Electronic Supplementary Material (ESI) for Green Chemistry.

Environmental and economic assessment of global and German production locations for CO_2-based methanol and naphtha

Simon Kaiser[a1], Katharina Prontnicki Stefan Bringezu[a]

Supplementary Information

Content:

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[a] *Center for Environmental Systems Research, University of Kassel, Wilhelmshoeher Allee 47, D-34117 Kassel, Germany*

[1] Corresponding author, Email address: simon.kaiser@uni-kassel.de, Tel.: +49 561 804 6122

S1: Method and Database for the GIS Analysis

Step 1: Characterization of the regions

The Geoinformation System (GIS) analysis was conducted with the software *ArcGis, Version 10.6.* For the analysis, the different data layers described in Table 1 were combined in a GIS-model using Gauß-Krueger coordinates (WGS 1984). The different regions were delineated according to the watersheds described in Boulay et al. [1]. Since there is no varying of the AWARE factor within one watershed, a further differentiation was not possible. In case a raster point could not be unambiguously assigned to one region, it was completely assigned to the region in which the majority of its area is located. In the next step, the mean value, and the standard deviation for each capacity factor as well as the number of CO_2-point sources were calculated for every region using the *zonal statistics* tool. The transport distance from each region to Germany was calculated using the Euclidean distance between the respective centroids. While the locations of waste incineration and cement plants could be directly extracted from the respective datasets, the locations of the steel plants were derived from company reports of the largest global steel producers and cross-checked with domestic production capacities.

Table 1: Parameters and Data used in the location analysis (IEC = International Electrotechnical Commission).

Resource	Parameter	Description	Resolution/ Nr. of plants	Data Source
Wind Energy	Capacity Factor	IEC Class I	9 " x 9 "	[2]
Solar Energy	Capacity Factor	kWh/kWp	9 " x 9 "	[3]
Water	AWARE (Available Water Remaining)	m^3/m^3	0.5 ° x 0.5 °	[1]
CO_2	Number of industrial CO_2 Point sources	Waste Incineration Plants	177	[4, 5]
		Cement Plants	1561	[6]
		Steel Plants (Blast Furnace)	115	[7, 8]

Step 2: Selection of representative examples

After the combination of the different data layers and the characterization of the different regions, best case examples for every system type and distance category were identified according to the decision procedure described in Figure 1. The selected regions were later used as representative locations in the environmental and economic assessments.

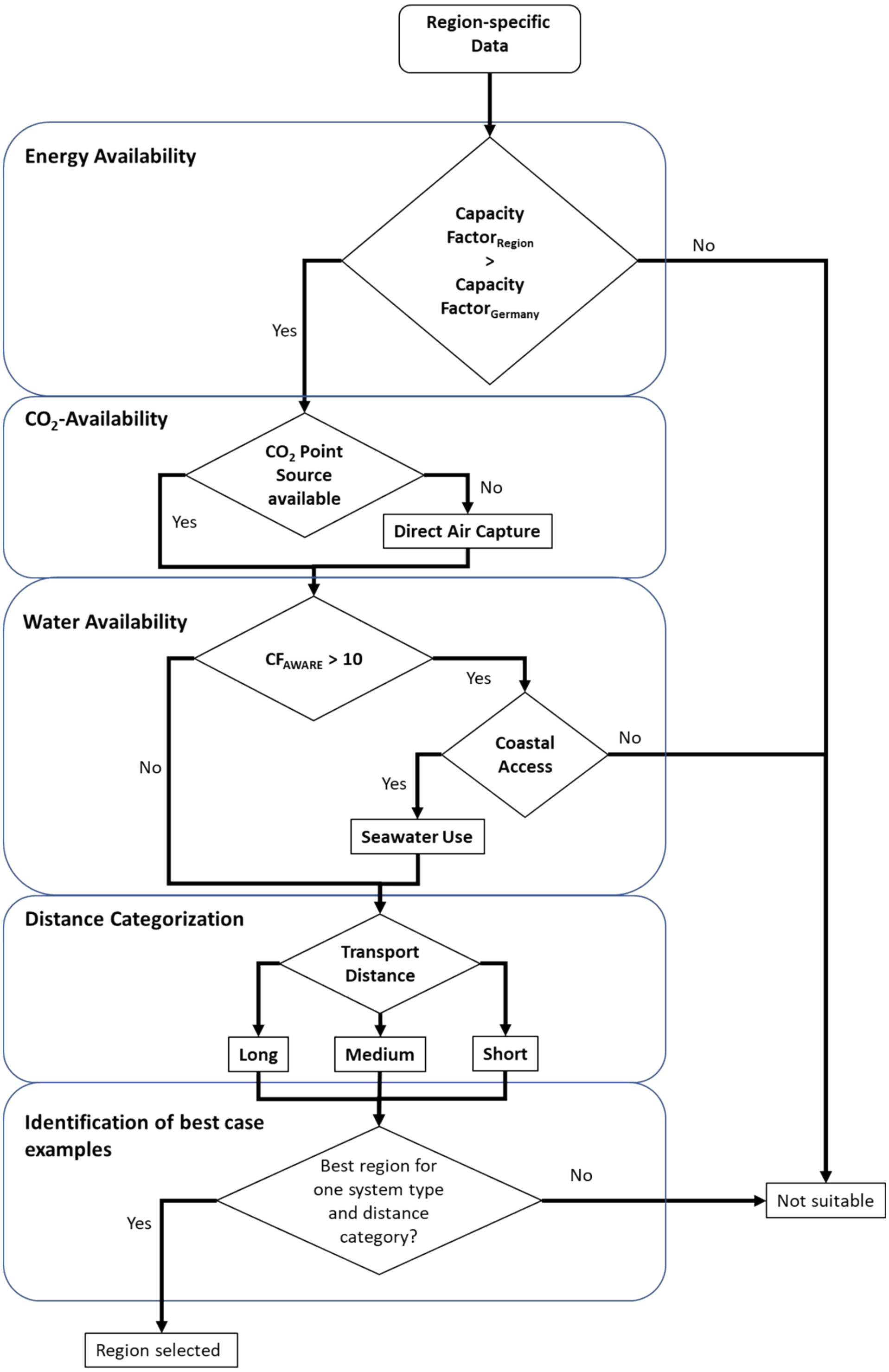

Figure 1: Selection procedure for the identification of best cases for the different system types.

