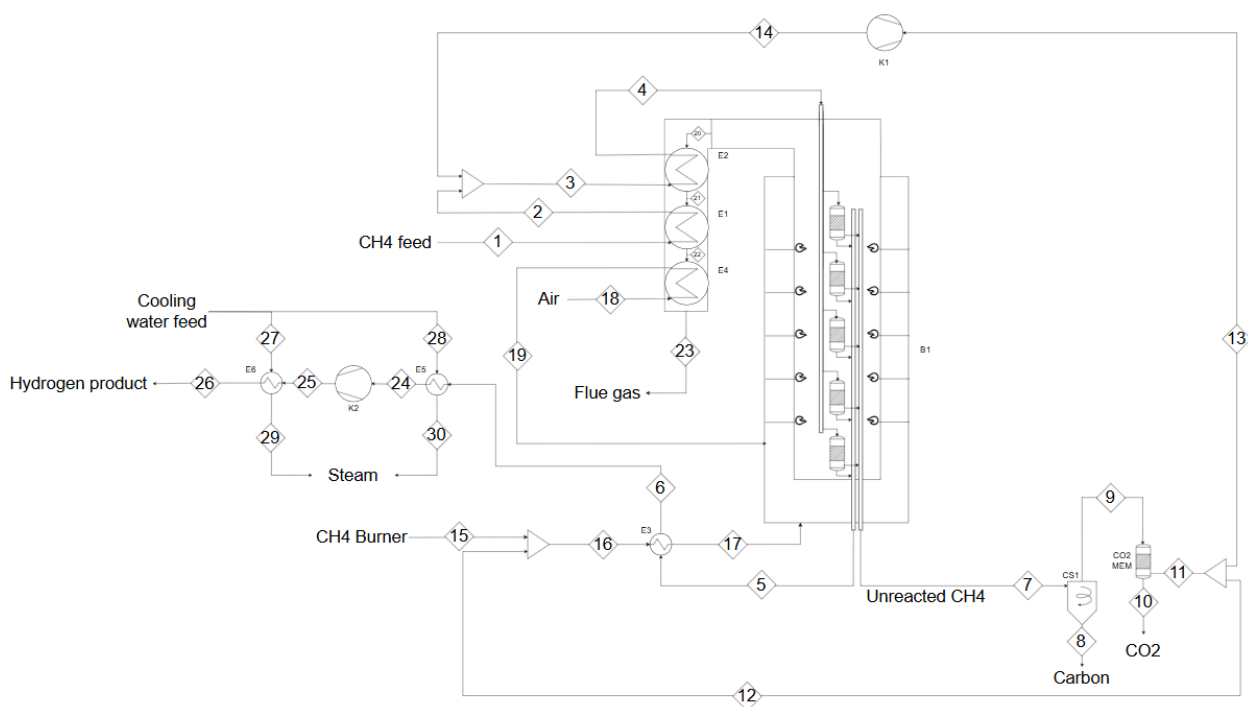


Figure S1. Flowsheet of a heat-integrated methane decomposition plant.

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Table S1. Stream information of the methane decomposition plant.

