<u>Supplementary Information:</u> Energy efficiency and economic assessment of imported energy carriers based on renewable electricity

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S1: Energy efficiency analysis: parameter Inventory

Table 1 Process parameters for the PtX pathways (values for the optimistic cases indicated in italics)

PtX pathway for renewable liquid hydrogen – LH_2							
H_2O desalination & deionization		**PEM water electrolysis**		**H2 liquefaction**		**Ship transport LH2**	
Electricity Desal. [kWh$_{el}$ (Nm^3)$^{-1}$]	3.75	Electricity [kWh$_{el}$ Nm^3(H_2)$^{-1}$]	4.81 *4.46*	Electricity [kWh$_{el}$ kg(LH_2)$^{-1}$]	6.0 *8.0*	Fuel demand [kWh tkm^{-1}]	0.181
Electricity Deioniz. [kWh$_{el}$ (Nm^3)$^{-1}$]	0.45	H_2O [kg(H_2O) kg(H_2)$^{-1}$]	10	H_2 [kg(H_2) kg(LH_2)$^{-1}$]	1.016	Boil-off rate [% d^{-1}]	0.20
PtX Pathway for renewable H_2 via LOHC – LOHC-H_2							
H2O desalination & deionization		**PEM water electrolyis**		**Ship transport LOHC**		**Dehydrogenation**	
Electricity Desal. [kWh$_{el}$ (Nm^3)$^{-1}$]	3.75	Electricity [kWh$_{el}$ Nm^3(H_2)$^{-1}$]	4.81 *4.46*	Fuel demand [kWh tkm^{-1}]	0.141 (related to LOHC mass)	Heat demand [% of $H_{2,LHV}$]	30 *25*
Electricity Deioniz. [kWh$_{el}$ (Nm^3)$^{-1}$]	0.45	H_2O [kg(H_2O) kg(H_2)$^{-1}$]	10	Boil-off rate [% d^{-1}]	-		
PtX Pathway for renewable liquid methane - LCH_4							
H2O desalination & deionization		**PEM water electrolyis**		**Direct Air Capture**			
Electricity Desal. [kWh$_{el}$ (Nm^3)$^{-1}$]	3.75	Electricity [kWh$_{el}$ Nm^3(H_2)$^{-1}$]	4.81 *4.46*	Electricity [kWh$_{el}$ kg(CO_2)$^{-1}$]	0.25 *0.20*		
Electricity Deioniz. [kWh$_{el}$ (Nm^3)$^{-1}$]	0.45	H_2O [kg(H_2O) kg(H_2)$^{-1}$]	10	Heat [kWh$_{th}$ kg(CO_2)$^{-1}$]	1.75 *1.50*		
Methanation		**Liquefaction**		**Ship transport**			
H2_in [kg(H_2) kg(CH_4)$^{-1}$]	0.52	Electricity [kWh$_{el}$ kg(CH_4)$^{-1}$]	0.50 *0.25*	Fuel demand [kWh tkm^{-1}]	0.026		
CO2_in [kg(CO_2) kg(CH_4)$^{-1}$]	2.94			Boil-off rate [% d^{-1}]	0.15		
Electricity_in [kWh$_{el}$ kg(CH_4)$^{-1}$]	0.14						
Excess heat for DAC [kWh$_{th}$ kg(CH_4)$^{-1}$]	2.99						
PtX Pathway for renewable methanol - CH_3OH							
H2O desalination & deionization		**PEM water electrolyis**		**Direct Air Capture**			
Electricity Desal. [kWh$_{el}$ (Nm^3)$^{-1}$]	3.75	Electricity [kWh$_{el}$ Nm^3(H_2)$^{-1}$]	4.81 *4.46*	Electricity [kWh$_{el}$ kg(CO_2)$^{-1}$]	0.25 *0.20*		
Electricity Deioniz. [kWh$_{el}$ (Nm^3)$^{-1}$]	0.45	H_2O [kg(H_2O) kg(H_2)$^{-1}$]	10	Heat [kWh$_{th}$ kg(CO_2)$^{-1}$]	1.75 *1.50*		
Methanol step		**Ship transport**					
H2_in [kg(H_2) kg(CH_3OH)$^{-1}$]	0.20	Fuel demand [kWh tkm^{-1}]	0.010				
CO2_in [kg(CO_2) kg(CH_3OH)$^{-1}$]	1.43	Boil-off rate [% d^{-1}]	-				
Electricity_in [kWh$_{el}$ kg(CH_3OH)$^{-1}$]	0.31						
Excess heat for DAC [kWh$_{th}$ kg(CH_3OH)$^{-1}$]	0.09						
PtX pathway for renewable ammonia - NH_3							
H2O desalination & deionization		**PEM water electrolyis**		**Cryogenic Air Separation**			
Electricity Desal. [kWh$_{el}$ (Nm^3)$^{-1}$]	3.75	Electricity [kWh$_{el}$ Nm^3(H_2)$^{-1}$]	4.81 *4.46*	Electricity [kWh$_{el}$ kg(LN_2)$^{-1}$]	0.80 *0.50*		
Electricity Deioniz. [kWh$_{el}$ (Nm^3)$^{-1}$]	0.45	H_2O [kg(H_2O) kg(H_2)$^{-1}$]	10				
Ammonia step		**Ship transport**					
H2_in [kg(H_2) kg(NH_3)$^{-1}$]	0.18	Fuel demand [kWh tkm^{-1}]	0.016				
N2_in [kg(N_2) kg(NH_3)$^{-1}$]	0.83	Boil-off rate [% d^{-1}]	0.04				
Electricity [kWh$_{el}$ kg(NH_3)$^{-1}$]	0.48						

