Supplementary Information: Comparative well-to-wheel Life Cycle Assessment of OME₃₋₅ synfuels production via the Power-to-Liquids pathway

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S1: Other LCA focused on OME_x via PtL pathways

Recently Deutz et al. conducted a comprehensive LCA for a OME₁-diesel-blend (35 vol.% OME₁) on a WtW basis.¹ The use phase was represented by combustion in a mid-size passenger car based on 1 km distance as the functional unit (FU). The OME1 production processes assessed were both based on methanol, the first via its condensation of formaldehyde (FA; produced via classical oxidative dehydrogenation chemistry) and the second via a novel pathway involving reduction of methanol in the presence of H₂ and CO₂. Electrolytic H₂ production was powered by different electricity sources accounting for global warming potential (GWP) differences on European electrical grids. CO₂ was sourced from a Direct Air Capture (DAC) module or as burden-free from a biogas upgrading plant. The latter is based on the authors premise that the biogas pathway is fully dedicated to the production of biomethane (CH₄). The impact of DAC is fully attributed to the feedstock CO₂. This report indicated that an OME₁-diesel-blend produced based on renewable or nuclear electricity has a potential CO₂ reduction in comparison to conventional diesel fuelled cars. Overall GWP for the 35 vol.% OME₁-blend equated to 101 g(CO_{2eq})/km for the best case (Biogas CO₂, wind electricity, thermal energy by electric heater) and 198 g(CO_{2eq})/km worst case (DAC of CO₂, 2020 EU grid mix, thermal energy by natural gas) respectively. The conventional diesel reference emits 129 g(CO_{2eq})/km. When focusing on the PtL process' electricity supply, the break-even point at which an OME₁-blend powered car performs better than a conventional diesel car is found in the range of 124-136 g(CO_{2eq})/kWh_{el} (GWP of the process' input electricity). OME₁ as analyzed in this report is commercially known as "Methylal". It has a high vapor pressure, relatively lower specific volumetric energy and low flash point. These are drawbacks when blended with diesel fuel and long term storage in current infrastructure is considered.

In contrast, higher OME_n (with n > 3) are of increasing interest in the engine research and development field due to their similar thermophysical properties to diesel.^{2–4} Mahbub *et al.* analysed the WtW GHG emission performance of OME_{1-8} a derived from the gasification of forestry biomass and downstream OME_{1-8} synthesis. ⁵ Either diesel with 10% OME_{1-8} additive or pure OME_{1-8} as diesel substitute were investigated. Whole-tree and forest residue biomass were used as the carbon source. Regarding the assessment, results were provided based on a FU of 1 MJ heat produced from OME_{1-8} , with WtW GWP results indicating that in case of 100% OME_{1-8} fuel, emissions could be reduced to 18-26 g(CO_{2eq})/MJ compared to 127 g(CO_{2eq})/MJ for the conventional diesel fuel reference case. Furthermore the considered theoretical combustion processes for the 10% OME₁₋₈-diesel blend indicated that soot emissions can be reduced by 30%.

S2: Defintion of "multifunctionality" in the context of CCU systems

Multifunctionality is described as a unit-process delivering more than one function. A function can either be in the form of generating *output* flow(s) with a *positive* market value and therefore a valuable product, energy or service unit. Or *via* the *uptake* of flow(s) with a *negative* market value as is the case for recycling transforming wastes into valuable products. Where the "emission" CO₂ is turned into a "feedstock" and temporarily bound into products, an accurate procedure for solving multifunctionality can become even more important. In principle the CCU production chain will comprise one or more multifunctional production steps. In most cases the CO₂-delivering process will be multifunctional since it is delivering a main-product (e.g. electricity, ammonia, biomethane) and a new feedstock: the captured CO₂ for downstream valorization. As described by [Guinée *et al.*]⁶ and exemplified by [Assen, Jung *et al.*]^{7,8} captured CO₂ can have a *positive* (captured, purified and ready-to-transport or -use CO₂) and a *negative* market value (unpurified fossil CO₂ emissions). The latter can be justified with the introduction of the European Emission Trading System (EU ETS) where specific CO₂ emissions are legitimately labeled as *waste*. In case of a *negative* market value, environmental impacts of the downstream CO₂-utilisation step can be assigned 'backward' to the CO₂-emitting process. But whether a CO₂ emission will be traded with a *positive* market value can be a matter of system boundaries and if the CO₂-emitter is as well the operator of the downstream CO₂-utilisation plant.

S3: Process Flow Diagram assessed OME₃₋₅ synthesis

A brief description of the considered synthesis steps is following next: Green methanol is produced from electrolytic H₂ and captured CO₂ at T > 180 °C and P = 50 bar. Therefore H₂ is compressed from 30 bar after the electrolysis to 50 bar and captured CO_2 from 1 bar after capturing and purification to 50 bar. A three-stage compressor unit is considered for CO_2 compression. Synthesized methanol is separated from unconverted H₂ and CO₂ as well as the side products CO and H₂O via Flash units and a distillation column before entering the formaldehyde synthesis step. Here the methanol, saturated in N₂ as carrier gas, is split via partial endothermic dehydrogenation into anhydrous formaldehyde (T > 650 °C, 1.5 bar) whereby H₂ is produced as the main side product. This step is characterised by competing side reactions and a selective catalyst improves selectivity to the desired target products formaldehyde (and H₂).⁹ After absorption of this intermediate product in the recycle stream, H₂ is compressed and recycled to the methanol synthesis while formaldehyde and unconverted methanol are fed into the OME reactor. The methanol acts as a methyl end capping agent in the oligomerisation of formaldehyde (CH₂O).^{10,11} Following the reaction to OME_n at P = 2.8 bar and T > 50 °C the mixture enters the distillation columns. The same short-cut distillation approach as considered in the previous work is applied in this work.^{11,12} The extended model considering the reactivity of the distillation feed mixture for a better process description is under development and will be described in further study. OME_{<3,>5} and unconverted formaldehyde and methanol are recycled to the OME synthesis, the side product H₂O is separated and removed as a wastewater stream. The desired product mixture of OME₃₋₅ can further be used for different applications.