Stream	Units	1	2	3	4	5	6	7					
W	Kg/h	6272.187	6272.187	13750.68	13750.68	1500	1500	12250.68					
F	Kmol/h	372.0821	372.0821	713.5476	713.5476	744.0919	744.0919	740.885					
Q	M3/h	452.4536	1048.366	2214.304	2754.247	52871.64	50029.06	2118.822					
FH	Kj/s	-7828.66	-5984.52	-6675.02	-4691.16	3371.424	2991.004	-96.7524					
T	C	30	400.5792	470.1589	650	581.2371	519.1236	666.7273					
P	kPa	2001	2000	2000	1999	99.99996	97.99996	1999					
VF		1	1	1	1	1	1	1					
VFm		1	1	1	1	1	1	1					
MW	Kg/Kmol	16.857	16.857	19.27087	19.27087	2.01588	2.01588	21.22705					
Wc[H2]	Kg/h	0.150015	0.150015	49.02922	49.02922	1500	1500	68.30235					
Wc[N2]	Kg/h	52.11657	52.11657	5211.657	5211.657	0	0	5211.657					
Wc[O2]	Kg/h	0	0	0	0	0	0	0					
Wc[C]	Kg/h	0	0	241.2611	241.2611	0	0	4873.961					
Wc[CO]	Kg/h	0	0	54.65481	54.65481	0	0	55.20687					
Wc[CO2]	Kg/h	49.12577	49.12577	171.6615	171.6615	0	0	171.2278					
Wc[CH4]	Kg/h	5654.048	5654.048	7293.433	7293.433	0	0	1655.944					
Wc[C2H6]	Kg/h	469.9117	469.9117	615.004	615.004	0	0	146.5578					
Wc[C3H8]	Kg/h	32.81505	32.81505	55.85877	55.85877	0	0	23.27649					
Wc[C4H10]	Kg/h	8.65067	8.65067	29.02113	29.02113	0	0	20.57623					
Wc[C5H12]	Kg/h	5.369165	5.369165	29.10344	29.10344	0	0	23.97401					
Wc[H2O]	Kg/h	0	0	0	0	0	0	0					
8		9		10		11		12		13		14	
4630.263		7620.42		66.38375		7554.037		75.54037		7478.496		7478.496	
385.5019		355.3831		10.46842		344.9147		3.449147		341.4655		341.4655	
697.2749		1421.548		35.57817		1385.969		12.73277		1260.544		1213.321	
-1198.29		1101.539		-71.3951		1172.934		-7.44119		-736.678		-690.497	
985.4766		666.7273		540.0766		567.6914		567.6906		567.6906		579.0074	
1999		1999		1999.975		1899		1899		1899		2000	
1		1		1		1		1		1		1	
1		1		1		1		1		1		1	
12.011		28.49922		6.341336		22.65089		21.90117		21.90117		21.90117	
0		68.30235		18.92941		49.37294		0.493729		48.87921		48.87921	
0		5211.657		0		5211.657		52.11657		5159.54		5159.54	
0		0		0		0		0		0		0	
4630.263		243.6981		0		243.6981		2.436981		241.2611		241.2611	
0		55.20687		0		55.20687		0.552069		54.65481		54.65481	
0		171.2278		47.45433		123.7735		1.237735		122.5358		122.5358	
0		1655.944		0		1655.944		16.55944		1639.384		1639.384	
0		146.5578		0		146.5578		1.465578		145.0923		145.0923	
0		23.27649		0		23.27649		0.232765		23.04372		23.04372	
2.26E-18		20.57623		0		20.57623		0.205762		20.37046		20.37046	
0		23.97401		0		23.97401		0.23974		23.73427		23.73427	
0		0		0		0		0		0		0	

