Supplementary Materials for: “Holistic view on synthetic natural gas production: A technical, economic and environmental analysis”

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1. Process Simulation

Table S1: Stream tables of PtSNG plant's simulation.

Stream name	From	To	Phase	Temperature [°C]	Pressure [bar]	Molar vapor fraction	Molar liquid fraction	Mass flow [kg/h]	Volume flow [m^3/h]	Mole fractions					
										H_2O	CO_2	H_2	CH_4	T-OIL	O_2
H2O		PEM	Liquid	20	7	0	1	150.58	0.15	1	0	0	0	0	0
H2	PEM	K-2	Vapor	80	7	1	0	16.85	35.06	0	0	1	0	0	0
O2	PEM		Vapor	80	7	1	0	133.73	17.53	0	0	0	0	0	1
CO2		K-1	Vapor	20	55	1	0	91.95	0.93	0	1	0	0	0	0
S3	K-1	K-2	Vapor	20	7	1	0	91.95	7.28	0	1	0	0	0	0
S4	K-2	HX-1	Vapor	65	7	1	0	108.80	41.98	0	0.20	0.80	0	0	0
S5	HX-1	R-1	Vapor	270	7	1	0	108.80	67.40	0	0.20	0.80	0	0	0
S6	R-1	HX-2	Vapor	338	7	1	0	108.80	46.73	0.62	0.01	0.05	0.31	0	0
S7	HX-2	ST-1		120	7	0.52	0.48	108.80	15.70	0.62	0.01	0.05	0.31	0	0
S8	ST-1		Liquid	120	7	0	1	55.58	0.06	0.99	0.00	0.00	0.00	0	0
S9	ST-1	HX-3	Vapor	120	7	1	0	53.22	15.67	0.28	0.02	0.10	0.60	0	0
S10	HX-3	R-2	Vapor	260	7	1	0	53.22	21.25	0.28	0.02	0.10	0.60	0	0
S11	R-2	HX-3	Vapor	282	7	1	0	53.22	21.31	0.33	0.01	0.03	0.64	0	0
S12	HX-3	HX-4	Vapor	142	7	1	0	53.22	15.94	0.33	0.01	0.03	0.64	0	0
S13	HX-4	ST-2		30	7	0.67	0.33	53.22	7.78	0.33	0.01	0.03	0.64	0	0
S14	ST-2		Liquid	30	7	0	1	19.40	0.02	0.99	0.00	0.00	0.01	0	0
S15	ST-2	CO-1	Vapor	30	7	1	0	33.82	7.75	0.00	0.01	0.04	0.95	0	0
S16	CO-1	HX-5	Vapor	107	16	1	0	33.82	4.24	0.00	0.01	0.04	0.95	0	0
SNG	HX-5		Vapor	30	16	1	0	33.82	3.38	0.00	0.01	0.04	0.95	0	0
A1	R-1	HX-1	Liquid	337	1	0	1	1000	1.28	0	0	0	0	1	0
A2	HX-1	HX-R1	Liquid	312	1	0	1	1000	1.25	0	0	0	0	1	0
A3	HX-R1	R-1	Liquid	200	1	0	1	1000	1.13	0	0	0	0	1	0
A4	HX-R2	R-2	Liquid	250	1	0	1	100	0.12	0	0	0	0	1	0
A5	R-2	HX-R2	Liquid	282	1	0	1	100	0.12	0	0	0	0	1	0

2. Determination of capital expenditures (CAPEX)

The fixed capital investment (FCI) is determined as per Eq. (S1), where EC_e represents the equipment cost and F_j Lang factors based on typical values for the chemical industry. Lang factors are summarized in the following table.

$$\mathrm{FCI} = \sum_{k=1}^{m} \mathrm{EC}_e \left(1 + \sum_{j=1}^{12} F_{e,j}\right) \tag{S1}$$

Table S2: Lang-factors for estimating FCI on the basis of EC, adapted from Peters, et al. [1]

Capital cost item	***j***	**Electrochemical equipment Lang-factor F_j**	**Thermochemical equipment Lang-factor. F_j**
Direct costs			
Installation	1	0.47	0.47
Instrumentation	2	0.00	0.36
Piping	3	0.00	0.68
Power supply	4	0.00	0.11
Building	5	0.00	0.18
Yard improvements	6	0.10	0.10
Service facilities	7	0.00	0.70
Indirect costs			
Engineering and	8	0.00	0.33
Construction expenses	9	0.00	0.41
Legal expenses	10	0.04	0.04
Contractor's fee	11	0.22	0.22
Contingency	12	0.44	0.44