Figure 1: Simplified process flow diagram for the assessed synthesis process including the step of methanol synthesis

S4: Selected Impact Categories for Midpoint Impact calculation

Table 1 - Selected life cycle midpoint impact assessment calculation for the assessed product system

Impact Category	Model
Climate Change, GWP 100a [kg CO _{2eq}]	IPCC 2013
Resources, mineral, fossil and renewables $[{\rm kg}~{\rm Sb}_{\rm eq}]$	ILCD 2016
Ecosystem quality, freshwater and terrestrial acidification [Mol H^{+}_{eq}]	ILCD 2016
Ecosystem quality, freshwater eutrophication $[kg \ P_{eq}]$	ILCD 2016
Ecosystem quality, marine eutrophication [kg N _{eq}]	ILCD 2016
Ecosystem quality, terrestrial eutrophication $[mol \ N_{eq}]$	ILCD 2016
Human health, ozone layer depletion [kg CFC-11 _{eq}]	ILCD 2016
Human health, respiratory effects, inorganics [kg PM2.5 _{eq}]	ILCD 2016
Human health, photochemical ozone creation [kg ethylene _{eq}]	ILCD 2016
Cumulative Energy Demand, total [MJ _{eq}]	Non-renewable and renewable energy resources used
Cumulative Energy Demand, non-renewable [MJ _{eq}]	HHV of non-renewable energy resources extracted

S5: Life Cycle Inventory – OME Product System

Electricity

Description of the electricity modelling: The 40% share of RE is based on load profiles of local wind and PV plants in the south of Germany. The wind load profiles are derived from two year measurements (15-min measurement intervals) from a wind park consisting of Enercon turbines (Type E-66/10) with 1.8 MW_p each. Data for the solar electricity generation is provided from a PV park with an installed capacity of 2.5 MW_p over a two year measurement (5-min measurement intervals). The combined renewable load curves of wind and PV served as a basis and were scaled to fit the demand of the product system studied with 36 kta OME₃₋₅ and a resulting steady state power input of the 35 or 40 MW_{el} PEM electrolysis¹. The applied RE scaling factor has been calculated as the optimum ratio between RE utilized and necessary RE installation capacities. The optimum scaling factor leads to hypothetical installed capacities of a 76 MW_p wind and a 24 MW_p PV park. At this configuration the RE utilization efficiency² results in 85 % and the RE coverage³ in 40%. Consequently, to balance the fluctuating renewable electricity generation, necessary coverage via grid electricity amounts to 60%. These shares apply for both the [2018 GR+RE] and the [2050 GR+RE] electricity scenario.

The 60% share of grid based electricity is either based on data for the German grid in 2018 or a prediction for the year 2050. The grid data for 2018 is based on published data of the publicly accessible *ISE energy charts.*¹³

¹ Demand in installed PEM electrolysis capacity dependent on the assumed PEM system efficiency of 65%LHV (2018) or 74%LHV (2050), (Further described in section *PEM electrolysis*).

² RE utilization efficiency: ratio between renewable electricity used for electrolytic H₂ generation and the renewable electricity produced.

³ RE coverage: Share of renewable energy of the total energy consumed by the OME3-5 product system.

Predictions for a future grid electricity mix for Germany are inseparably linked to uncertainties which will increase with an expanding time horizon of the aspired forecast. Two uncertainty aspects become relevant when assessing future energy systems: First of all technology improvements such as increased efficiencies and enhanced plant lifetimes will lead to potentially lower environmental footprints for most impact categories. We didn't account for this aspect in case of the ecoinvent background processes. The second aspect of uncertainty is a prediction for the composition of the future grid electricity mix which is an integral part of several studies and models. ^{14–20}

For an estimation of the 2050 grid electricity mix and its resulting footprint the REMod Model developed at Fraunhofer ISE has been used.^{21–23} REMod analyses different energy system transition pathways for the German economy until 2050. ^{17,18,24} For the applied 2050 grid electricity in this study results of a REMod "S90-Scenario" have been used as a basis. For the REMod S90-Scenario a 90%-reduction of GHG-emissions compared to 1990 is aspired. The total amount of electricity consumed in 2050 sums up to 1,132 TWh_{el}. Electricity provided directly from RE located within Germany make up a share of 74%.⁴ The remaining electricity production is based on a mix of technologies either fueled by H₂ or CH₄ and include electricity production in central and decentralized combined heat and power plants (CHP) such as gas turbines and fuel cells (both CH₄ and H₂). H₂ as well as CH₄ are to a large proportion based on imported synthetic gases. A 70% share of H₂ is imported and assumed to be produced in Spain and North Africa via large scale water electrolysis powered by photovoltaic electricity. 26% of H₂ is based on electrolytic production in Germany powered by the RE mix and a small share is based on gasification of biomass (3%) and steam reforming of methane (<1%).

These technology pathways have been modelled in Umberto[®] using specific conversion efficiencies for the single process steps. By this a first estimate for the environmental impacts of a potential 2050 grid electricity mix has been obtained. Hardware demand has only been considered for the electricity producing technologies and is based on ecoinvent background processes. Transport of the imported synthetic gases has been excluded in the Umberto[®] modelling. Technologies such as wind or PV power plants undergo rapid improvements in the technology itself but also changes in the production of the necessary hardware. It should be noted that the ecoinvent processes for these technologies based on data from 2012 should be revised for future assessments. The respective assumed technologies and the ecoinvent processes used for the assessment are part of the SI.

The electricity mix applied for the **[2018 HY+RE]** scenario is based on the 40% share of local RE and a 60% share of hydropower. The ecoinvent process "hydro, run-of-river [DE]" is used as background process. When it comes to using limited forms of electricity generation such as it is the case for hydropower in Germany the argument for the PtL plants' *additional* electricity demand is justified. It can be argued that in case of a large-scale PtL plant in Germany an electricity supply by dedicated hydroelectric power plants remains unlikely. However, the [2018 HY+RE] scenario is included to provide estimation for PtL scenarios supplied by low-carbon electricity as it is already the case for anticipated pilot-projects in Scandinavia.^{25–27} By now hydroelectricity provides the largest share of electricity from all RE sources within the EU member-states.

Material	Value	Unit
electricity production, wind, 1-3MW turbine, onshore [DE]	0.154	kWh
heat and power co-generation, biogas, gas engine [DE]	0.057	kWh
electricity production, lignite [DE]	0.232	kWh
electricity production, hard coal [DE]	0.120	kWh
electricity production, nuclear, pressure water reactor [DE]	0.105	kWh
heat and power co-generation, natural gas, conventional power plant, 100MW electrical [DE]	0.051	kWh
electricity production, nuclear, boiling water reactor [DE]	0.028	kWh
electricity production, hydro, run-of-river [DE]	0.020	kWh
heat and power co-generation, hard coal [DE]	0.018	kWh
electricity production, natural gas, combined cycle power plant [DE]	0.014	kWh

Table 2 – LCI: Electricity Mix for 2018 Grid Electricity Germany based on Fh ISE energy charts

⁴ PV: 25%; Wind onshore: 39%; wind offshore: 9%; hydropower: 1%.

heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014 [DE]	0.025	kWh
electricity production, natural gas, conventional power plant [DE]	0.008	kWh
treatment of blast furnace gas, in power plant [DE]	0.005	kWh
electricity production, wind, <1MW turbine, onshore [DE]	0.028	kWh
electricity production, hydro, pumped storage [DE]	0.008	kWh
heat and power co-generation, lignite [DE]	0.010	kWh
electricity production, oil [DE]	0.002	kWh
electricity production, wind, >3MW turbine, onshore [DE]	0.017	kWh
electricity production, hydro, reservoir, non-alpine region [DE]	0.004	kWh
heat and power co-generation, oil [DE]	0.001	kWh
treatment of coal gas, in power plant [DE]	0.002	kWh
electricity production, wind, 1-3MW turbine, offshore [DE]	0.006	kWh
heat and power co-generation, natural gas, combined cycle power plant, 400MW electrical [DE]	0.001	kWh
electricity production, deep geothermal [DE]	0.000	kWh
electricity production, natural gas, 10MW [DE]	0.000	kWh
electricity production, photovoltaic	0.084	kWh
Total	1.0000	kWh