S2: Calculation Formulars and Economic Parameters

S2-1: Levelized Cost of Energy (LCOE)

$$LCOE_{ij} = \frac{\sum_{t=1}^{n} \frac{Capex_t + \ Opex_t}{(1 + r_i)^t}}{\sum_{t=1}^{n} \frac{E_t}{(1 + r_i)^t}} \ [€/GJ]$$

t: Period

i: Produced Chemical

j: Location

$Capex_t$: Capital Expenditures (Investment Costs)

$Opex_t$: Operation Expenditures (Maintenance, Fuel and Personnel Costs)

E_t: Cumulated Energy bound in the yearly production volume

r: project specific interest rate/weighted average costs of capital

S2-2: Avoidance Costs (AC)

$$AC_{ij} = \frac{LCOE_{ij} - \ MP_{fossil}}{GWI_{ij} - GWI_{fossil}} \left[\frac{€}{t\ CO_2 eq.\ avoided}\right]$$

i: Produced Chemical

j: Location

$LCOE_{ij}$: Levelized Costs of Energy

MP_{fossil}: Net market price for fossil fuels in the status quo

S2-3: Net Present Value (NPV)

$$NPV_{ij} = \ -\sum_{1}^{t} \frac{Capex_t + Opex_t}{(1 + r_i)^t} + \sum_{1}^{t} \frac{(MP_{fossil} \ * \ (1 + \Delta PF_t)^t + \ CP_t * \Delta GWI) * \ PV_t}{(1 + r_i)^t} [€]$$

t: Period

i: Produced Chemical

j: Location

ΔGWI: Avoided emissions $\left[\frac{t\ CO_2\ eq.\ avoided}{t\ Chemical}\right]$

PV_t: Yearly production volume $[t]$

CP_t: Carbon Price

ΔPF_t: Relative Price change for fossil fuels compared to the status quo

S2-4: Economic Parameters

Table 2: Description of Cost Parameters. (Sq = Status quo, Capex = Capital Expenditures, Opex = operational expenditures, PV = Photovoltaic, FLH = Full load hours, PS = Point Source, DAC = Direct Air Capture, RSWO = Reverse Seawater Osmosis, WACC = Weighted Average Costs of Capital).

Process	Parameter	Value Sq	References	Value 2030	References
Onshore wind plant	Capex [€/MW]	1,605,000	[9]	1,000,000	[10]
	Opex [% Capex]	2		2	
	Lifetime [years]	20		20	
PV plant	Capex [€/MW]	900,000.00	[11]	750,000	[11]
	Opex [% Capex]	1		1	
	Lifetime [years]	30		30	
Electrolysis	Capex [€/MW]	1,470,000	[12]	500,000	[12,13]
	Opex [% Capex]	1		1	
	Lifetime [FLH]	60,000		90,000	[14]
	Energy Requirement	55 kWh/kg H_2	[12]	50 kWh/kg	[12]
CO_2 Capture (PS)	Capex [€] (Scaling Factor: 0.6)	26,680,367	[15]	18,676,256	[16]
	Opex [% Capex]	6	[17]	6	[17]
	Lifetime [years]	20		20	
	Heat Costs [€/kWh]	Country specific	[18]	Country specific	[18]
CO_2 Capture (DAC)	Capex [€/t CO_2 per year]	730.00	[19]	263.50	[19]
	Opex [% Capex]	4		4	
	Heat Costs [€/kWh]	Country specific	[18]	Country specific	[18]
	Lifetime [FLH]	105,120	[20]	105,120	[20]
RSWO	Capex [€/m³ H_2O per year]	2.25	[21]	2.25	[21]
	Opex [% Capex]	4	[22]	4	[22]
Freshwater Production	[€/m³]	Region specific	[23]	Region specific	[23]
Methanol Synthesis	Capex [€/t MeOH per year]	200.00	[24]	200.00	[24]
	Opex [% Capex]	5		5	
	Lifetime [years]	20		20	
FT-Synthesis	Capex [€/t Naphtha per year]	300	[24]	300	[24]
	Opex [% Capex]	5		5	
	Lifetime	20		20	
Transport Methanol	[€/km * kg]	1.96 * 10^-6	[25]	1.96 * 10^-6	[25]
Transport FT-	[€/km * kg]	9.38 * 10^-7		9.38 * 10^-7	

Synthesis					
WACC	[%]	Country Specific	[26]	Country Specific	[26]

S3: Location Specific Data

Due to the condition that the production locations must show a higher capacity factor than in Germany, it was not possible to identify regions with a point source and wind as energy for the distance categories short and medium. The identified location in Germany is used as a proxy for these distance categories.

Table 3: Specific Data for the analyzed locations. The basin number is taken from ref. [1]. (DAC = Direct Air Capture, PS = Point Source, PV = Photovoltaic, Wind = Onshore Wind).

Country	Basin Number	Energy Source	Capacity Factor	Aware Factor	CO_2-Source	Transport Distance [km]	Installed Energy Capacity [MW]			Installed Electrolyzer Capacity [MW]		
							Methanol	**Naphtha**	**Delta**	**Methanol**	**Naphtha**	**Delta**
Argentina	10,967	Wind	72 %	1	DAC	13,613	221	316	30 %	172	272	37 %
Argentina	10,851	Wind	64 %	17	PS	13,068	239	343		194	306	
Argentina	10,987	Wind	71 %	100	DAC	13,651	223	319		174	275	
Ireland	4,569	Wind	63 %	8	DAC	1,433	245	350		197	311	
Germany	4,583	Wind	58 %	1	PS	0	253	364		214	339	
Germany	4,650	Wind	52 %	4	DAC	0	293	418		238	376	
United Kingdom	4,073	Wind	62 %	11	DAC	1,310	248	354		198	314	
Venezuela	8,199	Wind	69 %	6	DAC	8,312	269	384		179	284	
Western Sahara	7,564	Wind	75 %	94	DAC	4,091	211	301		165	261	
Turkey	6,395	PV	19 %	1	PS	2,248	800	1,151		666	1,054	
Saudi Arabia	7,333	PV	21 %	9	PS	4,372	711	1,023		592	937	
Bolivia	10,043	PV	24 %	4	PS	10,742	624	897		519	821	
Spain	6,353	PV	19 %	1	DAC	2,095	799	1,141		638	1,010	
China	6,914	PV	24 %	8	DAC	6,425	644	919		514	814	
Argentina	10,243	PV	27 %	1	DAC	11,266	564	805		450	713	
Morocco	6,530	PV	20 %	91	PS	2,221	728	1,048		606	959	
Saudi Arabia	7,119	PV	22 %	65	PS	3,342	671	965		558	883	
Chile	10,209	PV	25 %	100	PS	11,333	592	851		492	779	
Egypt	6,870	PV	20 %	59	DAC	2,583	757	1,081		605	957	
Namibia	10,295	PV	23 %	35	DAC	8,583	670	956		535	846	
Chile	10,138	PV	26 %	97	DAC	11,179	607	867		485	767	

S4: LCA Results

Table 4: LCA Results for the different impact categories. If water desalination was used as water source, a water incorporation of 0 was assumed. (GWI = Global Warming Impact, RMI = Raw Material Input, TMR = Total Material Requirement, M = Methanol, N = Naphtha).