3. Equipment sizing and cost

Detailed information on:

Heat exchangers

The sizing of the heat exchanger network was carried out based on the calculation of the heat transfer area A using the correlation shown in Eq. (S2).

$$\dot{Q} = A \times k \times \Delta T_{\mathrm{ln}}, \tag{S2}$$

where k is the heat transfer coefficient, $\dot{Q}$ the heat duty and ΔT_{ln} the logarithmic mean temperature difference. ΔT_{ln} is defined by:

$$\Delta T_{\mathrm{ln}} = \frac{(T_{h,1} - T_{c,1}) - (T_{h,2} - T_{c,2})}{\ln\left[\frac{(T_{h,1} - T_{c,1})}{(T_{h,2} - T_{c,2})}\right]}, \tag{S3}$$

where the index *h* refers to the hot fluid, *c* to the cold fluid, 1 to inlet conditions, and 2 to outlet conditions. The heat transfer coefficient was estimated from Ulrich and Vasudevan [2], while the heat duty was extracted from Aspen Plus®.

Reactors

The methanation reactors were modelled as shell and tube heat exchangers. However, their sizing was determined based on the mean residence time, as discussed in Section 2.1.2. of the main text. Reactor R-1 and reactor R-2 each have 20 tubes of 7.5 cm diameter and respective lengths of 85 cm and 45 cm.

Separators

The lengths and diameters of both process vessels, ST-1 and ST-2, were determined by using the sizing function from Aspen Plus®. In both cases the flash drums are horizontally oriented and the length-to-diameter ratio is three, coinciding with design guidelines of Ulrich and Vasudevan [2] for gas to liquid separators operating at low pressure (< 10 bar).

Compressor

The shaft power of the centrifugal compressor and the fluid power were determined from the Aspen Plus® simulation. The pressure ratio is less than 4:1 and therefore staged compression is not required.

Electrolyser

The selected electrolyser is a 1 MW_{el} commercially available PEM electrolyser. Since Ulrich and Vasudevan [2] do not include costs for electrochemical equipment in their book, the cost of the electrolyser was extracted from the IndWEDe study published by NOW GmbH [3]. This study reports a cost of 700 €/kW for AEL and 1460 €/kW for PEMEL in 2018. Details of all the equipment sizing are provided in Table S3.

Table S3: Summary of plant equipment sizing.

Unit	Characteristic input 1	Characteristic input 2	Characteristic input 3
Compressor			
Gas compressor (CO-1) [a]	Fluid power: 10 kW		
	Shaft power: 1,805 kW		
Electrolyser			
PEM Electrolyser	Nominal power: 1000 kW		
Heat Exchangers			
Heat Exchanger 1 (HX-1)	Surface area: 0.40 m^2	Pressure: 7 bar	
Heat Exchanger 2 (HX-2)	Surface area: 1.15 m^2	Pressure: 7 bar	
Heat Exchanger 3 (HX-3)	Surface area: 0.43 m^2	Pressure: 7 bar	
Heat Exchanger 4 (HX-4)	Surface area: 1.91m^2	Pressure: 7 bar	
Heat Exchanger 5 (HX-5)	Surface area: 0.10 m^2	Pressure: 16 bar	
Rectors			
Methanation Reactor 1 (R-1)	Surface area: 3.86 m^2	Pressure: 7 bar	
Methanation Reactor 2 (R-2)	Surface area: 2.12 m^2	Pressure: 7 bar	
Separators			
Separator 1 *	Length: 2.75 m	Diameter: 0.91 m	Pressure: 7 bar
Separator 2 *	Length: 2.75 m	Diameter: 0.91 m	Pressure: 7 bar

*Characteristic values for equipment sizing were extracted from Aspen Plus® process simulation

Table S4: Equipment cost estimation parameters.