Table 3 - LCI: Simplified technology mix for the 2050 electricity based on REMod

Technology	Value	Unit
PV based electricity	286	TWhel
Hydro, run-off river	14	TWhel
Wind onshore	438	TWhel
Wind offshore	104	TWhel
Gas turbine, H2	14	TWhel
CHP, central, H2 & CH4	43	TWhel
CHP, decentralized, H2 & CH4	206	TWhel
Imported Electricity	27	TWhel
Electric Energy Total	1132	TWhel

CO₂ Sourcing

Biomethane

Description of the considered biomethane upgrading process: For the carbon dioxide supply case '**Biomethane [BM]**' the CO_2 is assumed to be supplied from a biogas upgrading plant used for the feed-in of biomethane into the natural gas grid. Biogas upgrading is a multi-step procedure including CO_2 removal from the raw biogas which usually contains concentrations of $40 < CO_2 < 50$ vol.% depending on the biomass-feed.²⁸ Pressurised water scrubbing was selected for this study which is the most common method for biogas upgrading in Europe due to the simple setup and the use of non-toxic solvents.²⁹ Data sources were literature values, ecoinvent and manufacturer inquiries. For the initial production of biogas from biomass and necessary materials and hardware demand the ecoinvent dataset "biogas production from grass [CH]" was modified and adjusted to average substrate feeds for the German market.^{29,30} The feed influences the shares of i.a. CH₄, CO₂, H₂S in biogas. For renewable crops CH₄ shares of ~50 - 55 vol.% are common. CH₄ content was thus assumed at an average share of 53 vol.%. A CH₄ loss of 1 vol.% has been considered as emission to the atmosphere. CO₂ content if using renewable resources sums up to ~44 vol.%, resp. 0.87 kg(CO₂)/Nm³(biogas).³¹ Biogas upgrading includes a desulphurisation step for the protection of downstream components and as an efficiency enhancement of the biomethane pathway. H₂S adds up to 100 - 1500 ppm(H₂S)/Nm³ of raw biogas.²⁹ After the biogas upgrading step the resulting CO₂ stream is assumed to contain at least 500 ppm of H₂S which is still too high for the downstream methanol synthesis and the involved catalyst. This aspect has been covered by a fine-desulphurisation step with a specific demand of granular activated carbon (282x 10⁻⁶ kg(AC)/kg(CO₂)) and electricity (17x10⁻⁶ kWh_{el}/kg(CO₂)). The data is based on manufacturer enquiries.³² Removed H₂S (4x10⁻⁶ kg(H₂S)/kg(CO₂)) is considered as emission to the atmosphere. Desulphurised CO₂ is available at ambient pressure.

Input	Value	Unit
heat, district or industrial, natural gas	1.07	MJ
maize silage, organic	6.90E-01	kg
grass silage, organic	1.70E-01	kg
electricity, low voltage	6.49E-02	kWh
manure, liquid, swine	3.00E-02	kg
manure, liquid, cattle	3.00E-02	kg
Water, river [natural resource/in water]	1.54E-03	m3
ethanol fermentation plant	1.57E-11	unit
Output	Value	Unit
biogas	1.00	m3
wastewater from grass refinery	1.27E-03	m3
Water [air/unspecified]	2.31E-04	m3

Table 4 - LCI: Biogas production, adapted to substrate composition Germany; FNR-Leitfaden 2014

Table 5 – LCI: Coupled biogas purifictaion

Input	Value	Unit
biogas	1.00	m3
electricity, medium voltage	2.05E-01	kWh
chemical factory, organics	1.49E-10	unit
Output	Value	Unit
methane, 96% by volume	5.20E-01	Nm3
CO2, 4 bar, gaseous from biogas	8.70E-01	kg
Hydrogen sulfide [air/non-urban air or from high stacks]	7.60E-06	kg

Methane slip, non-fossil [air/non-urban air or from high stacks]	7.16E-05	kg

Table 6 - LCI: CO2 Desulphurisation

Input	Value	Unit
CO2, 4 bar, gaseous from biogas	8.38E-01	kg
activated carbon, granular	2.82E-04	kg
electricity, low voltage	1.70E-05	kWh
Output	Value	Unit
CO2, 4 bar, gaseous from biogas	8.38E-01	kg
Hydrogen sulfide [air/non-urban air or from high stacks]	3.04E-06	kg

Ammonia

Description of the considered ammonia process: The CO₂ supply case '**Ammonia [AM]**' assumes that fossil CO₂ is captured from an ammonia production facility. Ammonia production as CO₂ point source has the appeal that the CO₂ removal *via* an amine solvent (MDEA) process is usually a process related step after the shift conversion of the reformation products H₂O and CO to H₂ and CO₂. More than 96% of the CO₂ content in the syngas is removed in the MDEA wash. The resulting CO₂ stream shows high purities (CO₂ > 99 vol.%).^{33,34} Hence many ammonia plants are either coupled with urea plants which reuse 70-90% of the separated CO₂^{30,35} or, at smaller scale, further utilisation pathways such as enhanced oil recovery (in the Unites States)³⁶ or *via* application in the food industry. Still a considerable part of the removed high concentrated CO₂ streams remains unused for many cases.^{37,38} Van der Assen *et al.* evaluate CO₂ from ammonia plants as the point source with the lowest indirect emissions due to the low demand of further treatment.³⁹ Although the total potential of CO₂ emitted by European ammonia facilities is smaller compared to other lower concentrated point-sources ammonia plants remain a promising candidate for CO₂ utilisation.^{39,40}

Input	Value	Unit
natural gas, high pressure	5.95E-01	m3
heavy fuel oil	1.97E-01	kg
Water, cooling, unspecified natural origin [natural resource/in water]	1.40E-01	m3
electricity, medium voltage	6.94E-02	kWh
natural gas, high pressure	4.91E-03	m3
Water, unspecified natural origin [natural resource/in water]	9.00E-04	m3
nickel, 99.5%	3.50E-04	kg
solvent, organic	3.00E-05	kg
chemical factory, organics	4.00E-10	unit
Output		
ammonia, liquid	1.00E+00	kg
CO2, 1bar, gaseous from ammonia, captured for CCU	1.23E+00	kg