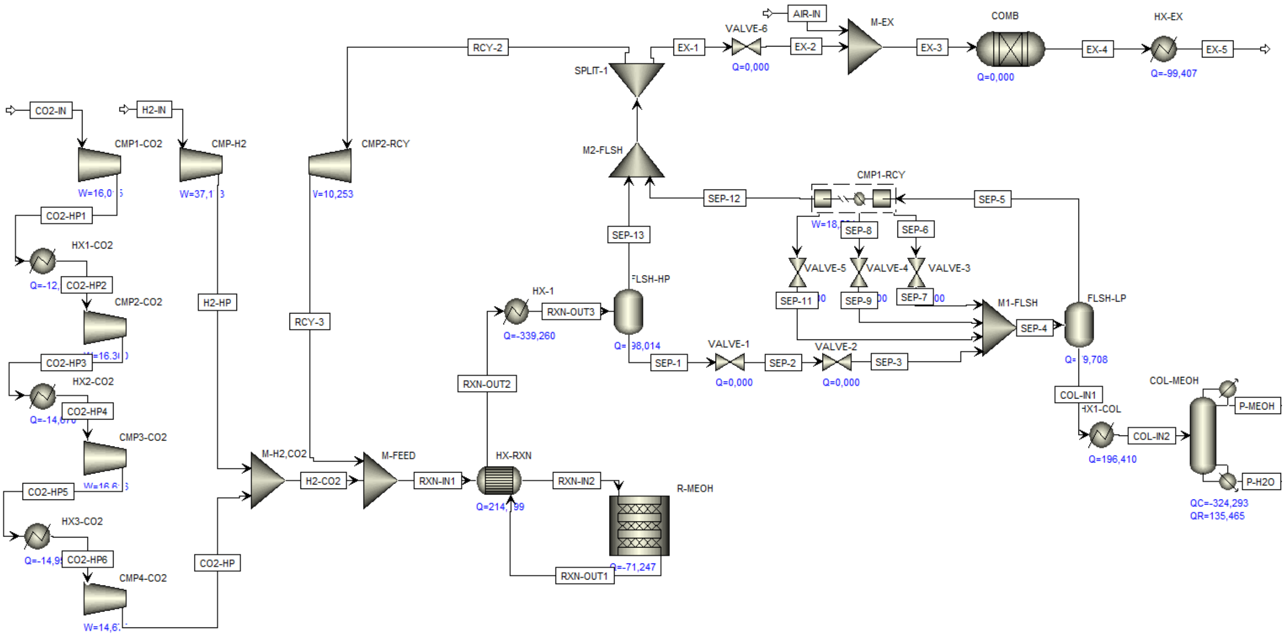


Figure 1 Process flow diagram for the methanol synthesis step (3.65 kt(CH3OH) a^{-1}) as modeled in ASPEN

S2: simulation background processes for the methanol and ammonia syntheses

The CO_2 based methanol process is based on the concept published by Bongartz et al.[1] which, in turn, used information on the concept from Pontzen et al.[2] and Van-Dal and Bouallou[3]. The process has been modeled in an ASPEN simulation for a capacity of 3.65 kt(CH3OH) a^{-1} (Figure 1) and uses a new kinetic model for a commercial state-of-the-art methanol catalyst (developed and published in near-term by Nestler et al., Fraunhofer ISE) for generation of conversion efficiencies and energy demands. The ammonia synthesis has also been modeled in ASPEN (Figure 2). The concept for heat integration has been assessed via Pinch methodology and enables heat integration for the DAC desorption cycle.

S3: Case study: simulation background for the RE plants

Calculation of wind electricity generation required information on wind speed and direction, temperature, air pressure at the respective hub height (80m) and the performance curve for a respective wind turbine (Siemens Gamesa G128 4.5 MW). Wind speeds have been extracted from the TMY by extrapolation from the measurement height (10 meters above ground level) to hub height applying the logarithmic wind profile:

$$\sum_n v_2 = v_1 * \frac{ln(\frac{h_2}{z_0})}{ln(\frac{h_1}{z_0})}$$

The roughness length (0.03, class 3) is derived from roughness layers of the DTU Global Wind Atlas. The change of air pressure with height was adjusted using the barometric formula.

The resulting representative weather year has been used in combination with the RE-simulation software “System Advisor Model” (SAM)[4] for simulation of fluctuating electricity generation via wind (Siemens Gamesa G128 4.5 $MW_{p,el}$) and photovoltaic (4 $kW_{p,el}$, 1-axis tracking) power plants (as exemplified by Figure 1).

S4: Case study: parameters for the economic assessment of the PtX pathways

This chapter is intended for further detailed description of the installed capacities, investment (CAPEX) and operational cost (OPEX).