Unit	Base equipment cost 2004, C^0_{2004} (\$)	Base equipment cost 2018, C^0_{2018} (€) [d]	Material factor F_M^{ss}	Pressure factor F_P	Equipment cost 2018, C^{ss}_{2018}(€)
Compressor [a]					
Gas compressor (CO-1)	\$15,000.00	17,262.07 €	4.4	1.0	76,419.20 €
	\$270.00	310.72 €			
Electrolyser					
PEM Electrolyser					1,460,000.00 €
Heat Exchangers [b]					
Heat Exchanger 1 (HX-1)	\$1,600.00	1,841.29 €	3.0	1.0	5,523.86 €
Heat Exchanger 2 (HX-2)	\$1,900.00	2,186.53 €	3.0	1.0	6,559.59 €
Heat Exchanger 3 (HX-3)	\$1,600.00	1,841.29 €	3.0	1.0	5,523.86 €
Heat Exchanger 4 (HX-4)	\$2,500.00	2,877.01 €	3.0	1.0	8,631.04 €
Heat Exchanger 5 (HX-5)	\$1,600.00	1,841.29 €	3.0	1.0	5,523.86 €
Rectors [b]					
Reactor 1 (R-1)	\$3,500.00	4,027.82 €	3.0	1.0	12,083.45 €
Reactor 2 (R-2)	\$3,500.00	4,027.82 €	3.0	1.0	12,083.45 €
Separators [c]					
Separator 1	\$3,500.00	4,027.82 €	2.5	1.5	15,104.32 €
Separator 2	\$3,500.00	4,027.82 €	2.5	1.5	15,104.32 €

All data was extracted from Ulrich and Vasudevan [2], details of the exact source are given below:

[a] Compressor cost is divided in driver (motor) cost and the compressor cost. Driver cost was extracted from Figure 5.20 and an installation factor of 1.5 was considered. The compressor cost was obtained from Figure 5.30.

[b] Values were gathered from Figure 5.36

[c] Values were extracted from Figure 5.44 and Figure 5.45

[d] Calculated utilizing $CEPCI_{2004}$ = 444.2 € and $CEPCI_{2018}$ = 603.1 €

4. Determination of operational expenditures (OPEX)

To estimate a fix production cost of item y, a corresponding ratio factor W_y was multiplied by a defined basis B_y. The total OPEX amounts to the sum of all cost items y.

Table S5: Method for the estimation of fixed production costs.

Fixed production cost item	y	**Factor** W_y	**Basis** B_y
Insurance and taxes	1	0.02	FCI
Maintenance labour (ML)	2	0.01	FCI-$CAPEX_{electrolyser}$
Maintenance material (MM)	3	0.01	FCI-$CAPEX_{electrolyser}$
Maintenance electrolyser	4		12.50 €/kW*
Operating supplies (OS)	5	0.15	ML+MM
Operating labour (OL)	6		
Operating supervision (OV)	7	0.15	OL
Laboratory charges	8	0.20	OL
Plant overhead costs (PO)	9	0.50	OL+OV+OS
Administrative costs	10	0.25	PO
Distribution and selling costs	11	0.00	NPC
Research and development costs	12	0.00	NPC

*Maintenance of electrolyser amounts to 12.50 €/kW for PEMEL and 18 €/kW for AEL in 2018 [3]

5. Base case net production cost estimation

Following the method described in the main text the net production cost (NPC) of produced SNG in the base case was calculated. The following Table S6 provides the detailed values and assumptions used in the aforementioned calculation.

Table S6: Base case NPC estimation summary.