Table 7 – LCI: Coupled ammonia production

Acetaldehyde [air/urban air close to ground]	1.24E-06	kg
Acetic acid [air/urban air close to ground]	8.37E-06	kg
Acetone [air/urban air close to ground]	1.21E-06	kg
Ammonia [air/urban air close to ground]	8.10E-08	kg
Arsenic [air/urban air close to ground]	1.05E-07	kg
Benzene [air/urban air close to ground]	9.36E-06	kg
Benzo(a)pyrene [air/urban air close to ground]	4.61E-10	kg
Butane [air/urban air close to ground]	1.64E-05	kg
Cadmium [air/urban air close to ground]	2.67E-07	kg
Calcium [air/urban air close to ground]	6.48E-07	kg
Carbon dioxide, fossil [air/urban air close to ground]	1.46E+00	kg
Carbon monoxide, fossil [air/urban air close to ground]	8.40E-05	kg
Chromium [air/urban air close to ground]	1.28E-07	kg
Chromium VI [air/urban air close to ground]	1.30E-09	kg
Cobalt [air/urban air close to ground]	2.67E-07	kg
Copper [air/urban air close to ground]	3.97E-07	kg
Dinitrogen monoxide [air/urban air close to ground]	1.53E-05	kg
Dioxins, measured as 2,3,7,8-tetrachlorodibenzo-p-dioxin [air/urban air close to ground]	4.35E-15	kg
Ethanol [air/urban air close to ground]	2.43E-06	kg
Formaldehyde [air/urban air close to ground]	5.99E-06	kg
Hydrocarbons, aliphatic, alkanes, unspecified [air/urban air close to ground]	4.86E-06	kg
Hydrocarbons, aliphatic, unsaturated [air/urban air close to ground]	2.43E-07	kg
Hydrocarbons, aromatic [air/urban air close to ground]	1.21E-06	kg
Hydrogen chloride [air/urban air close to ground]	1.17E-05	kg
Hydrogen fluoride [air/urban air close to ground]	1.17E-06	kg
Iron [air/urban air close to ground]	1.46E-06	kg
Lead [air/urban air close to ground]	4.62E-07	kg
Mercury [air/urban air close to ground]	1.92E-09	kg
Methane, fossil [air/urban air close to ground]	1.20E-05	kg
Methanol [air/urban air close to ground]	4.13E-06	kg
Molybdenum [air/urban air close to ground]	1.30E-07	kg
municipal solid waste	2.00E-04	kg

Nickel [air/urban air close to ground]	5.27E-06	kg
Nitrogen [water/surface water]	1.00E-04	kg
Nitrogen oxides [air/urban air close to ground]	1.00E-03	kg
PAH, polycyclic aromatic hydrocarbons [air/urban air close to ground]	2.39E-07	kg
Particulates, < 2.5 um [air/urban air close to ground]	2.88E-04	kg
Particulates, > 10 um [air/urban air close to ground]	8.10E-05	kg
Particulates, > 2.5 um, and < 10um [air/urban air close to ground]	4.05E-05	kg
Pentane [air/urban air close to ground]	2.81E-05	kg
Propane [air/urban air close to ground]	4.92E-06	kg
Propionic acid [air/urban air close to ground]	4.68E-07	kg
Selenium [air/urban air close to ground]	9.72E-08	kg
Sodium [air/urban air close to ground]	6.08E-06	kg
Sulfur dioxide [air/urban air close to ground]	1.00E-05	kg
Toluene [air/urban air close to ground]	4.92E-06	kg
Vanadium [air/urban air close to ground]	2.11E-05	kg
Water [air/unspecified]	5.44E-02	m3
Water [water/unspecified]	8.65E-02	m3
Zinc [air/urban air close to ground]	3.24E-07	kg

Direct Air Capture

Description of the considered DAC process: For the monofunctional CO₂ supply case '**Direct Air Capture [DAC]**' the CO₂ is sourced directly from the atmosphere. Capturing technologies based on reversible sorbents are gaining increasing attention for the development of materials and processes towards pilot-scale and several start-ups pushing from the lab to demonstration in the open field.^{41–44} The Swiss company Climeworks introduced DAC-modules whose core technology is based on sorbents consisting of amines supported in porous adsorbents. For the DAC modules in this study we considered process energies (electrical and thermal) as well as the manufacturing of the modules.^{45–47} The assumed electricity demand (0.25 kWh_{el}/kg(CO₂ captured and desorbed) is implemented under consideration of the three defined electricity scenarios. Low temperature thermal energy (<105 °C) for desorption of the captured CO₂ (1.75 kWh_{th}/kg(CO₂)) is necessary. Available synthesis and distillation exhaust heat (>115 °C) sums up to 0.23 kWh_{th}/kg(CO₂) which is assumed to partially cover the thermal demand of the DAC plant. The remaining thermal demand of the DAC plant (1.52 kWh_{th}/kg(CO₂)) is assumed to be covered either by additional available exhaust (burden free) heat or by the burning of natural gas. Low temperature exhaust heat at temperature levels <150°C is available in all industry sectors.⁴⁸ The local availability of exhaust heat is, thus, dependent on the specific case. Thermal coverage by natural gas considers the indirect emissions from the natural gas supply chain and the direct CO₂ emissions from natural gas oxidation.

Material data for the manufacturing of the DAC facility is based on a publication of Zhang *et al.*⁴⁷ and has been extended with the original life cycle inventory kindly provided by the authors. To cover the daily demand of 227.6 t of atmospheric CO₂ a total of 93 'DAC-18' systems is necessary.⁴⁹ The resulting DAC facility would cover an area of ~0.8 hectares which corresponds the size of a soccer field. Due to little experience with the longstanding operation of these modules a lifetime of 10 years has been assumed.

Table 8 - LCI: Direct Air Capture Process

Input	Value	Unit
heat, excess heat, from synthesis & distillation	2.30E+02	kWh
heat, additional	1.52E+03	kWh
electricity	2.50E+02	kWh
DAC-18 unit based on Zhang (2017)	1.22E-07	unit
Water, cooling, unspecified natural origin [natural resource/in water]	1.95E-05	m3
chemical, organic	3.56E-03	kg
Output		
CO2, 1 bar gaseous	1.00E+00	kg

PEM Electrolysis

Table 9 - LCI: PEM Electrolysis

Input	Value	Unit
electricity	3.21E+05	MWh
water, deionised, from tap water, at user	5.57E+04	ton
Water, cooling, unspecified natural origin [natural resource/in water]	1.01E+04	m3
Electrolyzer, 5MW (incl. Stack-Exchange)	4.01E-01	unit
Output	Value	Unit
H2, 30 bar, gaseous	6.25E+03	ton
exhaust heat	1.17E+05	MWh
Oxygen [natural resource/in air]	4.93E+04	ton
Water, cooling, unspecified natural origin [natural resource/in water]	1.01E+04	m3

Table 10 - LCI: PEM coupled Stack System Hardware, 5MW

Input	Value	Unit
heat, district or industrial, natural gas	1.09E+06	MJ
electricity, medium voltage	1.60E+05	kWh
Electrolyser Stack, 1MW	1.60E+04	unit
inverter, 2.5kW	2.00E+03	unit
Occupation, industrial area [natural resource/land]	1.88E+03	m2*year
building, hall	4.00E+02	m2

Water, unspecified natural origin [natural resource/in water]	3.65E+02	m3
Transformation, to industrial area [natural resource/land]	3.75E+01	m2
Transformation, from unspecified [natural resource/land]	3.75E+01	m2
Endplates(2x), 1 MW Stack	5.00E+00	unit
intermodal shipping container, 40-foot	3.00E+00	unit
Current Collectors for 5MW Ely	1.00E+00	unit
Output	Value	Unit
Electrolyzer, 5MW (incl. Stack-Exchange)	1.00E+00	unit
wastewater, from residence	3.65E+02	m3
Water [air/unspecified]	5.48E+01	m3