Table 1 and 2 list the capacities, the investment and operational cost for the PtX pathways and their respective components. Key capacities are already described in the main article but at this point we will add more information on the remaining capacities.

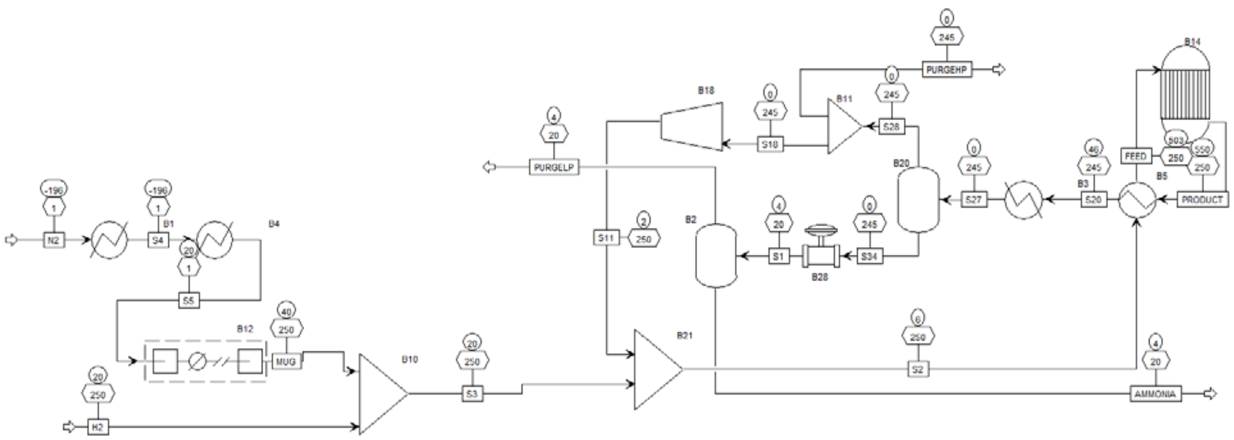


Figure 2 Process flow diagram for the ammonia synthesis step (236 kt(CH3OH) a^{-1}) as modeled in ASPEN

The desalination capacity is derived from the water demand of the PEM electrolysis of 10 kg(H_2O) kg$(H_2)^{-1}$. For the sake of simplicity no dynamic behaviour has been considered for the desalination. Buffering of water production and fluctuating electrolysis water demand could easily be realized by means of cost efficient water tanks.

The remaining capacities are a result of the H2ProSim simulation and the process and conversion parameter for the optimistic scenario as explained in Part I of the main article.

If investment cost data from literature has been available for different capacities the rule of six-tenths has been applied for estimation of investments at different capacities:

$$I_B = I_A * \left(\frac{C_B}{C_A}\right)^x$$

with

I_B = Investment cost for the component at capacity B

I_A = Known investment cost for the component at capacity A

C_B/C_A = Capacity ratio of the two components

x = Size exponent with 0.6 as chosen “hands-on” value for process equipment

For the steady state components (i.e. synthesis, capturing, liquefaction) a capacity factor of 91.3% (8500 h a^{-1}) is assumed to bear for maintenance and repair services.

The derivation of cost for the wind and PV electricity is described in the main article. **Electricity transmission** over a distance of 100 km from the RE location to the PtX plant site (next to the coast) is assumed to be realised via HVDC transmission. Corresponding costs of 2 € Mwh_{el}^{-1} are derived from published values for a 200 km HVDC line (4 € Mwh_{el}^{-1}).[5]

Specific investment and operational cost for the seawater reverse osmosis (SWRO) **desalination plant** is derived from Caldera et al.[6] who provide an extensive techno-economic assessment for SWRO plants for the cost year 2030.

PEM electrolysis system cost account for large-scale PEM systems in 2030 and are derived from a recent sector survey including manufacturer estimations for future electrolysis system performances depending on system size.[7] Lifetime of the PEM electrolysis system is assumed with 20 years whereas a replacement of the stacks is necessary once per system lifetime. This value is as well represented by the median value obtained from stakeholder statements in sector surveys.[7]

The share of stack replacement costs on total system cost is derived from cost share values for 5-100 MWel PEM systems.[8]

The assumed efficiency of the H_2 motor is based on manufacturer interviews[9] and can be assumed as almost constant over the entire power range by switching individual modules on and off.[10] Corresponding investment costs for the year 2030 are obtained from a study assessing H_2 production and large-scale cavern storage as well applying an H_2 motor.[10]

The parameters for the **H2 cavern** orientate on a cost curve for caverns differentiating in total storage capacity, the number of caverns and “green” and “brown” sites. Depending on the present H2 storage requirements, the costs vary between 50-100 € (m³ cavern)$^{-1}$. The initial H2 cavern pressure is considered with 115 bar. The resulting H2 cost have been included in the overall cost.

The cost for the **gas compressors** (H2, CO2, N2) are as well based on cost curves taking into account the installed compressor power.[11,12] The cost curves have been validated with existing offers for gas compressors at the Fraunhofer ISE.