Capital costs		**Yield estimate**			
	k€				
Direct Capital Costs	2,877.41	Annual operating hours (h/y)			8000
Indirect Capital Costs	1,256.08	SNG mass flow rate (kg/h)			33.82
Fixed Capital Investment	4,133.49	SNG higher heating value (kWh/kg)			15.18
Working Capital	729.44	Annual SNG prod. estimate (kWh/y)			4,106,744
Total Capital Investment	4,862.93				
Raw materials					
	Units	Units/y	Price €/unit		k€/y
Distilled Water	t	1,204.62	1		1.20
CO_2	t	735.64	20		14.71
Catalyst	kg	13.44	1288		17.31
Total raw materials					33.22
Utilities					
	Units	Units/y	Price €/unit		k€/y
Electricity	MWh	8,014.44	50		400.72
Cooling water	t	46,308.50	0		0.00
Total utilities					400.72
Fixed operational costs					
					k€/y
Operating labour (OL)	3 shifts	1 operators/shift	66 693€/operator/yr		200.08
Insurance and taxes		2%	of	FCI	82.67
Maintenance labour (ML)		1%	of	$FCI-CAPEX_{electrolyser}$	8.19
Maintenance material (MM)		1%	of	$FCI-CAPEX_{electrolyser}$	8.19
Maintenance PEM electrolyser		12,50		€/kWh	12.50
Operating supplies (OS)		15%	of	ML+MM	2.46
Operating supervision (OV)		15%	of	OL	30.01
Laboratory charges		20%	of	OL	40.02
Plant overhead costs (PO)		50%	of	OL+OV+OS	116.27
Administrative costs		25%	of	PO	29.07
Fixed cost of production					529.46
Annualized capital charges					
	k€	Interest Rate	Life (y)	AACR	k€/y
Fixed Capital Investment	4,133.49	5%	20	0.0802	331.68
Summary					
					k€/y
				Variable cost of production	443.95
				Fixed cost of production	529.46
				Annual capital charge	331.68
				Total annualized cost	1,295.09
				Net production cost (€/kWh)	**0.32**

Sale of by-products

Since the PtSNG plant produces not only SNG but also as by-products oxygen and heat, both of which can be sold to obtain an economic gain. It is assumed that oxygen will be sold at 70% of its conventional purchase price of 50 €/t to account for the pilot plant's electrical consumption during oxygen compression [4]. On the other hand, the price of heat provision was determined by analogy with biogas plants. An empirical study conducted in Germany showed that the prices for heat provision from biogas plants differed substantially from free to maximum of 90 €/MWh [5]. To keep the values as close to reality as possible, the average heat supply price reported in the aforementioned study was selected. All heat sources (electrolyser and methanation reactors) are considered with the same price

6. SNG cost literature comparison

Table S7: Compilation of literature utilized for the SNG cost comparison.

Source	Operating hours	Assumptions	Year	SNG Cost (€/kWh$_{SNG}$)	CAPEX	OPEX (€/kW$_{SNG}$)	Cost estimation method
Becker, et al. [6]	7,740 5,590 3,440	66 MW$_{H2}$ / 51 MW$_{SNG}$ capacity No electrolysis Free electricity 40y plant lifetime	2013	0.06–0.18 0.15 0.132	1,045 €/kW$_{SNG}$	80.7 4.14 M€ 8.4% of total installed cost	H2A tool developed by the National Renewable Energy Laboratory. 15% working capital
Benjaminsson, et al. [7]	8,600	1 MW$_{el}$ capacity Alkaline electrolysis Electricity 30 €/MWh Free CO_2	2014	0.14–0.24	6,500–8,666 €/kW$_{SNG}$ 7.8 –10.4 M€	468–624 234–312 k€ Maintenance and service 3% of investment	Based on cost estimated on contact with equipment suppliers
De Saint Jean, et al. [8]	4,500	1 MW$_{el}$ capacity SOEC electrolysis Electricity 0–50 €/MWh	2014	0.42–0.58	7,070–9,630 €/kW$_{SNG}$	664–9,144 Maintenance 4% of investment, tax 2%. 0.2 operators required	The Chauvet method excluded working capital
Giglio, et al. [9]	8,000	10 MW$_{el}$ capacity Steam and co-electrolysis Electricity 0–65 €/MWh CO_2 cost 4–88 €/t	2011	0.05–0.18	700–800 €/kW$_{SNG}$	38–40 Maintenance: 2% of total plant cost. considers one plant operator	Methodology developed by NETL, several levels of capital cost were calculated. Includes capital for inventory
Jentsch, et al. [10]		6-12 GW capacity	2014	0.05	750 €/kW$_{SNG}$	Fixed Operating costs 4% of investment costs	Investment cost, fixed operating costs, interest rate, depreciation method