15	16	17	18	19	20	21	22
1124.731	1200.272	1200.272	39530.04	39530.04	40730.31	40730.31	40730.31
67.24276	70.69191	70.69191	1370.173	1370.173	1442.084	1442.084	1442.084
238.6706	273.2209	2129.328	17263.78	32573.22	57140.86	48551.32	40418.76
-1400.59	-1408.03	-1063.27	50.64338	3048.13	-5998.62	-7982.48	-9826.62
30	55.92415	449.3941	30	295.3478	669.9823	524.1052	383.7971
701.325	701.325	199	200	199	198	197	195
1	1	0.99713	1	1	0.999859	0.999859	0.999859
1	1	0.99797	1	1	0.99994	0.99994	0.99994
16.72643	16.97891	16.97891	28.8504	28.8504	28.24406	28.24406	28.24406
0.027318	0.521048	0.521048	0	0	0.098999	0.098999	0.098999
0.379626	52.49619	52.49619	30322.82	30322.82	30375.32	30375.32	30375.32
0	0	0	9207.218	9207.218	5537.394	5537.394	5537.394
0	2.436981	2.436981	0	0	2.436981	2.436981	2.436981
0	0.552069	0.552069	0	0	0.552069	0.552069	0.552069
0.596401	1.834136	1.834136	0	0	2552.316	2552.316	2552.316
1029.626	1046.186	1046.186	0	0	198.7753	198.7753	198.7753
85.57291	87.03849	87.03849	0	0	16.53731	16.53731	16.53731
5.975759	6.208524	6.208524	0	0	1.17962	1.17962	1.17962
1.575324	1.781086	1.781086	0	0	0.338406	0.338406	0.338406
0.977748	1.217488	1.217488	0	0	1.217488	1.217488	1.217488
0	0	0	0	0	2044.1467 73	2044.147	2044.147
23	24	25	26	27	28	29	30
40730.31	1500	1500	1500	5400	5400	5400	5400
1442.084	744.09	744.09	744.09	299.75	299.75	299.75	299.75
25845.74	19918.95	2730.48	1095.67	5.40	5.40	5.40	5.40
-12824.1	83.50	3528.45	317.84	187.31	187.31	3097.68	3397.93
144.9324	39	605.77	77.65	29.85	29.85	494.02	541.91
194	97	2001	2000	101.325	101.325	100.325	100.325
0.999859	1	1	1	0	0	1	1
0.99994	1	1	1	0	0	1	1
28.24406	2.01588	2.01588	2.01588	18.01526 8	18.015268	18.015268	18.015268
0.098999	1500	1500	1500	0	0	0	0
30375.32	0	0	0	0	0	0	0
5537.394	0	0	0	0	0	0	0
2.436981	0	0	0	0	0	0	0
0.552069	0	0	0	0	0	0	0
2552.316	0	0	0	0	0	0	0
198.7753	0	0	0	0	0	0	0
16.53731	0	0	0	0	0	0	0
1.17962	0	0	0	0	0	0	0
0.338406	0	0	0	0	0	0	0
1.217488	0	0	0	0	0	0	0
2044.147	0	0	0	5400	5400	5400	5400

Table S2. Utilities information of the methane decomposition plant.

Heat Exchangers	Units	E1	E2	E3	E4	E5	E6
Duty	kW	1844.135	1983.857	380.4199	2997.487	2910.37	3210.62
Shell Temp in	C	524.1056	470.1589	581.2376	383.7971	29.85	29.85
Shell Temp out	C	383.7971	650	519.1236	144.9324	494.02	541.91
Tube Temp in	C	30	669.9823	53.8635	30	519.59	605.77
Tube Temp out	C	400.5792	524.1052	449.3941	295.3478	39	77.65
Effeciency	%	75	90	75	75	98	92
Furnace	Units	B1					
Pressure	kPa	199					
Flame Temp	C	1221.462					
Combustion Extent	%	90					
Burner Excess O2	%	12					
Cyclone Scrubber							
Duty	kW	-1699.78					
CO2 Mem							
Duty	kW	-213.388					
Compressor K1							
Pressure in	kPa	1899					
Pressure out	kPa	2000					
Power	kW	46.18035					
Efficiency	%	75					
Compressor K2							
Pressure in	kPa	97.99					
Pressure out	kPa	2000					
Power	kW	3445					
Efficiency	%	75					
Membrane Reactors (10 units)							
Duty	kW	8197.691					

Table S3. CAPEX, OPEX, and LCOH of the methane decomposition plant.

CAPEX

Equipment Cost	USD	Notes
Total	4,850,880	Sum of equipment cost
Other Fixed Capital Costs	USD	Notes
Installation	2,279,913	47% of equipment cost ¹
Instrumentation & Control	485,088	10% of equipment cost
Piping	3,880,704	80% of equipment cost
Electrical	970,176	20% of equipment cost
Buildings & Infrastructure	970,176	20% of equipment cost
Engineering	1,600,790	33% of equipment cost ¹
Construction Expenses	970,176	20% of equipment cost
Contingency	242,544	5% of equipment cost
Yard Improvements	727,632	15% of equipment cost
Sum of equipment and other fixed costs	16,978,079	
Service Facilities	1,697,808	10% of the above
Total Fixed Capital Investment	USD	Notes
Total	18,675,887	Sum of equipment, other fixed costs, and service facilities
Working Capital	USD	Notes
Total	4,668,972	25% of fixed capital
Total Capital Investment	USD	Notes
Total	23,344,858	Sum of Fixed and Working capital