Provision of N_2 via cryogenic air separation units (**ASU**) is based on publication of Matzen at al. for a 1010 t(N_2) d^{-1} ASU plant. For the present case study and a capacity of 556 t(N_2) d^{-1} the investment sums up to ~55 € (t(N_2)*a)$^{-1}$. The

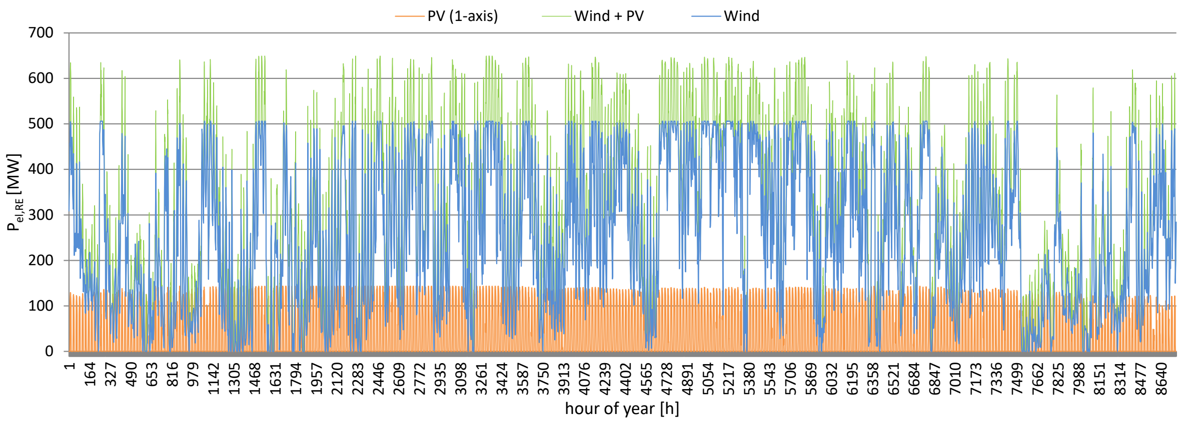


Figure 3 Renewable electricity generation data based on weather data for the assessed Moroccan location. Installed wind and PV capacities orientate on the PtX pathway LH2.

corresponding cost for capturing of atmospheric CO2 via direct air capturing (**DAC**) is obtained from Fasihi et al.[13] providing a techno-economic assessment of CO2 DAC plants.

Synthesis of CO2-based CH4 via the **Sabatier** process and related economics are based on a recent study[14] by the ludwig bölkow systemtechnik GmbH considering a 54 $MW_{LHV,CH4}$ PtG plant which has been scaled to the needed capacity of 135 $MW_{LHV,CH4}$ resulting in 456 €/$kW_{LHV,CH4}$. The CO_2 based synthesis of **methanol** is based on the same study and a 50 $MW_{LHV,CH3OH}$ plant and, after correction of plant capacity (143 $MW_{LHV,CH3OH}$), resulting in 368 €/$kW_{LHV,\,CH3OH}$. Compared to other published values (308-399€/$kW_{LHV,\,CH3OH}$) of Otto et al.[15] the calculated value in our study can be seen as medium conservative for the cost year 2030. The reason for the lower specific methanol plant investment (although characterised by higher pressures (steel demand) and larger reactors) compared to sabatier can be assumed as a result from higher heat integration efforts in case of the sabatier process. The specific investment demand for the synthesis of NH_3 via the **Haber-Bosch** concept at a capacity of 150 $MW_{LHV,NH3}$ is derived from values published by Matzen et al.[16] and, after correction of capacity, amount to 690 €/$kW_{LHV,NH3}$.

The **liquefaction** process for H2 is based on the IDEALHY project report giving CAPEX estimations for a 120 t(H2) d^{-1} liquefaction plant with 105 M€.[17]. Liquefaction of CH4 orientates on a techno-economic study for a LNG-plant. Since the study focused on processing of fossil natural gas we excluded the cost for gas treatment, fractionation and the flares as well as storage and jetty since product storage is considered as part of the other costs in our study.

As for the efficiency analysis the information on investment and operational cost for the **(de-)hydrogenation units of DBT** are based on discussion with an industrial stakeholder and manufacturer of LOHC pilot plants. An investment of 60M € for both units at the necessary scale (120 t d^{-1}; reference hydration unit: 20 t d^{-1}; reference de-hydration unit 2 t d^{-1}) has been considered.[18] A dehydrogenation loss of 0.1 wt% of DBT per cycle is considered in the cost. In case of the LOHC-H2 pathway and the respective ship transporting the loaded LOHC an on-board dehydrogenation unit at necessary scale has been considered as well. The respective cost are in this case connected to higher uncertainties but with minor impact on overall economics.

The cost of **product storage** take into account the storage conditions of the respective PtX product. For CH3OH and the LOHC-H2 pathway conventional floating roof tanks at atmospheric conditions and the respective scale have been considered without any boil-off.[19] For the storage of NH3 we considered low-temperature storage (t ~-33°C) since this technology is favored over pressurized (p > 17 bar) storage in case large-volume storages are required.[20,21] The CAPEX for low-temperature NH3 storage have been considered with 350€ $t(NH3)^{-1}$ representing large scale storage vessels (>30,000 t(NH3)).[22] Losses due to boil-off (~0.04% d^{-1}) have been neglected since at these capacities a recompression and flash loop are statutory and hence assumed as part of the storage cost.