Source	Operating hours	Assumptions	Year	SNG Cost (€/kWh$_{SNG}$)	CAPEX	OPEX (€/kW$_{SNG}$)	Cost estimation method
Mohseni, et al. [11]	8,000	2.5 MW$_{el}$ or 1.2 MW$_{SNG}$ Alkaline electrolysis Sale of heat and oxygen Free CO_2	2014	0.13	1,516 €/kW$_{SNG}$ 1.82 M€	1,095 O&M are 5% of investment	Uses cost estimation tool CAPCOST, a set price for SNG is determined
Parra and Patel [12]	8,000	0.01–1000 MW$_{el}$ capacity PEM electrolyser Revenue for frequency control Sale of heat and oxygen Free CO_2	2016	0.1–0.25	0.07–141 M€	O&M cost is 5% of CAPEX for methanation and 2% for electrolyser. BoP OPEX is 7%	Calculated total levelized cost. Used the cost curve method to account for scale dependencies
Peters, et al. [13]	8,000	13.2 MW$_{SNG}$ capacity No electrolysis CO_2 cost 80–800€/t	2019	0.25–0.47	649–1,274 €/kW$_{SNG}$	2,140–3,827	Cost of manufacture by using Lang factors and initial equipment cost. Working capital 15%
Schiebahn, et al. [14]	3,000	84 GW$_{el}$ capacity PEM Electrolysis Free CO_2	2015	0.23	1,809 €/kW$_{SNG}$	Operation and maintenance are 3% of total investment	Cost estimated based in component scaling and process design
Tremel, et al. [15]	6,000	32 MW$_{SNG}$ capacity No electrolysis	2015	0.17	1,000 €/kW$_{SNG}$	Operation and maintenance are 4% of total investment per year	Used cost curve method to account for scaling effects.
Tichler, et al. [16]	5,630	1–10 MW$_{el}$ capacity Alkaline electrolysis Electricity 33–105 €/MWh CO_2 cost 30–90 €/t	2013	0.26–0.44	1,500–2,197 €/kW$_{el}$		

7. Natural gas price

Table S8 reports the German natural gas market price for private and industrial customers as well as the cross-border price, for 2017, 2021 (first half), and its average in this period. Industrial and private customers have seen a price development without major fluctuations between 2017 and 2021, and their taxes amounted to 33% of the price shown in Table S8.

Table S8: Natural gas price in Germany. Prices include taxes for private and industrial customers, but not for cross-border.

Type of tariff	Price 2017 (€-cent/kWh)	Price 2021 (1st half) (€-cent/kWh)	Average price 2017 – 2019 (€-cent/kWh)	Source
Private customers	6.11	6.47	6.13	Eurostat [17]
Industrial customers	3.72	3.95	3.72	Eurostat [18]
Cross-border	1.70	2.30	-	BAFA [19]

8. Life Cycle Analysis – Background data

The electricity source plays a major role regarding the global warming potential of SNG. Thus, different electricity scenarios were defined according to Table S9.

Table S9: Definition of electricity scenarios in the life cycle analysis.

Electricity scenario	Global warming potential in g CO_2-eq/kWh	Specification	Name of data set (ecoinvent 3.7.1 cut-off)	Source
German grid mix	619.66	Shares of electricity technology are based on IEA World Energy Statistics for 2017	market for electricity, medium voltage | electricity, medium voltage | Cutoff, U(DE)	ecoinvent 3.7.1 cut-off
Wind Mix	26.51	20% offshore wind power	electricity production, wind, 1-3 MW turbine, offshore | electricity, high voltage | Cutoff, U(DE)	Umweltbundesamt [20]
		80% onshore wind power	electricity production, wind, >3 MW turbine, onshore | electricity, high voltage | Cutoff, U(DE)	
		Transmission losses (high-to-medium voltage): 0.37%	see market for electricity, medium voltage | electricity, medium voltage | Cutoff, U(DE)	ecoinvent 3.7.1 cut-off
Wind offshore	14.43	100% offshore wind power	electricity production, wind, 1-3 MW turbine, offshore | electricity, high voltage | Cutoff, U(DE)	ecoinvent 3.7.1 cut-off
		Transmission losses (high-to-medium voltage): 0.37%	see market for electricity, medium voltage | electricity, medium voltage | Cutoff, U(DE)	
PV Mix	93.91	75% PV on roof	electricity production, photovoltaic, 3 kW slanted-roof installation, multi-Si, panel, mounted | electricity, low voltage | Cutoff, U (DE)	BMWi [21]
		25% PV on open ground	electricity production, photovoltaic, 570 kW open ground installation, multi-Si | electricity, low voltage | Cutoff, U (DE)	
German grid mix (2030)	368.81	10.2% Lignite	electricity production, lignite | electricity, high voltage | Cutoff, U(DE)	Revolution Scenario for 2030 in EWI Energy Research and Scenarios [22]
		8.6% Hard coal	electricity production, hard coal | electricity, high voltage | Cutoff, U(DE)	
		12.5% Gas	electricity production, natural gas, combined cycle power plant | electricity, high voltage | Cutoff, U(DE)	
		2.4% Oil	electricity production, oil | electricity, high voltage | Cutoff, U(DE)	