Country	Basin Number	Energy Source	Capacity Factor	Aware Factor	Carbon Footprint		Material Footprint				Water Footprint				Land Footprint	
					GWI [kg CO_2 eq./MJ]		RMI [kg/kg]		TMR [kg/kg]		Incorporation [l/MJ]		Evaporation [l/MJ]		Occupation [m^2*a]	
					M	N	M	N	M	N	M	N	M	N	M	N
Argentina	10,851	Wind	64%	17	-0.049	-0.056	0.04	0.05	0.05	0.07	0.00	0.00	0.460	0.566	0.001	0.001
Argentina	10,967	Wind	72%	1	-0.040	-0.042	0.04	0.06	0.06	0.08	0.92	0.98	0.644	0.714	0.001	0.001
Argentina	10,987	Wind	71%	100	-0.040	-0.045	0.04	0.06	0.06	0.08	0.00	0.00	0.645	0.767	0.001	0.001
Argentina	10,243	PV	27%	1	-0.022	-0.021	0.07	0.08	0.10	0.12	5.33	5.69	3.232	4.266	0.012	0.016
Bolivia	10,043	PV	24%	4	-0.034	-0.034	0.05	0.07	0.07	0.10	0.22	0.23	3.102	4.188	0.012	0.017
Chile	10,209	PV	25%	100	-0.035	-0.036	0.05	0.06	0.07	0.10	0.00	0.00	6.309	8.651	0.012	0.016
Chile	10,138	PV	26%	97	-0.020	-0.019	0.07	0.09	0.10	0.13	0.00	0.00	3.452	4.547	0.012	0.017
China	6,914	PV	24%	8	-0.019	-0.017	0.07	0.10	0.11	0.14	0.44	0.47	3.641	4.823	0.013	0.018
Egypt	6,870	PV	20%	59	-0.015	-0.010	0.08	0.11	0.12	0.16	0.00	0.00	4.213	5.644	0.015	0.021
Germany	4,583	Wind	58%	1	-0.050	-0.054	0.04	0.05	0.05	0.07	0.22	0.24	0.374	0.515	0.000	0.001
Germany	4,650	Wind	52%	4	-0.034	-0.034	0.06	0.07	0.07	0.10	0.06	0.06	0.613	0.779	0.001	0.001
Ireland	4,569	Wind	63%	8	-0.035	-0.035	0.05	0.06	0.06	0.09	0.42	0.45	0.551	0.693	0.001	0.001
Morocco	6,530	PV	20%	91	-0.033	-0.031	0.06	0.08	0.08	0.12	0.00	0.00	3.554	4.880	0.014	0.020
Namibia	10,295	PV	23%	35	-0.018	-0.015	0.08	0.10	0.11	0.14	0.00	0.00	5.096	6.812	0.014	0.019
Saudi Arabia	7,119	PV	22%	65	-0.035	-0.033	0.05	0.07	0.08	0.11	0.00	0.00	3.265	4.493	0.013	0.018
Saudi Arabia	7,333	PV	21%	9	-0.033	-0.028	0.05	0.07	0.08	0.11	0.05	0.06	3.475	4.743	0.014	0.019
Spain	6,353	PV	19%	1	-0.006	0.002	0.09	0.12	0.13	0.17	0.04	0.05	4.373	5.809	0.016	0.022
Turkey	6,395	PV	19%	1	-0.030	-0.027	0.06	0.08	0.09	0.13	0.49	0.52	3.891	5.341	0.016	0.022
United Kingdom	4,073	Wind	62%	11	-0.035	-0.035	0.05	0.07	0.07	0.09	0.00	0.00	0.554	0.700	0.001	0.001
Venezuela	8,199	Wind	69%	6	-0.040	-0.042	0.05	0.06	0.06	0.08	0.33	0.35	0.667	0.783	0.001	0.001
Western Sahara	7,564	Wind	75%	94	-0.043	-0.044	0.04	0.05	0.05	0.07	0.00	0.00	0.571	0.696	0.001	0.001
Fossil based Process		--			0.034	0.010	0.05	0.03	0.05	0.04	0.00	0.00	0.3697	0.3309	0.0003	0.0003

S5: Results of the contribution Analysis

For the climate footprint, the heat demand of the CO_2-capture process (36%) as well as the energy (27%) and material supply (23%) of the supply chain are the main drivers. This is especially the case for DAC production systems for which the contribution of the capture process is on average about 13% higher (41% vs. 28%) than for systems based on point sources. The product synthesis (7%) and the transport (6%) only have a minor impact. Hence, there is a large potential for further optimization in case for scope 1 as well as for scope 3 emissions. The resulting negative climate footprint could be twice as high if the whole supply chain and the CO_2-capture process would be defossilized.

In case of the material footprint, the demand for different metal ores (51 %) is the main driver for environmental impacts related to the material requirement. More specifically, for wind-based systems, copper and iron are the main drivers, while for PV-based systems copper, aluminum as well as silver are the dominating metal flows. Those metals are important for the construction processes of the respective energy plants. The fossil fuel supply within the supply chain makes up to 26 % of the RMI. In case of minerals (23 %), construction materials like cement are the main contributors. Hence, a higher secondary input rate for metals in combination with a defossilization of the energy supply would be necessary to significantly reduce the RMI of CO_2-based chemicals and accommodate trade-offs between climate footprint reduction and the material footprint.