In case of LH2 a ultimate target value (3.3M € at 3,500m³ LH2) for cryogenic LH2 storage tanks as published by the U.S. department of Energy has been considered.[23] Boil-off losses are considered with 0.03% d^{-1}.[23] The necessary investment for the LCH4 tank orientate on published values for 30 million gallon peak LNG tanks (full containment version).[24] These costs include in-tank LNG pumps and boil-off gas compression system. Hence, no boil-off losses during LCH4 storage have been considered.

Labor costs (in € a^{-1}) have been estimated based on the Wessel equation[25] giving the operating workhours per year:

$$\frac{operating\ workhours}{tons\ of\ product} = T * \left(\frac{\#process\ steps}{capacity^{0.76}}\right)$$

with

$T = 23$, as rather pessimistic assumption, representing batch operations with maximum workload

$\#\text{process steps}$ = each PtX component assumed as one process step: LH_2=5; NH_3=6; CH_3OH=6; LCH_4=7; LOHC-H_2=6

capacity = plant capacity in t/d

The cost of operating workhour has been assumed with 50€ h^{-1}.

Table 4 lists the values relevant for the economic assessment of the **shipping processes**. As described in the main article the shipping processes orientate on larger vessels with assumed transport capacities of 70,000 m³ (LOHC-H2) or 140,000 m³ (other assessed pathways) of PtX product. The main source for the ships necessary SMCR power (specified maximum continuous rating) and related speed (orientating on the ships transport capacity) are publications from MAN Diesel&Turbo for tankers[26] (assumed for the pathways LOHC-H2, CH3OH) and LNG carriers[27] (assumed for the pathways NH3, LH2, LCH4). The respective SMCR power defines the consumption of on-board PtX product considering an efficiency for the respective propulsion process (as described in Part I of the main article). The investment for the respective ship is derived from literature. The cost for a LH2 carrier is aligned to the cost assumed by Heuser et al.[28] and published by Kawasaki Heavy Industries[29]. The LCH4 and NH3 carrier orientates on costs published by Fasihi et al..[30] The LOHC and CH3OH carrier costs have been derived from a study of Konovessis et al.[31] providing costs for modern large-scale tankers. If boil-off occurred during ship transport (NH3, LH2, LCH4) it had been assumed to be used as fuel. For all cases the boil-off had been smaller than the respective fuel demand of the ships. Therefore no losses due to boil-off have been considered. The total fuel demand orientates on the two-distance bearing as well for the ship's return.

Table 2 Investment cost (CAPEX) for the assessed PtX pathways

CAPEX	NH3	LH2	LOHC-H2	LCH4	CH3OH
Renewables					
Wind Installed capacity [MWp]	506	506	453	509	578
Wind capacity factor	50%	50%	50%	50%	50%
PV Installed capacity [MWp]	144	172	142	153	220
PV capacity factor	27%	27%	27%	27%	27%
RE produced [GWhel/a]	2,573	2,638	2,331	2,606	3,067
RE cost [€/MWhel]	25	25	25	25	25
Seawater Desalination					
CAPEX specific [€/m³*a]	2.2	2.2	2.2	2.2	2.2
Installed capacity [m³/a]	425,000	425,000	425,000	425,000	425,000
CAPEX total [€]	947,750	947,750	947,750	947,750	947,750
Electrolysis					
CAPEX specific [€/MWel]	600,000	600,000	600,000	600,000	600,000
Installed capacity [MWel]	440	450	419	446	481
Lifetime system	20	20	20	20	20
Lifetime stack	10	10	10	10	10
Replacement cost	34%	34%	34%	34%	34%
CAPEX total [€]	353,100,000	361,125,000	336,247,500	357,915,000	387,607,500
H2 motor					
CAPEX specific [€/MWel]	715,000	715,000	715,000	715,000	715,000
Installed capacity [MWel]	26.2	32.6	2	29	68
CAPEX total [€]	18,711,550	23,273,250	1,670,955	55,677,000	48,540,635
H2 cavern					
Installed capacity [m³]	608,410	631,980	516,430	630,240	768,290
CAPEX total [€]	54,888,000	55,725,000	51,727,000	55,677,000	60,172,000
Compressors					
CAPEX total	34,900,260	12,268,000	11,768,000	14,608,866	20,827,737
ASU / DAC					
CAPEX specific [€/t*a]	54	-	-	200	200
Installed capacity [t/d]	556	-	-	708	872
CAPEX total [€]	10,903,769	-	-	50,130,391	61,793,651
Synthesis					
CAPEX specific [€/t*a]	427	-	-	723	227
Installed capacity [t/d]	667	-	-	241	635
CAPEX total [€]	103,854,104	-	-	63,569,931	52,662,775
Liquefaction					
CAPEX specific [€/t*a]	-	4,054		604	-
Installed capacity [t/d]	-	120	-	241	-
CAPEX total [€]	-	177,548,106	-	51,455,251	-
(De-)Hydrogenation set					
CAPEX specific [€/t*a]	-	-	1,370	-	-
Installed capacity [t/d]	-	-	120	-	-
CAPEX (De-)Hydrogenation [€]	-	-	60,000,000	-	-
Initial Purchase of DBT [€], @2€/kg DBT	-	-	214,100,781	-	-
CAPEX total [€]	-	-	274,100,781	-	-
Product storage					
CAPEX specific [€/t]	350	11,952	68	2,284	75
Installed capacity [t]	114,576	11,928	87,696	71,000	132,367
CAPEX total [€]	40,101,600	142,560,000	5,940,000	162,171,390	9,900,000