OPEX (Annual)

Item	USD	Notes
Utility	11,942,982	
Raw materials	26,083,976	Main feedstock
Manpower	1,863,690	Includes operators, engineers, supervision
Maintenance	1,867,589	Approx. 10% of fixed costs
	USD	
Total OPEX	41,758,237	

Production Capacity & Costs

Parameter	Value	Notes
Hydrogen Production	13,140 t/year	Operating 90% a year
Operating Hours	7,884 hours/year	
Energy Consumption	44 MJ/kg H ₂	

Cost Metrics	USD	Notes
Levelized Cost of H₂ (LCOH) 3,383 Per ton H₂		

Equipment Cost Breakdown (USD)

Equipment	Cost (USD)	Notes
Heat Exchanger (E1)	32,809	
Compressor (K1)	138,873	
Furnace (B1)	1,193,322	
Heat Exchanger (E4)	87,417	
Heat Exchanger (E2)	175,930	
Membrane Reactor (MR1–MR10)	25,982 per reactor	10 reactors
Cyclone Scrubber (CS1)	17,424	
CO2 Membrane (CO2 MEM)	34,152	
Heat Exchanger (E3)	14,017	
Compressor (K2)	2,092,422	To deliver same H ₂ pressure and temperature as in SMR
Heat Exchanger (E5)	633,938	To deliver same H ₂ pressure and temperature as in SMR
Heat Exchanger (E6)	170,757	To deliver same H ₂ pressure and temperature as in SMR

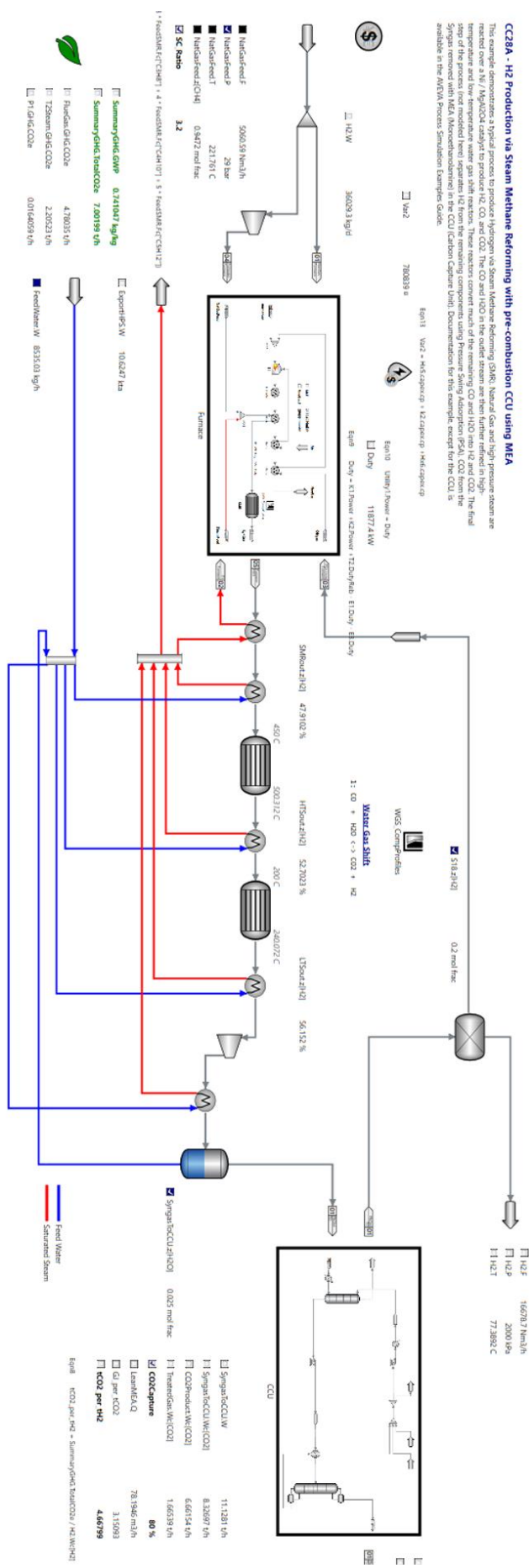


Figure S2. Flowsheet of a steam methane reforming (SMR) plant with carbon capture process.