The main drivers for water evaporation are manufacturing processes (42 %) with the production of chemicals and base metals showing the highest contribution. Furthermore, the energy supply has the second highest (39 %) impact, which is mostly related to fossil-based power plants. The mining processes for fossil fuels (14 %) and metals (5 %) show a minor impact. Therefore, an increased efficiency in water use in combination with a defossilization of the energy supply are the most important measures to reduce the water footprint for CO_2-based chemicals.

S5-1: Global Warming Impact

Table 5: Contribution to the climate footprint of CO_2-based Methanol production.

All Locations	**Relative**			**Absolute [kg CO_2equiv. /MJ]**		
	Mean	**Min**	**Max**	**Mean**	**Min**	**Max**
Scope 1 (Synthesis)	7%	4%	12%	0.05	0.05	0.05
Scope 2 (Capture)	36%	23%	57%	0.26	0.11	0.46
Scope 3 (Energy Supply)	27%	15%	42%	0.22	0.06	0.41
Scope 3 (Material Supply)	23%	16%	37%	0.17	0.07	0.29
Scope 3 (Transport)	6%	3%	13%	0.05	0.01	0.08
Total emissions	100%	100%	100%	0.74	0.37	1.28
Scope 1 (Sequestration)	-211%	-385%	-110%	- 1.41	- 1.42	- 1.41
Net emissions	-111%	-285%	-10%	- 0.67	- 1.05	- 0.13

S5-2: Raw Material Input

Table 6: Contribution of different Raw Materials to the Raw Material Input.

All Locations	Relative			Absolute [kg/kg]		
	Mean	Min	Max	Mean	Min	Max
Fossil Fuels	26%	18%	31%	0.32	0.14	0.61
Metals	51%	46%	58%	0.61	0.40	1.06
Minerals	23%	11%	32%	0.26	0.11	0.34

S5-3: Water Evaporation

Table 7:Contribution of different Raw Materials to Water Evaporation

All Locations	Relative			Absolute [m^3/MJ]		
	Mean	Min	Max	Mean	Min	Max
Energy Supply	39%	29%	55%	0.016	0.003	0.029
Fossil Fuel Mining	14%	9%	20%	0.005	0.001	0.010
Manufacturing Processes	42%	18%	60%	0.026	0.002	0.052
Metals Mining	5%	1%	15%	0.001	0.001	0.001

S6: Detailed Results of the economic assessment

To enhance the validity of the economic assessment, the calculated results for the levelized costs of electricity were compared with existing studies which contain measured cost data and prognoses for renewable electricity generation [10, 27, 28, 29]. For wind energy, accurate data was available for every region. Therefore, the endogenously calculated LCOE were modified accordingly. In case a range was available in the literature, the minimum LCOE value was chosen since the input data for the capacity factor which serves as basis for the plant modelling depicts the technical potential (see SI-8). According to Fraunhofer ISE [29] a LCOE reduction of 7 % was assumed for wind electricity between 2020 and 2030.

S6-1: Methanol

Table 8: Calculated levelized production costs of the different process steps and years for CO_2-based methanol. To calculate the CO_2-avoidance costs for each location, different yearly changes in the oil price were assumed (-1%; +2%; +4%). (WACC = Weighted average costs of capital; LCOH$_2$/CO$_2$/MeOH/Naphtha) = Levelized Costs of H_2/CO_2/Methanol/Naphtha production). [26]

Location	WACC[1]	LCOH$_2$ [€/kg]		LCOCO$_2$ [€/kg]		LCONaphtha [€/t]		CO_2-Avoidance Costs [€/t CO_2]					
	Status quo	Status quo	2030	Status quo	2030	Status quo	2030	Status quo			2030		
								-1%	2%	4%	-1%	2%	4%
Argentina	10.4%	6.9 €	3.0 €	143 €	68 €	1,666 €	773 €	1,167 €	1,102 €	1,076 €	429 €	270 €	194 €
Argentina	10.4%	4.4 €	2.5 €	136 €	64 €	1,179 €	691 €	567 €	518 €	498 €	271 €	150 €	93 €
Argentina	10.4%	4.4 €	2.5 €	136 €	64 €	1,181 €	691 €	568 €	519 €	499 €	271 €	150 €	93 €
Argentina	10.4%	4.6 €	2.5 €	42 €	32 €	1,072 €	653 €	440 €	397 €	380 €	218 €	112 €	61 €
Bolivia	7.4%	6.4 €	3.1 €	37 €	29 €	1,414 €	747 €	794 €	734 €	709 €	340 €	200 €	133 €
Chile	4.9%	4.9 €	2.3 €	114 €	58 €	1,208 €	624 €	806 €	725 €	691 €	315 €	134 €	46 €
Chile	4.9%	4.9 €	2.4 €	34 €	26 €	1,111 €	588 €	561 €	498 €	472 €	220 €	79 €	11 €
China	7.4%	6.3 €	3.1 €	127 €	63 €	1,519 €	780 €	1,091 €	1,016 €	985 €	457 €	281 €	197 €
Egypt	7.4%	7.4 €	3.6 €	130 €	65 €	1,742 €	889 €	1,396 €	1,315 €	1,281 €	599 €	410 €	318 €
Germany	3.0%	4.0 €	2.4 €	143 €	93 €	1,072 €	673 €	542 €	473 €	444 €	284 €	136 €	63 €
Germany	3.0%	4.0 €	2.4 €	52 €	45 €	933 €	602 €	364 €	308 €	284 €	191 €	71 €	11 €
Great Britain	7.3%	4.2 €	2.3 €	149 €	86 €	1,112 €	659 €	560 €	502 €	478 €	268 €	133 €	68 €
Ireland	8.4%	4.3 €	2.4 €	155 €	88 €	1,148 €	676 €	584 €	528 €	505 €	279 €	147 €	83 €
Morocco	10.4%	5.0 €	3.0 €	136 €	64 €	1,284 €	784 €	609 €	562 €	543 €	317 €	202 €	147 €
Morocco	7.4%	7.4 €	3.6 €	37 €	29 €	1,615 €	838 €	937 €	877 €	852 €	405 €	265 €	198 €
Namibia	7.4%	6.6 €	3.2 €	128 €	64 €	1,576 €	810 €	1,177 €	1,100 €	1,068 €	499 €	318 €	231 €
Saudi Arabia	4.2%	5.6 €	2.7 €	33 €	26 €	1,231 €	638 €	666 €	599 €	571 €	264 €	116 €	44 €
Saudi Arabia	4.2%	5.3 €	2.5 €	33 €	26 €	1,163 €	602 €	600 €	535 €	508 €	232 €	89 €	18 €
Spain	5%	6.7 €	3.2 €	180 €	123 €	1,661 €	888 €	1,619 €	1,512 €	1,467 €	735 €	495 €	377 €
Turkey	5.4%	7.0 €	3.4 €	41 €	34 €	1,523 €	789 €	907 €	840 €	812 €	386 €	236 €	162 €
Venezuela	10.4%	4.5 €	2.5 €	182 €	108 €	1,241 €	746 €	602 €	554 €	534 €	304 €	185 €	128 €