Table 11 - LCI: PEM Stack Hardware, 1 MW

Input	Value	Unit
titanium, primary	1.74E+05	g
heat, district or industrial, natural gas	2.23E+04	MJ
electricity, medium voltage	1.69E+04	kWh
phenolic resin	1.10E+03	kg
Iridium, imported from PROBAS	3.75E+02	g
platinum	2.00E+02	g
glass fibre	1.00E+02	kg
isopropanol	9.50E+00	kg
tetrafluoroethylene	9.49E+00	kg
sulfuric acid	7.04E+00	kg
water, deionised, from tap water, at user	6.00E+00	kg
carbon black	8.00E-01	kg
Output	Value	Unit
Electrolyser Stack, 1MW	1.00E+00	unit
Propanol [air/urban air close to ground]	9.50E+00	kg
waste plastic, industrial electronics	6.61E+03	kg
waste polyvinylfluoride	5.20E+01	kg
Water [air/unspecified]	9.00E-04	m3
Water [water/unspecified]	5.10E-03	m3

Methanol and OME3-5 synthesis steps

Description of the considered Methanol & OME₃₋₅ **Synthesis Steps:** The methanol step comprises one adiabatic reactor (12.6 m³) and one isothermal reactor (8.0 m³). In the OME step an adiabatic reactor for the dehydrogenation of methanol to FA (15.2 m³) and an isothermal reactor for the OME_n synthesis (19.4 m³) has been considered. Necessary steel demand (44.2 t) as well as BE (56.7 t) and enamel (12.5 t) has been estimated based on CAD models and personal communication with industry.^{50–52} The same procedure has been applied for the estimations of material demands for the 19 heat exchangers (26.4 t) estimated after processing the heat integration *via* pinch analysis. Further hardware material demand for compressors, pumps, distillation and flash units as well as other chemical plant equipment has been estimated based on secondary data from ecoinvent background processes which is listed in the supplementary information (S4 – *Methanol and OME synthesis steps and distillation column*).

Process data includes electricity for compressors and pumps (1.20 MWhel/t(OME₃₋₅)), heat for the dehydrogenation of methanol to FA (1.22 MWh_{th}/t(OME₃₋₅)) and steam for the necessary 5 distillation columns (3.62 MWh_{th}/t(OME₃₋₅)). Thermal energy supply is either covered by natural gas (GRID2018+RE) or by the respective electricity mix (GRID2050+RE, HYDRO2018). For the methanol step a standard CuO/Al₂O₃/ZnO catalyst has been considered at a consumption rate of 33 mg(Cat)/kg(methanol).³⁴ The OME₃₋₅ reaction requires Amberlyst[™]-36 in dry state as catalyst which is not included in the ecoinvent database. Amberlyst™-36 is commercially available in dry state with a water content of 1.65 %.⁵³ Ecoinvent database provides data for the production of a cationic-resin in wet state which mostly represents the production of Amberlyst[™]-36 wet according to an inquiry at DOW. Thus, the electricity consumption required to dry the cationic-resin from wet to dry state has been considered.^{53,54} The wastewater (ww) created during distillation towards the desired products sums up to 0.78 t(ww)/t(OME₃₋₅) (methanol content in ww < 0.11 wt.%). Necessary treatment is considered as average industrial wastewater and the impact assessed by a respective ecoinvent market process for European waste water treatment processes. The distillation fractions OME_{1-2} and $OME_{n>5}$ are cycled back to the reactor. It could be argued that they are valuable side-products. Consideration of them as side-products would have two effects: On the one hand a possibility to allocate parts of the overall environmental footprint on these side-products and possibly a lower footprint of OME₃₋₅. On the other hand the decision not to recycle would have a significant decrease in OME₃₋₅ yields. Since this study focuses on OME₃₋₅ the distillations side-products have been cycled back to the reactor to enable an increased OME₃₋₅ yield.

Methanol synthesis and distillation step

Table 12 - LCI: Methanol synthesis step

Input	Value	Unit
Water, unspecified natural origin [natural resource/in water]	3.09E+06	m3
CO2, 1 bar, gaseous	7.59E+04	ton
electricity (incl. compression)	1.36E+04	MWh
H2, 30 bar, gaseous	6.24E+03	ton
copper oxide	9.49E+02	kg
zinc oxide	3.56E+02	kg
aluminium oxide	1.78E+02	kg
air compressor, screw-type compressor, 300kW	7.55E-01	unit
reactors & heat exchanger, methanol production	3.33E-02	unit
chemical factory, organics	8.99E-03	unit
Output	Value	Unit
methanol, unpurified	4.49E+04	t

Water, unspecified natural origin [natural resource/in	3.09E+06	m3
water]		

Table 13 - LCI: Methanol distillation

Input	Value	Unit
Water, cooling, unspecified natural origin [natural resource/in water]	3.47E+06	m3
steam	1.56E+05	GJ
methanol	4.49E+04	t
Output	Value	Unit
methanol	4.49E+04	t
CO2 Case [AM]: carbon dioxide fossil, from purge gas	5.87E+03	t
CO2 Case [BM], [DAC]: carbon dioxide biogenic, from purge gas	5.87E+03	t
CO2 Case [AM]: carbon monoxide fossil, from purge gas	7.42E-02	t
CO2 Case [BM], [DAC]: carbon monoxide biogenic, from purge gas	7.42E-02	t
Hydrogen [air/non-urban air or from high stacks]	1.10E+00	t
wastewater, average	2.37E+04	m3
Water, cooling, unspecified natural origin [natural resource/in water]	3.47E+06	m3

$\textbf{OME}_{\texttt{3-5}}$ synthesis steps and distillation column

Table 14 - LCI: FA Reactor

Input	Value	Unit
electricity, incl. electricity of H2 recycle compressor	2.86E+07	kWh
Water, cooling, unspecified natural origin [natural resource/in water]	2.85E+05	m3
heat	1.31E+05	GJ
methanol	4.49E+04	t
soda ash, light, crystalline, heptahydrate	2.57E+03	kg
nitrogen, liquid	4.80E+02	t
air compressor, screw-type compressor, 300kW	7.75E-01	unit
reactors & heat exchanger, OME production	1.67E-02	unit
chemical factory, organics	7.23E-03	unit
Output	Value	Unit
Formaldehyde – Methanol Mix	3.55E+04	t
CO2 Case [AM]: carbon dioxide fossil, from purge gas	4.19E+03	kg

CO2 Case [BM], [DAC]: carbon dioxide biogenic, from purge gas	4.19E+03	kg
CO2 Case [AM]: carbon monoxide fossil, from purge gas	0.00E+00	kg
CO2 Case [BM], [DAC]: carbon monoxide biogenic, from purge gas	0.00E+00	kg
Water, cooling, unspecified natural origin [natural resource/in water]	2.85E+05	m3

Table 15 - LCI: OME Reactor

Input	Value	Unit
Water, cooling, unspecified natural origin [natural resource/in water]	5.22E+05	m3
Formaldehyde – Methanol Mix	3.55E+04	t
electricity, incl. electricity of pumps	7.69E+03	kWh
Amberlyst DRY	1.55E+03	kg
pump, 40W	3.21E+00	units
reactors & heat exchanger, OME production	1.67E-02	units
Output	Value	Unit
OMEn	3.55E+04	t
Water, cooling, unspecified natural origin [natural resource/in water]	5.22E+05	m3