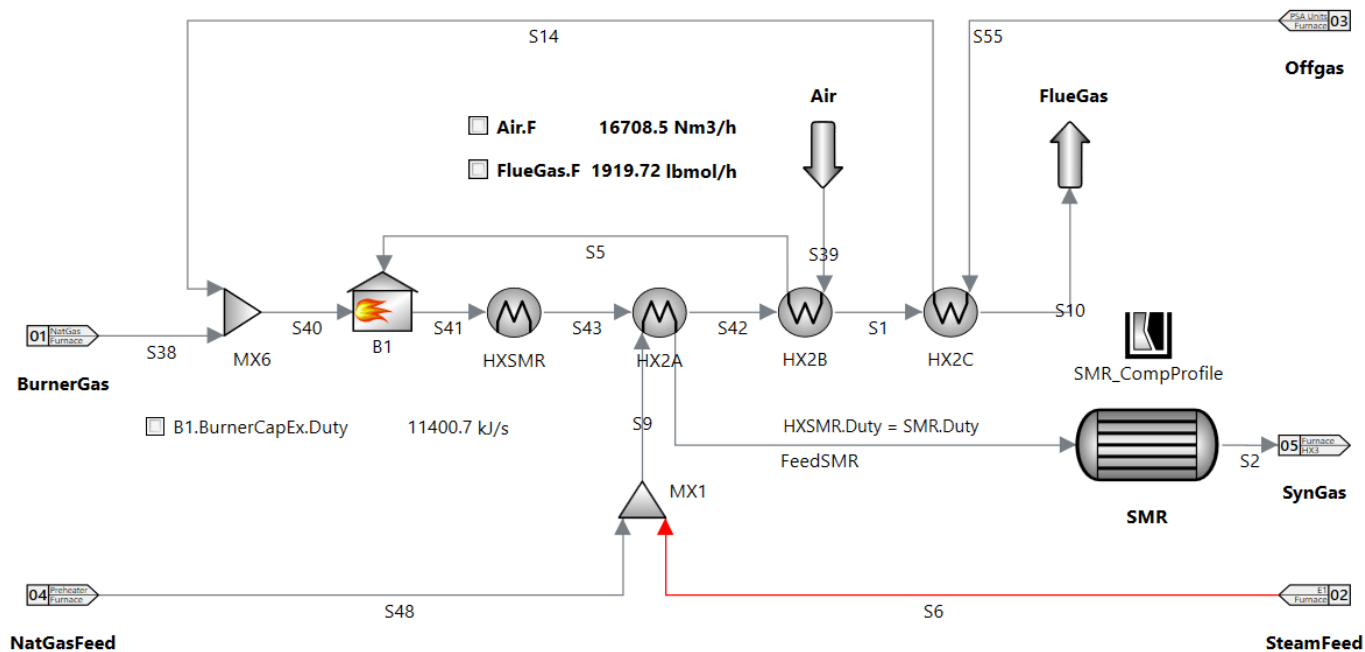


Figure S3. Furnace model of the SMR plant.