Engineering					
Share of CAPEX	5%	5%	5%	5%	5%
Engineering total [€]	30,870,352	38,672,355 €	23,415,060	38,865,176 €	32,122,602
Total CAPEX (incl. Enginnering)	648,277,385	812,119,461	705,817,046	816,168,704	674,574,650

Table 3 Operational expenditures (OPEX) for the assessed PtX pathways

OPEX	**NH3**	**LH2**	**LOHC-H2**	**LCH4**	**CH3OH**
Electricity cost					
Cost of RE electricity [€/MWhel]	25	25	25	25	25
Cost of 100km DC transmission [€/MWhel]	2	2	2	2	2
Electricity desalination [MWhel/a]	1,275	1,275	1,275	1,275	1,275
Electricity PEM electrolysis [MWhel/a]	2,142,600	2,151,100	2,113,000	2,148,300	2,223,700
Electricity Compressors [MWhel/a]	108,442	9,228	8,455	21,162	48,447
Electricity ASU / DAC [MWhel/a]	98,389	-	-	176,510	489,798
Electricity Liquefaction [MWhel/a]	-	255,000	-	20,433	-
Electricity Cost Total [€/a]	63,469,076	65,248,281	57,313,713	63,927,334	74,606,948
Fixed OPEX [% of CAPEX/a]					
Desalination 4%CAPEX/a [€]	37,910	37,910	37,910	37,910	37,910
Electrolysis 2%CAPEX/a [€]	5,280,000	5,400,000	5,028,000	5,352,000	5,796,000
H2 motor [17.5 €/MWhel]	83,351	129,305	5,848	108,072	431,265
Compressors 4%CAPEX/a [€]	1,396,010	490,720	470,720	584,355	833,109
H2 Cavern 1%CAPEX/a [€]	548,880	557,250	517,270	556,770	601,720
ASU / DAC 2%CAPEX/a [€]	218,075	-	-	2,005,216	2,471,746
Synthesis fixed 2%CAPEX/a [€]	2,077,082	-	-	1,271,399	1,053,255
Liquefaction 2%CAPEX/a [€]	-	3,550,962	-	1,029,105	-
(De-)Hydrogenation 4%CAPEX/a [€]	-	-	2,400,000	-	-
Product Storage 1-2%CAPEX/a [€]	802,032	2,851,200	59,400	3,243,428	99,000
Other fixed OPEX					
Insurance & Taxes [2% total CAPEX/a]	12,965,548	14,116,037	14,116,341	13,652,400	13,491,493
Labor [€/a]	7,710,105	6,425,087	7,710,105	8,995,122	7,710,105
Replacement of lost DBT [€/a]	-	-	1,318,500	-	-
Total OPEX (incl. Enginnering)	94,588,069	100,933,104	88,977,806	103,434,084	107,132,551

Table 4 Parameters for shipping of PtX products

Shipping	**NH3**	**LH2**	**LOHC-H2**	**LCH4**	**CH3OH**
Transport volume ship [m³]	140,000	140,000	70,000	140,000	140,000
Capacity Ship [t product]	95,480	9,940	73,080	59,167	110,306
Total CAPEX Ship [€]	152,309,263	440,000,000	42,361,844	152,309,263	54,231,949
Ship speed [knots]	20	18	15	20	15
Travel time, 2ways incl. (dis-)charge [d]	12	12	14	12	14
Ship utilization [% of year]	10%	17%	44%	6%	10%
Ship availability [% of year]	95%	95%	95%	95%	95%
Ship lifetime [a]	30	30	30	30	30
OPEX Ship [% CAPEX/a]	3.5%	0.02%	3%	3.5%	3%
Effective CAPEX Ship [€/a]	1,073,156	2,699,191	1,220,894	625,416	341,337
Boil-off rate [%/d]	0.04%	0.20%	-	0.10%	-
Boil-off: cover of ship fuel demand	15%	42%	-	61%	-
Total fuel demand two-ways [t]	2,122	383	219	791	1,400
Total shipping cost [€/MWh transported product]	0.9	2.0	1.3	0.5	0.3

Table 5 Levelised cost of PtX products in Morocco (w/o shipping)

LCoProduct Morocco [€/MWh]	**117**	**90($H2_g$)**	**90 ($H2_g$)**	**124**	**128**
LCoProduct Morocco [€/t]	604	2,991	2,991	1,724	715

Table 6 Levelised cost of PtX products in Germany (including shipping)

LCoProduct Germany [€/MWh]	**124**	**126**	**156**	**145**	**131**
LCoProduct Germany [€/t]	640	4,208	5,193	2,017	730