S6-2: Naphtha

Table 9: Calculated levelized production costs of the different process steps and years for CO2-based naphtha. To calculate the CO_2-avoidance costs for each location, different yearly changes in the oil price were assumed (WACC = Weighted average costs of capital; $LCOH_2/CO_2$/Naphtha) = Levelized Costs of H_2/CO_2/Naphtha production).[26]

Location	WACC[1]	LCOH$_2$ [€/kg]		LCOCO$_2$ [€/kg]		LCONaphtha [€/t]		CO_2-Avoidance Costs [€/t CO_2]					
	Status quo	Status quo	2030	Status quo	2030	Status quo	2030	Status quo			2030		
								-1%	2%	4%	-1%	2%	4%
Argentina	10.4%	6.8 €	3.4 €	163 €	84 €	4,911 €	2,465 €	3,307 €	3,235 €	3,207 €	1,548 €	1,372 €	1,289 €
Argentina	10.4%	4.4 €	2.9 €	159 €	79 €	3,398 €	2,198 €	1,307 €	1,265 €	1,248 €	803 €	699 €	650 €
Argentina	10.4%	4.4 €	2.5 €	159 €	79 €	3,400 €	1,914 €	1,241 €	1,200 €	1,184 €	645 €	546 €	499 €
Argentina	10.4%	4.6 €	2.5 €	49 €	38 €	3,109 €	1,801 €	938 €	905 €	891 €	501 €	418 €	379 €
Bolivia	7%	6.4 €	4.1 €	44 €	34 €	4,207 €	2,732 €	2,311 €	2,245 €	2,218 €	1,442 €	1,290 €	1,216 €
Chile	5%	4.9 €	2.3 €	124 €	66 €	3,527 €	1,749 €	2,509 €	2,415 €	2,375 €	1,122 €	912 €	809 €
Chile	5%	4.9 €	2.4 €	39 €	30 €	3,289 €	1,652 €	1,443 €	1,384 €	1,359 €	649 €	519 €	455 €
China	7.4%	6.3 €	4.0 €	143 €	76 €	4,498 €	2,844 €	3,498 €	3,406 €	3,368 €	2,125 €	1,910 €	1,807 €
Egypt	7%	7.4 €	3.6 €	148 €	80 €	5,205 €	2,591 €	5,392 €	5,271 €	5,220 €	2,511 €	2,229 €	2,093 €
Germany	3%	4.0 €	2.4 €	153 €	102 €	3,082 €	1,881 €	1,403 €	1,338 €	1,310 €	799 €	658 €	588 €
Germany	3%	4.0 €	2.3 €	55 €	47 €	2,723 €	1,687 €	836 €	791 €	772 €	480 €	383 €	335 €
Great Britain	7%	4.2 €	2.3 €	157 €	92 €	3,204 €	1,837 €	1,421 €	1,366 €	1,343 €	752 €	624 €	563 €
Ireland	8%	4.3 €	2.8 €	168 €	98 €	3,309 €	2,150 €	1,470 €	1,417 €	1,396 €	907 €	782 €	722 €
Morocco	10.4%	5.0 €	3.0 €	163 €	81 €	3,757 €	2,231 €	1,414 €	1,373 €	1,357 €	790 €	690 €	642 €
Morocco	7%	7.4 €	3.6 €	45 €	35 €	4,869 €	2,442 €	2,515 €	2,455 €	2,429 €	1,176 €	1,034 €	966 €
Namibia	7%	6.6 €	3.2 €	144 €	77 €	4,660 €	2,322 €	3,901 €	3,802 €	3,761 €	1,803 €	1,573 €	1,462 €
Saudi Arabia	4%	5.6 €	3.3 €	39 €	30 €	3,696 €	2,233 €	2,004 €	1,930 €	1,899 €	1,143 €	982 €	902 €
Saudi Arabia	4%	5.3 €	2.5 €	38 €	30 €	3,490 €	1,738 €	1,636 €	1,572 €	1,545 €	734 €	594 €	525 €
Spain	5%	6.7 €	4.1 €	186 €	125 €	4,873 €	3,046 €	13,200 €	12,857 €	12,713 €	7,943 €	7,175 €	6,801 €
Turkey	5%	7.0 €	4.3 €	47 €	38 €	4,588 €	2,863 €	2,580 €	2,509 €	2,479 €	1,546 €	1,386 €	1,308 €
Venezuela	10.4%	4.5 €	3.0 €	196 €	116 €	3,545 €	2,339 €	1,385 €	1,342 €	1,325 €	873 €	768 €	718 €