		3.7% Hydropower	electricity production, hydro, run-of-river | electricity, high voltage | Cutoff, U(DE)	
		7.7% Biomass	heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014 | electricity, high voltage | Cutoff, U(DE)	
		32.6% Wind onshore	electricity production, wind, >3 MW turbine, onshore | electricity, high voltage | Cutoff, U(DE)	
		8.6% Wind offshore	electricity production, wind, 1-3 MW turbine, offshore | electricity, high voltage | Cutoff, U(DE)	
		13.3% PV	electricity production, photovoltaic, 570kWp open ground installation, multi-Si | electricity, low voltage | Cutoff, U(DE)	
		1.13E-7 kg SF6/kWh	sulfur hexafluoride production, liquid | sulfur hexafluoride, liquid | Cutoff, U (RER)	ecoinvent 3.7.1 cut-off
		Transmission network, high voltage: 6.582E-09 km/kWh	market for transmission network, electricity, high voltage | transmission network, electricity, high voltage | Cutoff, U (GLO)	
		Transmission network, medium voltage: 1.863E-8 km/kWh	market for transmission network, electricity, medium voltage | transmission network, electricity, medium voltage | Cutoff, U (GLO)	
		Transmission network, long-distance: 3.17E-10 km/kWh	market for transmission network, long-distance | transmission network, long-distance | Cutoff, U (GLO)	
		Transmission losses (high-to-medium voltage): 0.37% N_2O emission: 5.0E-6 kg/kWh Ozone emissions: 4.1577E-6 kg/kWh SF6 emissions: 1.13E-7 kg/kWh	see market for electricity, medium voltage | electricity, medium voltage | Cutoff, U(DE)	
German grid mix (2040)	222.38	4.5% Lignite	electricity production, lignite | electricity, high voltage | Cutoff, U(DE)	Revolution Scenario for 2040 in EWI Energy Research and Scenarios [22]
		2.8% Hard coal	electricity production, hard coal | electricity, high voltage | Cutoff, U(DE)	
		9.4% Gas	electricity production, natural gas, combined cycle power plant | electricity, high voltage | Cutoff, U(DE)	

		1.3% Oil	electricity production, oil | electricity, high voltage | Cutoff, U(DE)	
		3% Hydropower	electricity production, hydro, run-of-river | electricity, high voltage | Cutoff, U(DE)	
		7.5% Biomass	heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014 | electricity, high voltage | Cutoff, U(DE)	
		39.9% Wind onshore	electricity production, wind, >3 MW turbine, onshore | electricity, high voltage | Cutoff, U(DE)	
		13.1% Wind offshore	electricity production, wind, 1-3 MW turbine, offshore | electricity, high voltage | Cutoff, U(DE)	
		18.6% PV	electricity production, photovoltaic, 570 kW open ground installation, multi-Si | electricity, low voltage | Cutoff, U(DE)	
		1.13E-7 kg SF6/kWh	sulfur hexafluoride production, liquid | sulfur hexafluoride, liquid | Cutoff, U (RER)	ecoinvent 3.7.1 cut-off
		Transmission network, high voltage: 6.582E-09 km/kWh	market for transmission network, electricity, high voltage | transmission network, electricity, high voltage | Cutoff, U (GLO)	
		Transmission network, medium voltage: 1.863E-8 km/kWh	market for transmission network, electricity, medium voltage | transmission network, electricity, medium voltage | Cutoff, U (GLO)	
		Transmission network, long-distance: 3.17E-10 km/kWh	market for transmission network, long-distance | transmission network, long-distance | Cutoff, U (GLO)	
		Transmission losses (high-to-medium voltage): 0.37% N_2O emission: 5.0E-6 kg/kWh Ozone emissions: 4.1577E-6 kg/kWh SF6 emissions: 1.13E-7 kg/kWh	see market for electricity, medium voltage | electricity, medium voltage | Cutoff, U(DE)	
German grid mix (2050)	127.15	9.6% Gas	electricity production, natural gas, combined cycle power plant | electricity, high voltage | Cutoff, U(DE)	Revolution Scenario for 2050 in EWI Energy
		3.3% Hydropower	electricity production, hydro, run-of-river | electricity, high voltage | Cutoff, U(DE)	