S5: Case study: Detailed cost and sensitivity results

Table 7 CAPEX shares of the respective components

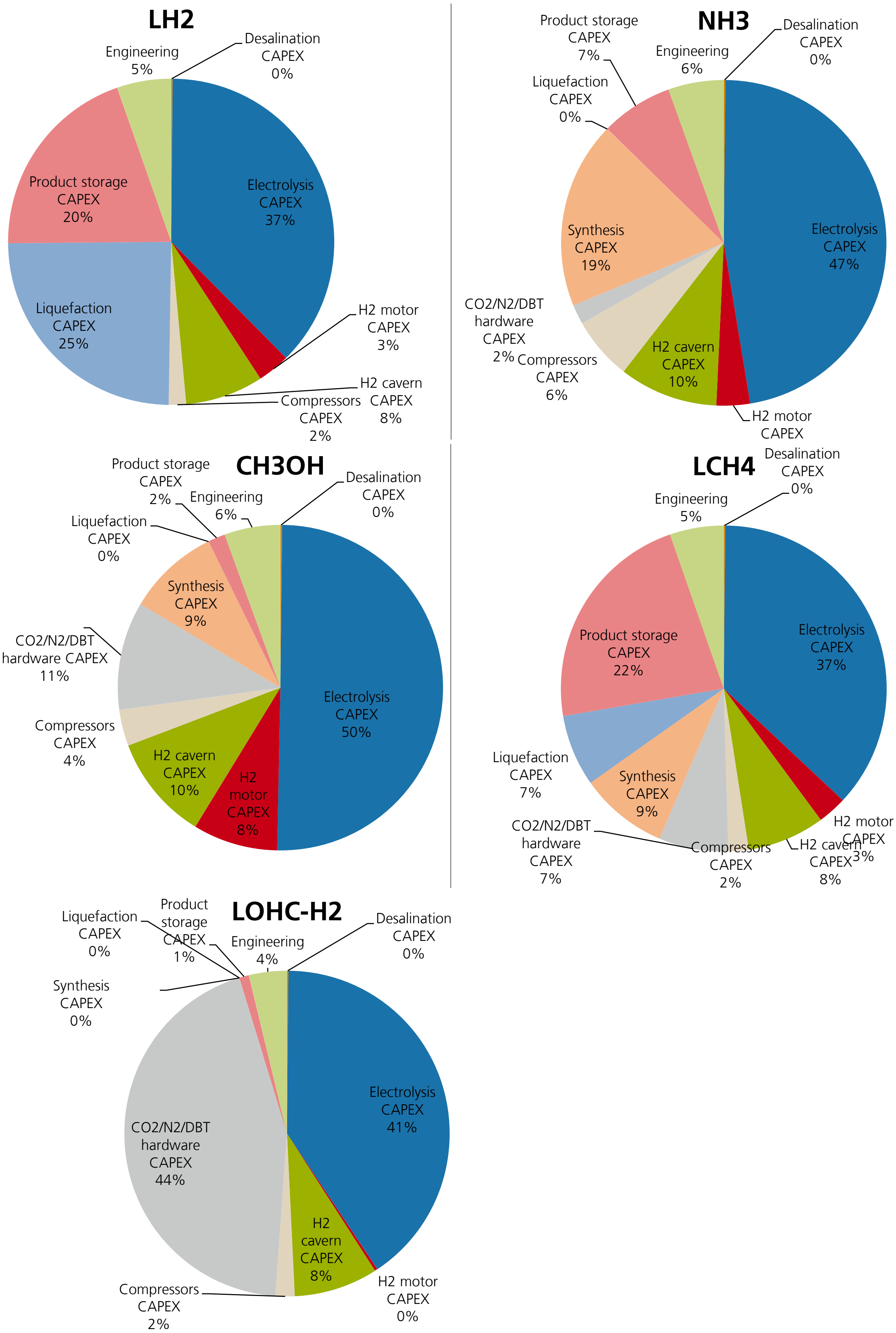


Table 8 Detailed composition of the final levelized cost of product. In case of the LOHC-H2 pathway, the "DBT step" CAPEX include the initial investment for the DBT and the "DBT step" OPEX include the 0.1% DBT cycle-loss.