S6-3: Cost Composition

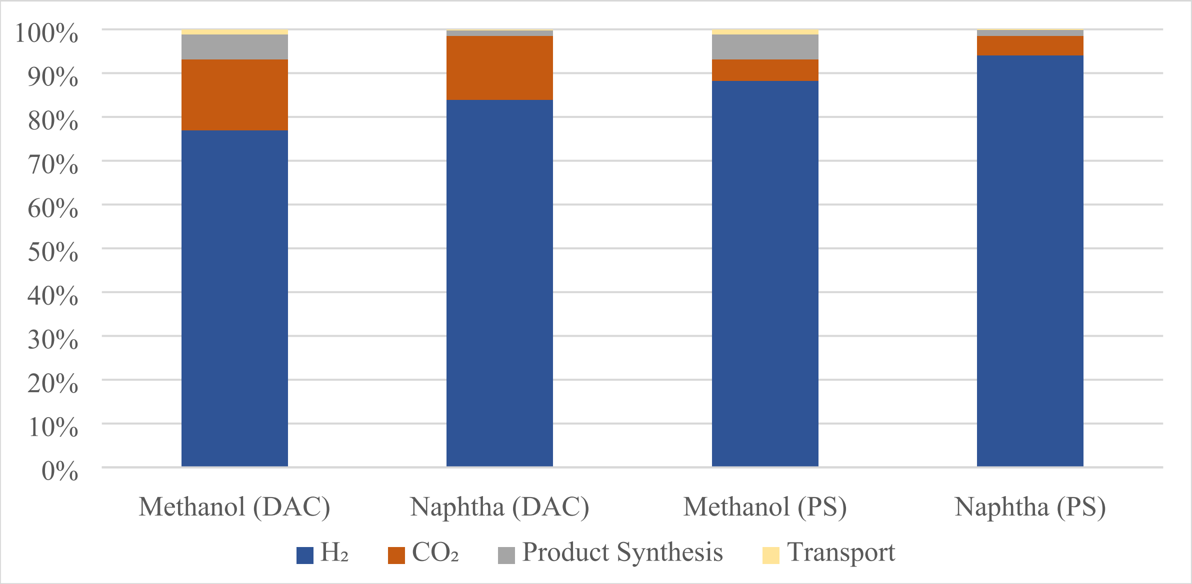

Figure 2: Average cost composition for the production and import of CO_2-based methanol and naphtha using Direct Air Capture (DAC) or a point source (PS) as CO_2 source.

S6-4: Net Present Value

For the NPV calculation the following prices were assumed for the fossil methanol (2020: 322€/t, 2030: 292 up to 477 €/t) and naphtha production (2020: 414€/t, 2030: 374 €/t up to 616 €/t).

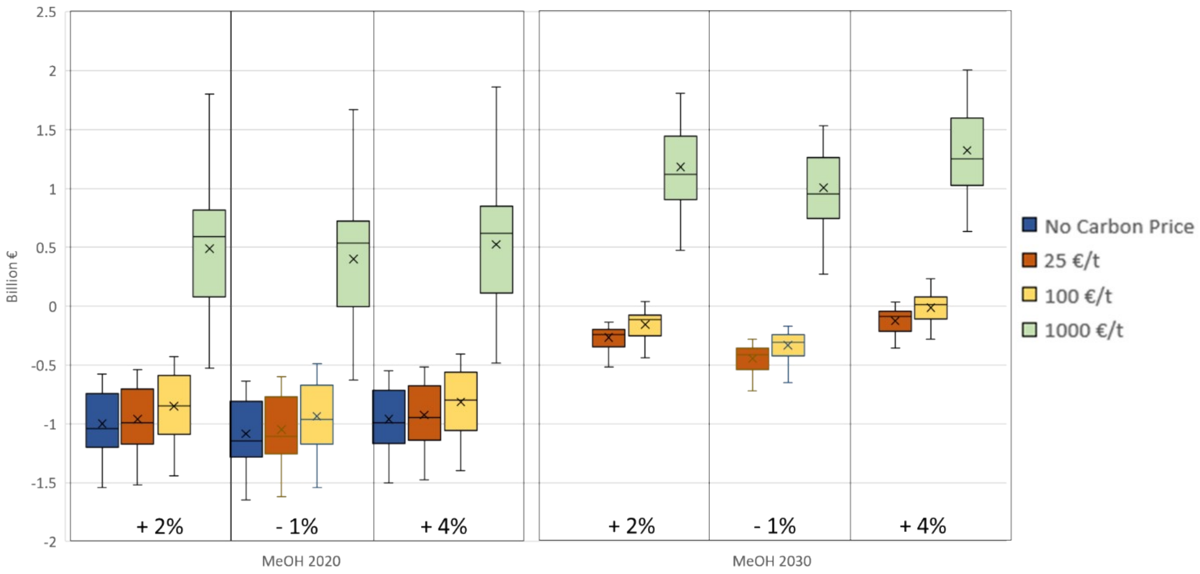

Figure 3: Results for the Net Present Value for CO_2-based Methanol production, depending on the oil price development (+4%, +2%, -1%) and the carbon price in € per ton CO_2 avoided.

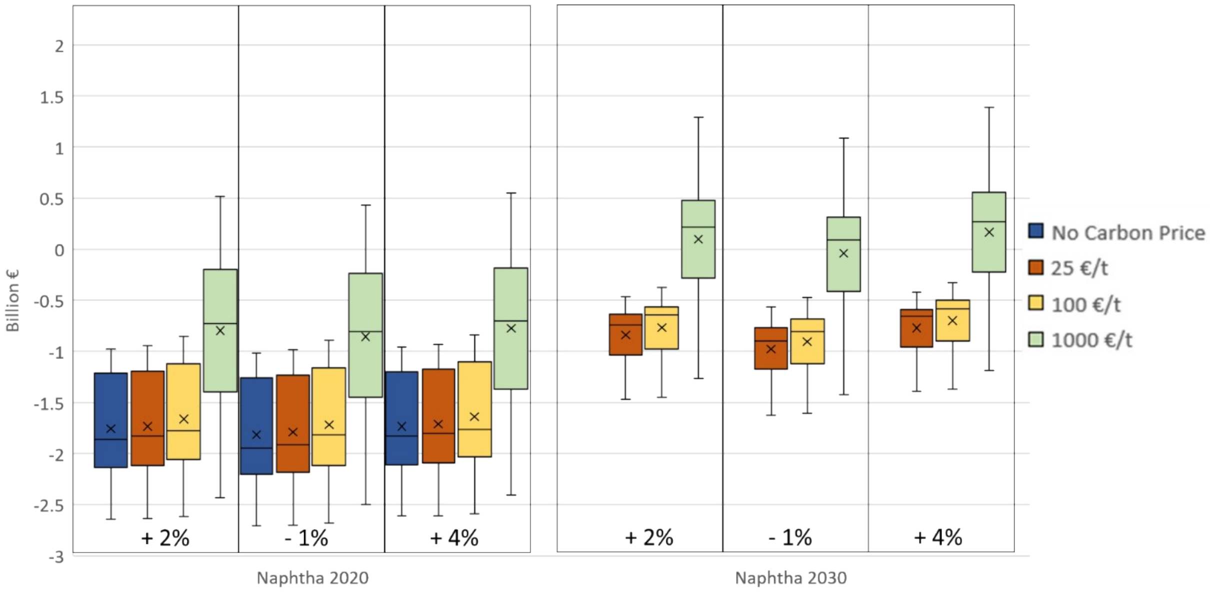

Figure 4: Results for the Net Present Value for CO_2-based Naphtha production, depending on the oil price development (+4%, +2%, -1%) and the carbon price in € per ton CO_2 avoided.