Table 16 - LCI: OME Distillation column

Water, cooling, unspecified natural origin [natural resource/in water]5.61E+06m3steam3.07E+05GJOME_3-5+3.55E+04telectricity, incl. electricity of pumps3.82E+03kWhpump, 40W1.42E+00unitsOutputValueUnitOME_3-53.55E+04tOME_3-52.07E+02toME_2 (no further consideration)2.07E+02twastewater, average4.06E+03m3Water, cooling, unspecified natural origin [natural resource/in water]5.61E+06m3	Input	Value	Unit
steam3.07E+05GJOME_3-5+3.55E+04telectricity, incl. electricity of pumps3.82E+03kWhpump, 40W1.42E+00unitsOutputValueUnitOME_3-53.55E+04tOME_2 (no further consideration)2.07E+02twastewater, average4.06E+03m3Water, cooling, unspecified natural origin [natural resource/in water]5.61E+06m3	Water, cooling, unspecified natural origin [natural resource/in water]	5.61E+06	m3
OME_3-5+3.55E+04telectricity, incl. electricity of pumps3.82E+03kWhpump, 40W1.42E+00unitsOutputValueUnitOME_3-53.55E+04tOME_2 (no further consideration)2.07E+02twastewater, average4.06E+03m3Water, cooling, unspecified natural origin [natural resource/in water]5.61E+06m3	steam	3.07E+05	GJ
electricity, incl. electricity of pumps3.82E+03kWhpump, 40W1.42E+00unitsOutputValueUnitOME_3-53.55E+04tOME_2 (no further consideration)2.07E+02twastewater, average4.06E+03m3Water, cooling, unspecified natural origin [natural resource/in water]5.61E+06m3	OME_3-5+	3.55E+04	t
pump, 40W1.42E+00unitsOutputValueUnitOME_3-53.55E+04tOME_2 (no further consideration)2.07E+02twastewater, average4.06E+03m3Water, cooling, unspecified natural origin [natural resource/in water]5.61E+06m3	electricity, incl. electricity of pumps	3.82E+03	kWh
OutputValueUnitOME_3-53.55E+04tOME_2 (no further consideration)2.07E+02twastewater, average4.06E+03m3Water, cooling, unspecified natural origin [natural resource/in water]5.61E+06m3	pump, 40W	1.42E+00	units
OME_3-53.55E+04tOME_2 (no further consideration)2.07E+02twastewater, average4.06E+03m3Water, cooling, unspecified natural origin [natural resource/in water]5.61E+06m3	Output	Value	Unit
OME_2 (no further consideration) 2.07E+02 t wastewater, average 4.06E+03 m3 Water, cooling, unspecified natural origin [natural resource/in water] 5.61E+06 m3	OME_3-5	3.55E+04	t
wastewater, average4.06E+03m3Water, cooling, unspecified natural origin [natural resource/in water]5.61E+06m3	OME_2 (no further consideration)	2.07E+02	t
Water, cooling, unspecified natural origin [natural resource/in water] 5.61E+06 m3	wastewater, average	4.06E+03	m3
	Water, cooling, unspecified natural origin [natural resource/in water]	5.61E+06	m3

OME₃₋₅ Distribution

Table 17 - LCI: OME₃₋₅ Distribution

Input	Value	Unit

transport, pipeline, onshore, petroleum	5.59E-01	metric ton*km
transport, freight, lorry, unspecified	5.67E-02	metric ton*km
transport, freight train	4.40E-02	metric ton*km
transport, freight, inland waterways, barge tanker	3.23E-02	metric ton*km
electricity, low voltage	6.70E-03	kWh
transport, freight, light commercial vehicle	1.80E-03	metric ton*km
tap water	6.89E-04	kg
heat, central or small-scale, other than natural gas	5.84E-04	MJ
infrastructure, for regional distribution of oil product	2.48E-10	unit
Output	Value	Unit
OME_3-5	1.00E+00	kg
fly ash and scrubber sludge	0.00E+00	kg
municipal solid waste	6.27E-06	kg
rainwater mineral oil storage	0.00E+00	m3
wastewater, average	6.89E-07	m3
Water [air/unspecified]	1.03E-07	m3
Water [water/unspecified]	5.86E-07	m3

OME₃₋₅ Utilization

Derivation of the emissions resulting from OME₃₋₅ combustion: Since no motor testing has been conducted in the framework of this paper a picture of the resulting exhaust pipe emissions is derived from existing literature.³⁰ The ecoinvent process has been adjusted accordingly: All emissions to ecosphere of mineral origin (Cd, Cr, Cu, Pb, Hg, Ni, Se, SO₂, Zn) were assumed as non-existent in case of OME₃₋₅ fuel. Remaining emissions have been modified: NO_x content has been adjusted to 1 g/kWh OME_{LHV} according to [Richter et al.; Fig. 6]³ who analyzed the trade-off between PM and NO_x emissions. By applying OME₃₋₆ (as well as OME₁) as fuel in a single-cylinder test engine they could resolve the conflict of NO_x -PM trade-off and show that the reduction of NO_x correlates with rising oxygen contents of the fuel. They state an efficiency increase of ~2%. [Omari et al.]⁵⁵ found similar numbers for an 80:20 OME₁-diesel blend. Additionally, they measured a hydrocarbon reduction of 40% at lower loads³⁰. [Härtl et al.]⁵⁶ measured hydrocarbon reduction by 90% with the use of OME₁. They moreover found that FA and ammonia concentrations were below the limit of detection. PM formation reduction reaches up to 100% for pure OME₁ fuels.^{57,58} Emissions of Hydrocarbons (10%), CO (20%), FA (0%), ammonia (0%), NO_x (100%) and PM (0%) were adjusted accordingly. All other emissions that could not be excluded, neither because of their chemical composition nor according to empirical studies, were assumed to remain the same as in the diesel process. Formation of methane has been detected outside of the optimum operating point (rich mixtures).^{3,4} Since diesel engines are usually operated with sufficient surplus of oxygen, methane was assumed as non-existent. Exhaust pipe emissions of carbon dioxide are by now surprisingly not in the scope of the cited publications since it was assumed that all CO₂ captured and used for OME production can be seen as "CO₂-neutral". With the given mixture of OME₃₋₅ and in case of an assumed complete oxidation of its C-content the stoichiometric maximum of CO₂ formation sums up to 1.595 kg CO_2/kg OME₃₋₅. With the assumed engine efficiency the specific direct CO₂ emissions sum up to 0.199 g CO₂/km. At this point it should be noted that the PtL process' considered CO₂ demand will always be higher than the stoichiometric maximum of the fuels CO₂ formation. Parts of the feed CO₂ is lost in the form of C-containing purge gases and waste

streams and not bound into the synfuels molecule. Thus for environmental evaluation of synfuels production it is important to consider the full CO_2 demand for correct impact assessment of CO_2 capturing, purification and compression.