		6.7% Biomass	heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014 | electricity, high voltage | Cutoff, U(DE)	Research and Scenarios [22]
		42.6% Wind onshore	electricity production, wind, >3 MW turbine, onshore | electricity, high voltage | Cutoff, U(DE)	
		15.9% Wind offshore	electricity production, wind, 1-3 MW turbine, offshore | electricity, high voltage | Cutoff, U(DE)	
		21.9% PV	electricity production, photovoltaic, 570 kW open ground installation, multi-Si | electricity, low voltage | Cutoff, U(DE)	
		1.13E-7 kg SF6/kWh	sulfur hexafluoride production, liquid | sulfur hexafluoride, liquid | Cutoff, U (RER)	ecoinvent 3.7.1 cut-off
		Transmission network, high voltage: 6.582E-09 km/kWh	market for transmission network, electricity, high voltage | transmission network, electricity, high voltage | Cutoff, U (GLO)	
		Transmission network, medium voltage: 1.863E-8 km/kWh	market for transmission network, electricity, medium voltage | transmission network, electricity, medium voltage | Cutoff, U (GLO)	
		Transmission network, long-distance: 3.17E-10 km/kWh	market for transmission network, long-distance | transmission network, long-distance | Cutoff, U (GLO)	
		Transmission losses (high-to-medium voltage): 0.37% N_2O emission: 5.0E-6 kg/kWh Ozone emissions: 4.1577E-6 kg/kWh SF6 emissions: 1.13E-7 kg/kWh	see market for electricity, medium voltage | electricity, medium voltage | Cutoff, U(DE)	

Table S10: Life cycle inventory for a 1 MW_{th} SNG plant.

Inventory	Value	Name of data set (ecoinvent 3.7.1 cut-off)	Source
CO_2 compression (1 bar to 55 bar)			
CO_2 captured	1.044 kg CO_2/kg CO_2 compressed	-	Process simulation
Electricity	0.125 kWh/kg CO_2 compressed	defined by electricity scenario (see Tab. S-4)	Process simulation
Reinforcing steel for HX-5 (see Fig. 2-2)	0.274 kg/kg CO_2 compressed and per overall SNG plant operating time in h	market for reinforcing steel I reinforcing steel I Cutoff, U-GLO	Process simulation
CO_2 transportation			
CO_2 compressed	1 kg CO_2/kg CO_2 transported	-	
Transport per lorry	0.05 t*km/kg CO_2 transported	transport, freight, lorry 7.5 – 16 metric ton, EURO 6 I transport, freight, lorry 7.5 – 16 metric ton, EURO 6 I Cutoff, U -RER	Assumption
Methanation unit			
Aluminum oxide (part of catalyst)	0.715 kg Aluminum oxide/kg SNG and per yearly SNG plant full load hours Assumption: replacement every 2 years of plant operation	market for aluminium oxide, non-metallurgical I aluminium oxide, non-metallurgical I Cutoff, U- IAI Area, EU27 & EFTA	Process simulation
CO_2 compressed, transported	1.73 kg CO_2/kg SNG	-	Process simulation
H_2	0.317 kg H_2/kg SNG	defined by H_2 source in scenario	Process simulation
Reinforcing steel for R-1, R-2, HX-1, HX-2, HX-3, ST-1 (see Fig. 2-2)	11.09 kg/kg SNG and per overall SNG plant operating time in h	market for reinforcing steel I reinforcing steel I Cutoff,U-GLO	Process simulation
SNG Upgrading (to 30 °C, 16 bar)			
Electricity	0.053 kWh/kg SNG upgraded	defined by electricity scenario (see Tab. S-4)	Process simulation

SNG	1.573 kg SNG/kg SNG upgraded	-	Process simulation
Reinforcing steel for HX-4, ST-2 (see Fig. 2-2)	3.538 kg/kg SNG upgraded and per overall SNG plant operating time in h	market for reinforcing steel I reinforcing steel I Cutoff,U-GLO	Process simulation

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