S7: Uncertainty Analysis

S7-1: Monte Carlo Analysis

Table 10: Results of the Monte Carlo Analysis for one onshore wind and one photovoltaic location for CO_2-based Methanol. (CF = Capacity Factor, GWI = Global Warming Impact, RMI = Raw Material Input, STD = Standard Deviation).

Energy Source	Country (CF)	Indicator	Mean	Min	Max	STD
Wind	Argentina (71 %)	GWI	-0.84	-0.95	-0.67	0.05
		RMI	0.95	0.75	1.24	0.07
Photovoltaic	Chile (26 %)	GWI	-0.36	-0.55	-0.01	0.08
		RMI	1.52	1.2	2.06	0.16

S7-2: Sensitivity Analysis

In the sensitivity analysis, the influence of a capacity factor alteration on the ecological and economic results was calculated for methanol and naphtha production, differentiated between the energy sources. To exclude the influence of different CO_2 sources, the sensitivity analysis was conducted only for systems using an identical CO_2 source. Because more results are available for systems using Direct Air Capture, this system type was selected for the sensitivity analysis. The resulting sensitivities correspond to the slope of the trend line calculated by linear regression analysis.

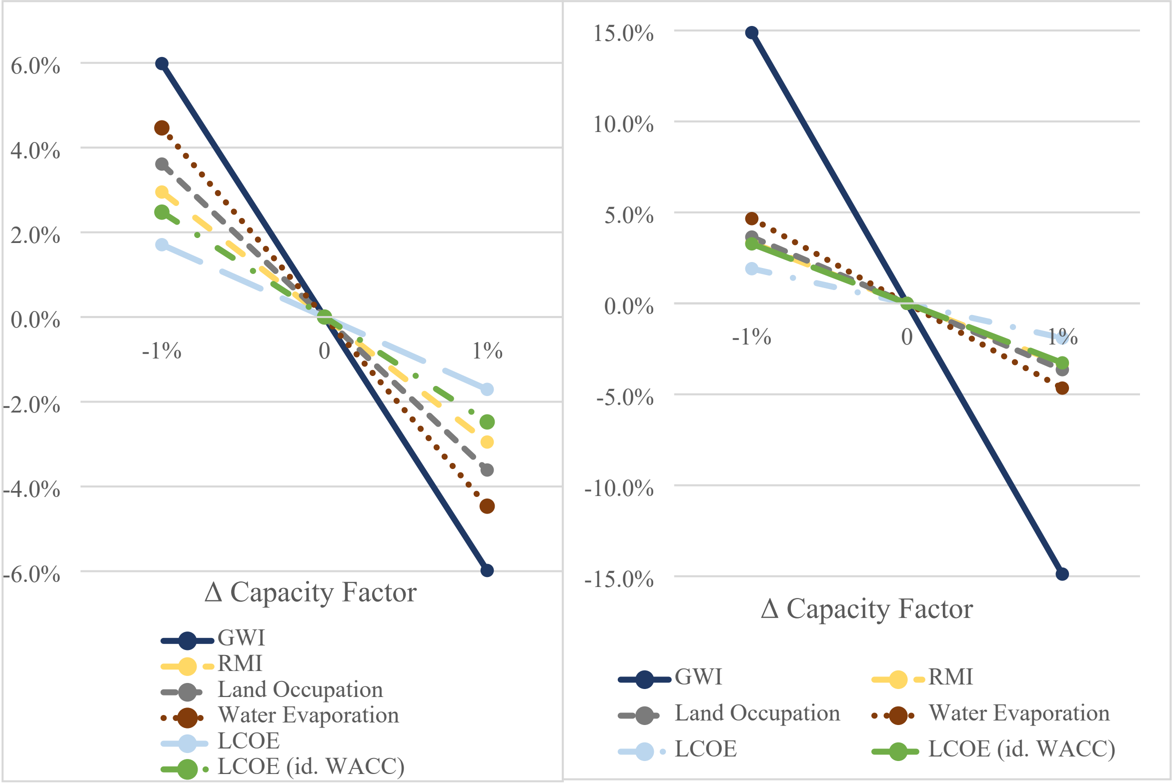

Figure 5: Results of the sensitivity analysis for CO_2-based methanol (left) and naphtha (right) production with photovoltaic plants as electricity and DAC as CO_2 source (GWI = Global Warming Impact; RMI = Raw Material Input; LCOE = Levelized Costs of Electricity; id. WACC = identical weighted average costs of capital of 5 % for all locations).