Table 18 - LCI: OME Utilization

Input	Value	Unit
OME_3-5	1.25E-01	kg
passenger car, diesel (not considered)	1.07E-02	kg
road (not considered)	9.11E-04	m*year
passenger car maintenance (not considered)	8.60E-06	unit
Output	Value	Unit
transport, OME3-5	1.00E+00	km
Acetaldehyde [air/urban air close to ground]	1.61E-06	kg
Acetone [air/urban air close to ground]	7.32E-07	kg
Acrolein [air/urban air close to ground]	8.91E-07	kg
Ammonia [air/urban air close to ground]	0.00E+00	kg
Benzaldehyde [air/urban air close to ground]	2.14E-07	kg
Benzene [air/urban air close to ground]	4.93E-07	kg
brake wear emissions, passenger car (not considered)	7.55E-06	kg
Butane [air/urban air close to ground]	2.74E-08	kg
CO2 Case [AM]: Carbon dioxide, fossil [air/urban air close to ground]	1.99E-01	kg
CO2 Case [BM], [DAC]: Carbon dioxide, biogenic [air/urban air close to ground]	1.99E-01	kg
Cyclohexane (for all cycloalkanes) [air/urban air close to ground]	1.62E-07	kg
Dinitrogen monoxide [air/urban air close to ground]	2.78E-06	kg
Ethane [air/urban air close to ground]	8.22E-08	kg
Ethylene oxide [air/urban air close to ground]	2.73E-06	kg
Formaldehyde [air/urban air close to ground]	0.00E+00	kg
Heptane [air/urban air close to ground]	4.98E-08	kg
Methane [air/urban air close to ground]	1.87E-06	kg
Methyl ethyl ketone [air/urban air close to ground]	2.99E-07	kg
m-Xylene [air/urban air close to ground]	1.52E-07	kg
Nitrogen oxides [air/urban air close to ground]	6.77E-04	kg
NMVOC, non-methane volatile organic compounds, unspecified origin [air/urban air close to ground]	1.32E-05	kg

o-Xylene [air/urban air close to ground]	6.72E-08	kg
PAH, polycyclic aromatic hydrocarbons [air/urban air close to ground]	1.03E-09	kg
Particulates, < 2.5 um [air/urban air close to ground]	0.00E+00	kg
Pentane [air/urban air close to ground]	9.96E-09	kg
Propane [air/urban air close to ground]	2.74E-08	kg
Propylene oxide [air/urban air close to ground]	8.96E-07	kg
road wear emissions, passenger car (not considered)	1.66E-05	kg
Styrene [air/urban air close to ground]	9.21E-08	kg
Toluene [air/urban air close to ground]	1.72E-07	kg
tyre wear emissions, passenger car (not considered)	9.72E-05	kg

S6: Life Cycle Impact Assessment Results for System Expansion

The system expansion LCIA results include the by-product of either 0.16m³ of biomethane (CO₂ cases [BM]) or 0.26 kg of ammonia (CO₂ cases [AM]). To enable comparable functional units the reference diesel process is expanded to include as well either an uncoupled production of biomethane or ammonia.

A comparison of system expansion LCIA results between the CO₂ cases [BM] and the CO₂ cases [AM] is not valid due to the differing functional units.

In the following we present the system expansion LCIA results at first for the CO₂ cases [BM] compared to the expanded diesel reference system resulting in a FU of [1km+0.16m³ of CH₄]. Subsequent we present the system expansion LCIA results for the CO₂ cases [AM] compared to the expanded diesel reference system resulting in a FU of [1km+0.26 kg NH3].

Table 19 - System Expansion Results for CO2 cases [BM]: GWP100a

System Expansion Results for CO ₂ cases [BM]: GWP100a				
CO2 Case Biomethane; $FU = 1km+0.16kg CH_4$	OME 2018GR+RE, BM	OME 2050GR+RE, BM	OME 2018HY+RE, BM	Diesel Ref.
PtL: CO2 sourcing	0.121	0.084	0.121	
PtL: H2 production	0.402	0.080	0.025	
PtL: methanol step	0.062	0.015	0.004	
PtL: OME distribution	0.004	0.004	0.004	
PtL: OME step	0.135	0.041	0.011	
PtL: OME utilization - exhaust pipe emissions	0.001	0.001	0.001	
Reference: Crude Petrol Production				0.015
Reference: Diesel distribution + desulphurisation				0.004
Reference: Diesel refinery step				0.014
Reference: Diesel utilization - exhaust pipe emissions				0.176
Reference: Expanded system value conv. biomethane				0.083



Table 20 - System Expansion Results for CO₂ cases [BM]: CED - Renewable

System Expansion Results for CO₂ cases [BM]: CED - Renewable

CO2 Case Biomethane; $FU = 1km+0.16kg CH_4$	OME 2018GR+RE, BM	OME 2050GR+RE, BM	OME 2018HY+RE, BM	Ref. Diesel
PtL: CO2 sourcing	2.267	2.433	2.267	
PtL: H2 production	2.995	3.839	4.461	
PtL: H2 production	0.136	0.766	0.782	
PtL: OME distribution	0.004	0.004	0.004	
PtL: OME step	0.290	2.019	2.061	
PtL: OME utilization - exhaust pipe emissions	0.000	0.000	0.000	
Reference: Crude Petrol Production				0.005
Reference: Diesel distribution + desulphurisation				0.005
Reference: Diesel refinery step				0.006
Reference: Diesel utilization - exhaust pipe emissions				0.000
Reference: Expanded system value conv. biomethane				2.433



Table 21 - System Expansion Results for CO2 cases [BM]: CED - Fossil

System Expansion Results for CO ₂ cases [BM]: CED - Fossil				
CO2 Case Biomethane; FU = 1 km+ 0.16 kg CH ₄	OME 2018GR+RE, BM	OME 2050GR+RE, BM	OME 2018HY+RE, BM	Ref. Diesel
PtL: CO2 sourcing	1.168	0.600	1.168	
PtL: H2 production	5.519	0.726	0.283	
PtL: H2 production	0.888	0.145	0.050	
PtL: OME distribution	0.059	0.059	0.059	
PtL: OME step	1.936	0.390	0.139	
PtL: OME utilization - exhaust pipe emissions	0.000	0.000	0.000	
Reference: Crude Petrol Production				2.938
Reference: Diesel distribution + desulphurisation				0.059
Reference: Diesel refinery step				0.203
Reference: Diesel utilization - exhaust pipe emissions				0.000
Reference: Expanded system value conv. Biomethane				0.596



Table 22 - System Expansion Results for CO2 cases [BM]: ecosystem quality, freshwater and terrestrial acidification

System Expansion Results for CO ₂ cases [BM]: ecosystem quality, freshwater and terrestrial acidification				
CO2 Case Biomethane; FU = 1km+0.16kg CH ₄	OME 2018GR+RE, BM	OME 2050GR+RE, BM	OME 2018HY+RE, BM	Ref. Diesel
PtL: CO2 sourcing	1.14E-03	1.10E-03	1.14E-03	
PtL: H2 production	8.81E-04	4.78E-04	1.49E-04	
PtL: H2 production	2.29E-04	9.68E-05	2.77E-05	
PtL: OME distribution	2.52E-05	2.52E-05	2.52E-05	
PtL: OME step	4.99E-04	2.54E-04	7.15E-05	
PtL: OME utilization - exhaust pipe emissions	5.01E-04	5.01E-04	5.01E-04	
Reference: Crude Petrol Production				2.28E-04
Reference: Diesel distribution + desulphurisation				2.76E-05
Reference: Diesel refinery step				1.22E-04
Reference: Diesel utilization - exhaust pipe emissions				5.05E-04
Reference: Expanded system value conv. biomethane				1.10E-03