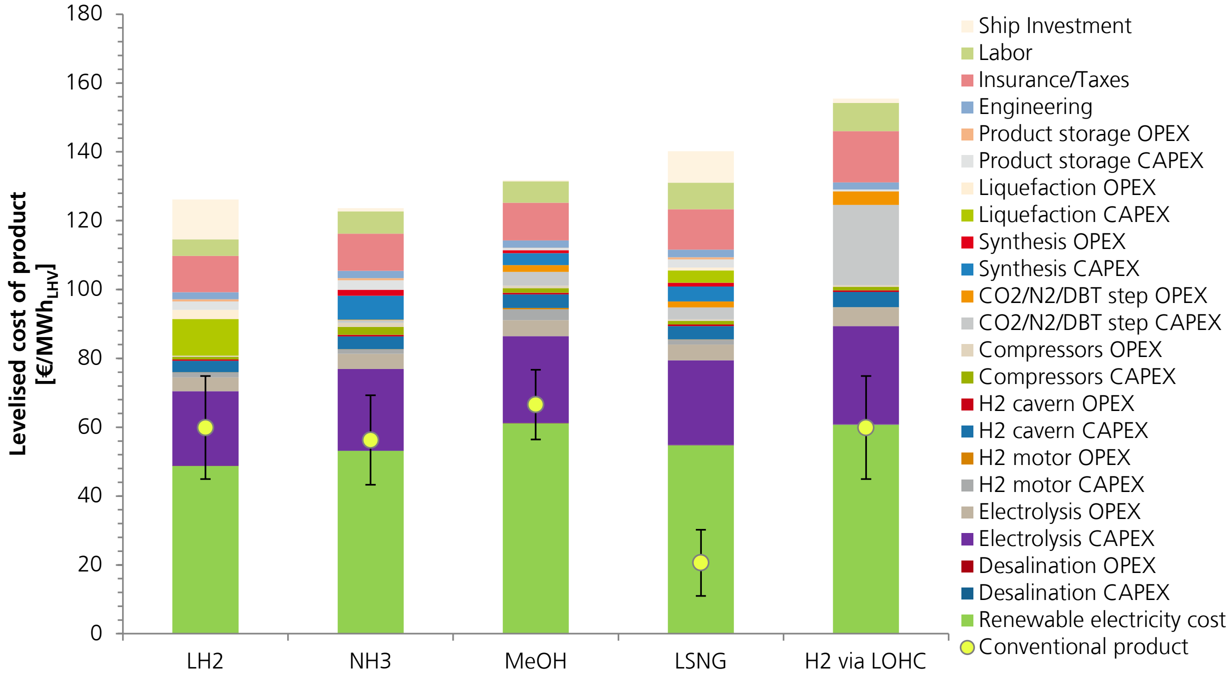
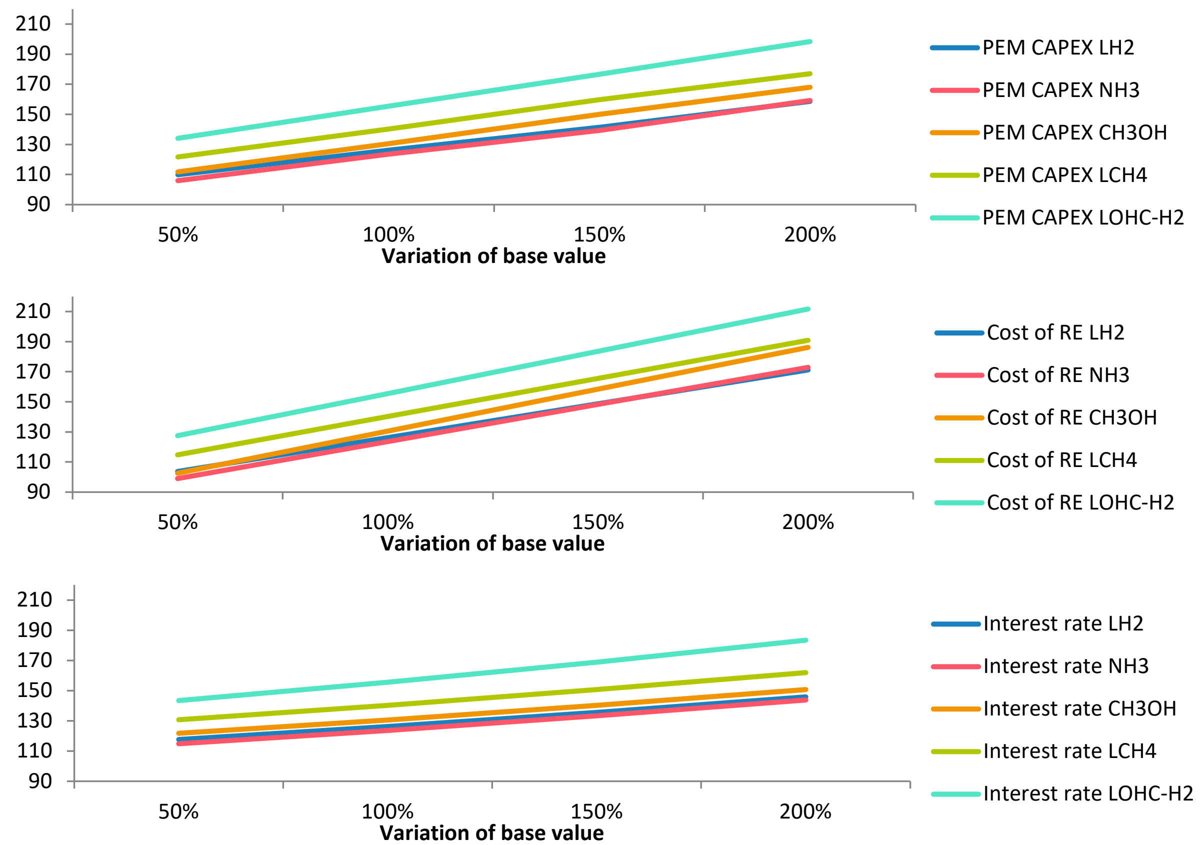


Table 9 Sensitivity: Influence of a variation of PEM CAPEX (base=600€/kWel), cost of RE electricity (base=25€/MWhel), interest rate (base=5%) on the levelised cost of product (€/MWh_{LHV})



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