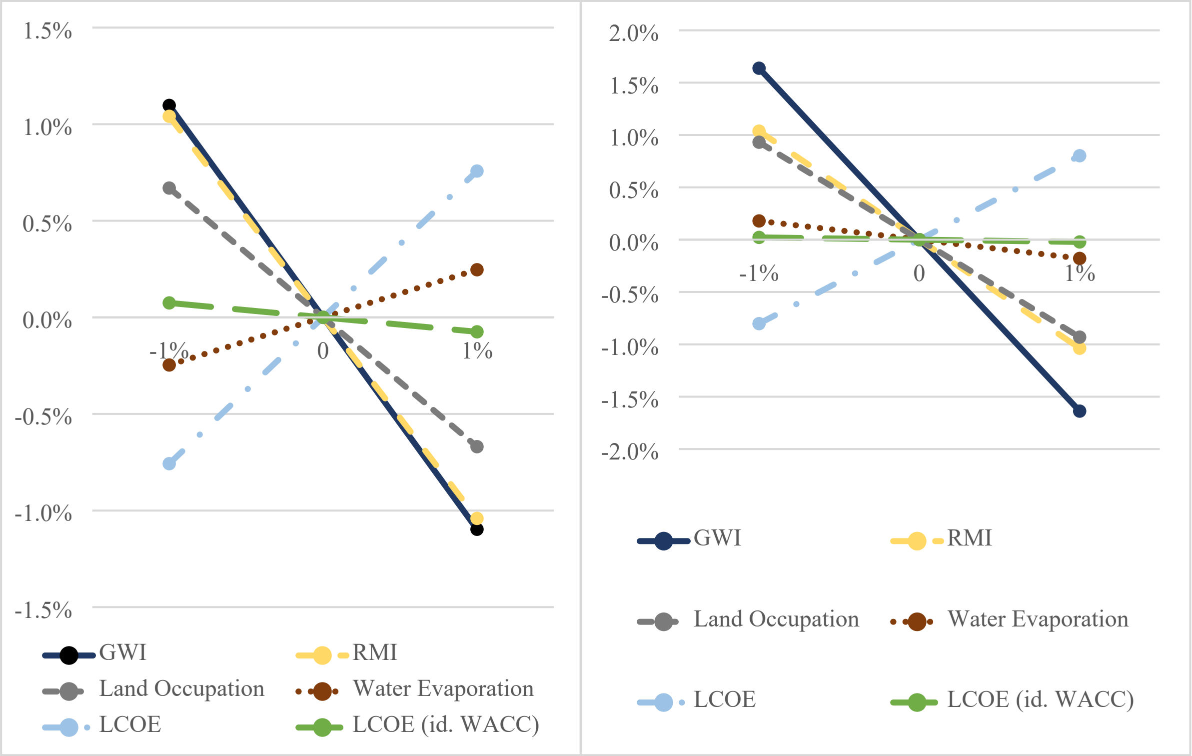

Figure 6: Results of the sensitivity analysis for CO_2-based methanol (left) and naphtha (right) production with onshore wind plants as electricity and DAC as CO_2 source. (GWI = Global Warming Impact; RMI = Raw Material Input; LCOE = Levelized Costs of Electricity; id. WACC = identical weighted average costs of capital of 5 % for all locations).

S7-3: Manova

A one-way Manova was conducted (n = 21) using the software SPSS Statistics, version 26. As significance level, an alpha-value of 0.05 was assumed. The results of the multivariate analysis (Table 11) show the significant effect ($p < 0.05$) of the variables *CO_2* and *Energy source* on the combined dependent variables, while the *Water Source* and *Transport Distance* do not show a significant effect.

Table 11: Results of the multivariate test for the independent variables

Independent Variable	Test procedure	Value	Hypothesis df	Error df	F	Significance
Water Source	Wilks-Lambda	0.583	5	9	1,288	0.348
CO_2 Source	Wilks-Lambda	0.075	5	9	22,087	0.000
Energy Source	Wilks-Lambda	0.006	5	9	281,474	0.000
Transport Distance	Wilks-Lambda	0.004	5	9	126,939	0.063

The results of the post-hoc tests (Table 12) show if there are significant effects of the independent variables *Energy* and *CO_2 source* on single dependent variables. While the values for the energy source show a significant effect on all dependent variables, the CO_2 source only shows a significant effect on the GWI and RMI.

Table 12: Results of the post-hoc tests for those independent variables with a significant effect on the combined variable (GWI = Global Warming Impact, RMI = Raw Material Input, Evaporation, LCO MeOH = Levelized Costs of Methanol production)

Independet Variable	Dependent Variable	Typ III Sum of Squares	Mean of squares	F	Significance
CO_2 Source	GWI	0.352	0.352	46.343	0.000
	RMI	0.538	0.538	24.056	0.000
	Water Evaporation	2.962E-05	2.962E-05	0.108	0.747
	Land Occupation	6.816E-08	6.816E-08	0.034	0.856
	LCO MeOH	31473.052	31473.052	0.867	0.369
Energy Source	GWI	0.648	0.648	85.248	0.000
	RMI	0.910	0.910	40.704	0.000
	Water Evaporation	0.022	0.022	79.360	0.000
	Land Occupation	0.001	0.001	351.602	0.000
	LCO MeOH	538712.805	538712.805	17.961	0.001

S8: Data Quality Assessment

Within this study, different types of data sets were utilized. To assess the resource availability for energy, water, and CO_2 datasets for their distribution on a global scale were applied. To be independent of periodical fluctuations of the regional resource availability, only data sources which depict long-term yearly averages were used. To enable a direct comparison between different locations, the actuality, consistency, and completeness of the datasets are very important aspects. Therefore, for energy and water availability state-of-the-art datasets were used which cover all global regions instead of combining data from different regions, sources, and publication dates. Even though site specific data might be more accurate, the use of several different datasets and sources would involve consistency errors due to the use of different methods and premises. This procedure was selected, because a valid comparability of the different locations was seen as a very important aspect in our analysis. However, the capacity factors for energy generation used in the models depict the technical optimum. Capacity factors reached in practice are typically lower but show a continuously increasing trend over the last decade[30]. In consequence, the results in this study possibly underestimate the actual absolute environmental impacts and production costs in the status quo, nevertheless the relations between the different locations would be identical if lower values for the capacity factors would have been used. In case of CO_2, the point sources were identified using publicly available information from industry reports, scientific studies, or company reports. However, the data availability differed between different regions and sectors. For example, while for Europe and North America detailed information about CO_2-point sources was available, no, or only few data were available for CO_2 point sources in China. Furthermore, the available data for cement and waste incineration plants was very good, while the available information about steel plants using a blast furnace only covers around 30 % of the global production capacity. Therefore, the completeness of the data can be enhanced for certain regions and sectors. Nevertheless, significant deviations of the results are not expected because of the number of already included point sources.

For life cycle modelling, process and cost data from the literature was combined with a state-of-the-art life cycle-database (ecoinvent 3.5). The process and cost data for the CO_2-based production processes were derived from recent publications. According to the data quality assessment for life cycle data introduced by Weidema et al. [31] their overall reliability and temporal correlation can be assessed as good. Since the material requirement for the electrolyzer and sequestration plants were also considered in this study the completeness can be assessed as good, too. However, especially for the CO_2-sequestration and electrolyzer plants only demonstration plants with smaller production volumes than considered in this study exist, wherefore the technological correlation is only sufficient. Energy and material requirements of production plants with the assumed production volume can only be estimated. To handle this aspect and shed light on the uncertainty and future values for the environmental impacts and LCOEs, value ranges were considered in combination with an MCA and scenario analysis, additional to the modelling with discrete values. Furthermore, the background data was extracted from the life-cycle database which was last actualized in 2018. Thus, the actuality of the database is good, nevertheless the specific actuality and technological correlation of the included processes differ. To increase the quality of the results important background processes, such as the construction of a wind power or solar power plant as well as RSWO were cross checked with literature data and actualized if more actual data was available.

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