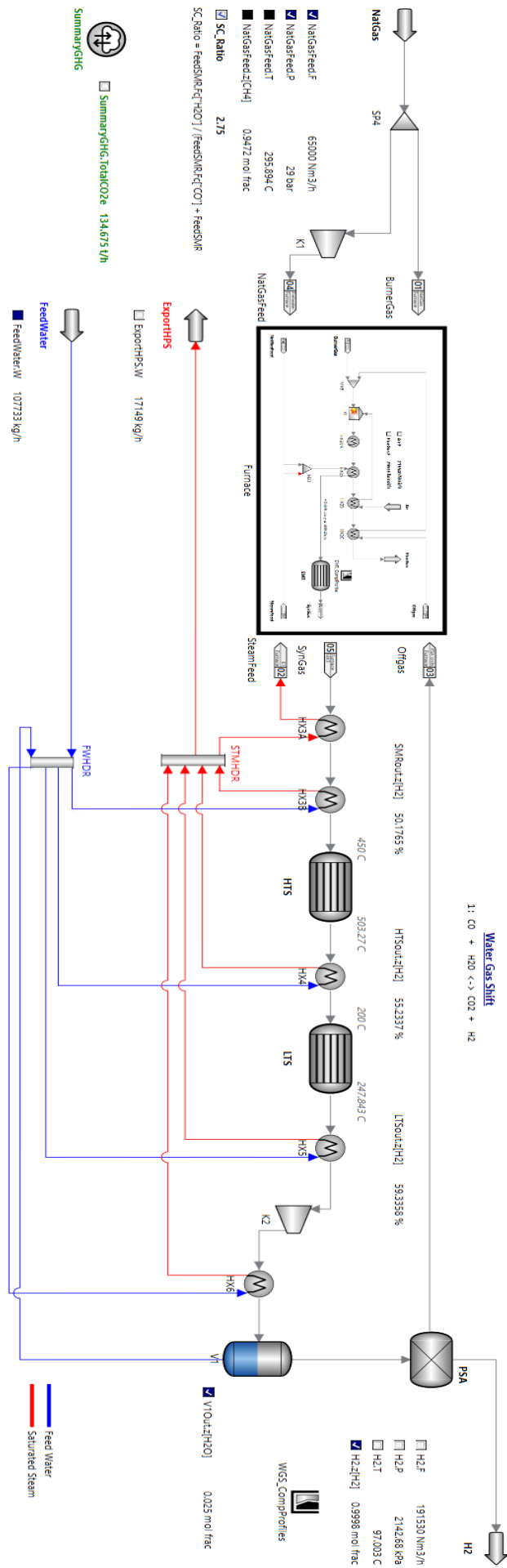


Figure S5. Flowsheet of a SMR plant without carbon capture process.

Table S4. CAPEX, OPEX, and LCOH of the SMR plant with carbon capture process.

CAPEX

Equipment Cost	USD	Notes
Total	9,430,815	Sum of equipment cost
Other Fixed Capital Costs	USD	Notes
Installation	4,432,483	47% of equipment cost ¹
Instrumentation & Control	943,082	10% of equipment cost
Piping	7,544,652	80% of equipment cost
Electrical	1,886,163	20% of equipment cost
Buildings & Infrastructure	1,886,163	20% of equipment cost
Engineering	3,112,169	33% of equipment cost ¹
Construction Expenses	1,886,163	20% of equipment cost
Contingency	471,541	5% of equipment cost
Yard Improvements	1,414,622	15% of equipment cost
Sum of equipment and other fixed costs	33,007,853	
Service Facilities	3,300,785	10% of the above
Total Fixed Capital Investment	USD	Notes
Total	36,308,640	Sum of equipment, other fixed costs, and service facilities
Working Capital	USD	Notes
Total	9,077,160	25% of fixed capital
Total Capital Investment	USD	Notes
Total	45,385,799	Sum of Fixed and Working capital

OPEX (Annual)

Item	USD	Notes
Utility	18,709,563	
Materials	16,271,515	Main feedstock
Manpower	1,862,571	Includes operators, engineers, supervision
Maintenance	3,630,864	Approx. 10% of fixed costs
Material Transport & Storage	1,448,752	Transporting and storing of captured CO ₂

Item	USD	Notes
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Total OPEX	USD	
	41,923,264	

Production Capacity & Costs

Parameter	Value	Notes
Hydrogen Production	13,151 t/year	Operating 90% a year
Operating Hours	7,884 hours/year	
Energy Consumption	56 MJ/kg H ₂	

Cost Metrics	USD	Notes
Levelized Cost of H ₂ (LCOH)	3,572	Per ton H ₂

Equipment Breakdown (USD)

Equipment	Cost (USD)	Notes
Compressor (K1)	626,950	
Furnace (B1)	1,033,029	
Heat Exchanger (HX2A)	45,642	
Heat Exchanger (HX2B)	95,171	
Heat Exchanger (HX2C)	23,562	
Reactor (SMR)	17,524	Steam Methane Reformer
Heat Exchanger (HX3A)	210,953	
Heat Exchanger (HX3B)	12,834	
Reactor (HTS)	5,922	High-Temperature Shift
Heat Exchanger (HX4)	38,845	
Reactor (LTS)	11,148	Low-Temperature Shift
Heat Exchanger (HX5)	29,259	
Compressor (K2)	689,129	
Heat Exchanger (HX6)	62,452	
Vessel (V1)	7,271	

Equipment	Cost (USD)	Notes
Heat Exchanger (E1)	50,805	
Column (T1)	62,268	
Heat Exchanger (E2)	604,138	
Column (T2)	65,384	
Pump (P1)	11,395	
Heat Exchanger (E3)	303,579	
PSA	1,010,368	Pressure Swing Adsorber Unit

Table S5. CAPEX, OPEX, and LCOH of the SMR plant without carbon capture process.

CAPEX		
Equipment Cost	USD	Notes
Total	10,486,587	Equipment breakdown cost below
Other Fixed Capital Costs	USD	Notes
Installation	4,928,696	47% of equipment cost ¹
Instrumentation & Control	1,048,659	10% of equipment cost
Piping	8,389,269	80% of equipment cost
Electrical	2,097,317	20% of equipment cost
Buildings & Infrastructure	2,097,317	20% of equipment cost
Engineering	3,460,574	33% of equipment cost ¹
Construction Expenses	2,097,317	20% of equipment cost
Contingency	524,329	5% of fixed costs
Yard Improvements	1,572,988	15% of fixed costs
Sum of equipment and other fixed costs	33,007,853	
Services Facilities	3,670,305	10% of the above
Total Fixed Capital Investment	USD	Notes
Total	40,373,359	Sum of equipment, other fixed costs, and service facilities
Working Capital	USD	Notes
Total	10,093,340	25% of fixed capital
Total Capital Investment	USD	Notes
Total	50,466,699	Sum of Fixed and Working capital
OPEX (Annual)		
Item	USD	Notes
Utility	1,746,922	
Raw materials	16,271,515	Main feedstock
Manpower	1,862,571	Includes operators, engineers, supervision
Maintenance	4,037,336	Approx. 10% of fixed costs
Material Transport	0	Transporting of captured CO ₂
Total OPEX	USD	
	25,598,176	

Production Capacity & Costs

Parameter	Value	Notes
Hydrogen Production	13,151 t/year	Operating 90% a year
Operating Hours	7,884 hours/year	
Energy Consumption	30 MJ/kg H ₂	

Cost Metrics	USD	Notes
Levelized Cost of H₂ (LCOH)	2,372	Per ton H₂

Equipment Breakdown (USD)

Equipment	Cost (USD)	Notes
Compressor (K1)	656,965	
Furnace (B1)	1,078,392	
Heat Exchanger (HX2A)	42,319	
Heat Exchanger (HX2B)	149,795	
Heat Exchanger (HX2C)	55,621	
Reactor (SMR)	17,524	Steam Methane Reformer
Heat Exchanger (HX3A)	228,568	
Heat Exchanger (HX3B)	13,049	
Reactor (HTS)	5,922	High-Temperature Shift
Heat Exchanger (HX4)	40,917	
Reactor (LTS)	3,781	Low-Temperature Shift
Heat Exchanger (HX5)	30,640	
Compressor (K2)	689,129	
Heat Exchanger (HX6)	62,452	
Vessel (V1)	7,271	
PSA	7,404,242	This cost is higher in the SMR plant without a carbon capture unit, as the PSA (pressure swing Adsorber) unit must also separate CO ₂ , a task typically handled by an amine process.

References:

1. Makhloufi C, Kezibri N. Large-scale decomposition of green ammonia for pure hydrogen production. Int. J. Hydrogen Energy 2021;46(70):34777-87. <https://doi.org/10.1016/j.ijhydene.2021.07.188>.