Table 23 - System Expansion Results for CO2 cases [BM]: ecosystem quality, freshwater eutrophication

System Expansion Results for CO ₂ cases [BM]: ecosystem quality, freshwater eutrophication				
CO2 Case Biomethane: ELL = 1km+0 16kg CH.	OME	OME	OME	Ref Diesel
	2018GR+RE, BM	2050GR+RE, BM	2018HY+RE, BM	
PtL: CO2 sourcing	8.77E-05	2.94E-05	8.77E-05	
PtL: H2 production	5.32E-04	4.39E-05	1.47E-05	
PtL: H2 production	2.83E-05	9.06E-06	2.88E-06	
PtL: OME distribution	1.49E-06	1.49E-06	1.49E-06	
PtL: OME step	5.99E-05	2.34E-05	7.17E-06	
PtL: OME utilization - exhaust pipe emissions	0.00E+00	0.00E+00	0.00E+00	
Reference: Crude Petrol Production				2.11E-06
Reference: Diesel distribution + desulphurisation				1.42E-06
Reference: Diesel refinery step				5.85E-07
Reference: Diesel utilization - exhaust pipe emissions				0.00E+00
Reference: Expanded system value conv. biomethane				2.92E-05



Table 24 - System Expansion Results for CO2 cases [BM]: ecosystem quality, marine eutrophication

System Expansion Results for CO ₂ cases [BM]: ecosystem quality, marine eutrophication				
CO2 Case Biomethane; FU = 1km+0.16kg CH ₄	OME	OME	OME	Ref. Diesel
	2018GR+RE, BM	2050GR+RE, BM	2018HY+RE, BM	
PtL: CO2 sourcing	4.16E-04	3.94E-04	4.16E-04	
PtL: H2 production	2.58E-04	7.21E-05	2.69E-05	
PtL: H2 production	3.70E-05	1.62E-05	6.53E-06	
PtL: OME distribution	6.49E-06	6.49E-06	6.49E-06	
PtL: OME step	7.69E-05	3.85E-05	1.31E-05	
PtL: OME utilization - exhaust pipe emissions	2.63E-04	2.63E-04	2.63E-04	
Reference: Crude Petrol Production				2.71E-05
Reference: Diesel distribution + desulphurisation				6.15E-06
Reference: Diesel refinery step				8.69E-06
Reference: Diesel utilization - exhaust pipe emissions				2.64E-04
Reference: Expanded system value conv. biomethane				3.94E-04



Table 25 - System Expansion Results for CO2 cases [BM]: ecosystem quality, terrestrial eutrophication

System Expansion Results for CO ₂ cases [BM]: ecosystem quality, terrestrial eutrophication				
CO2 Case Biomethane; FU = 1 km+ 0.16 kg CH ₄	OME 2018GR+RE, BM	OME 2050GR+RE, BM	OME 2018HY+RE, BM	Ref. Diesel
PtL: CO2 sourcing	4.32E-03	4.22E-03	4.32E-03	
PtL: H2 production	1.81E-03	8.23E-04	2.62E-04	
PtL: H2 production	3.33E-04	1.66E-04	4.77E-05	
PtL: OME distribution	7.18E-05	7.18E-05	7.18E-05	
PtL: OME step	7.23E-04	4.36E-04	1.24E-04	
PtL: OME utilization - exhaust pipe emissions	2.89E-03	2.89E-03	2.89E-03	
Reference: Crude Petrol Production				2.94E-04
Reference: Diesel distribution + desulphurisation				6.50E-05
Reference: Diesel refinery step				9.10E-05
Reference: Diesel utilization - exhaust pipe emissions				2.90E-03
Reference: Expanded system value conv. biomethane				4.21E-03



Table 26 - System Expansion Results for CO2 cases [BM]: human health, ozone layer depletion

System Expansion Results for CO ₂ cases [BM]: human health, ozone layer depletion				
CO2 Case Biomethane; FU = 1 km+ 0.16 kg CH ₄	OME 2018GR+RE, BM	OME 2050GR+RE, BM	OME 2018HY+RE, BM	Ref. Diesel
PtL: CO2 sourcing	5.41E-09	3.89E-09	5.41E-09	
PtL: H2 production	2.04E-08	6.94E-09	2.60E-09	
PtL: H2 production	6.06E-09	1.38E-09	4.53E-10	
PtL: OME distribution	4.64E-10	4.64E-10	4.64E-10	
PtL: OME step	1.33E-08	3.68E-09	1.23E-09	
PtL: OME utilization - exhaust pipe emissions	0.00E+00	0.00E+00	0.00E+00	
Reference: Crude Petrol Production				3.57E-08
Reference: Diesel distribution + desulphurisation				4.61E-10
Reference: Diesel refinery step				2.41E-09
Reference: Diesel utilization - exhaust pipe emissions				0.00E+00
Reference: Expanded system value conv. biomethane				3.89E-09



Table 27 - System Expansion Results for CO2 cases [BM]: Human health, respiratory effects, inorganics

System Expansion Results for CO ₂ cases [BM]: Human health, respiratory effects, inorganics					
CO2 Case Biomethaner EU - 1km+0 16kg CH	OME 2018GR+RE,	OME 2050GR+RE,	OME 2018HY+RE,	Ref.	
	BM	BM	BM	Diesel	
PtL: CO2 sourcing	5.52E-05	5.50E-05	5.52E-05		
PtL: H2 production	7.54E-05	6.51E-05	2.42E-05		
PtL: H2 production	2.24E-05	1.31E-05	4.34E-06		
PtL: OME distribution	2.92E-06	2.92E-06	2.92E-06		
PtL: OME step	4.88E-05	3.44E-05	1.13E-05		
PtL: OME utilization - exhaust pipe emissions	5.27E-06	5.27E-06	5.27E-06		
Reference: Crude Petrol Production				1.37E-05	
Reference: Diesel distribution + desulphurisation				3.30E-06	
Reference: Diesel refinery step				1.43E-05	
Reference: Diesel utilization - exhaust pipe emissions				1.18E-05	
Reference: Expanded system value conv. biomethane				5.46E-05	



Table 28 - System Expansion Results for CO2 cases [BM]: Human health, photochemical ozone creation

CO2 Case Biomethane: Ell = 1km+0 16kg CH.	OME 2018GR+RE,	OME 2050GR+RE,	OME 2018HY+RE,	Ref.
	BM	BM	BM	Diesel
PtL: CO2 sourcing	2.07E-04	1.81E-04	2.07E-04	
PtL: H2 production	4.57E-04	2.13E-04	8.57E-05	
PtL: H2 production	1.00E-04	4.29E-05	1.54E-05	
PtL: OME distribution	1.94E-05	1.94E-05	1.94E-05	
PtL: OME step	2.18E-04	1.13E-04	4.05E-05	
PtL: OME utilization - exhaust pipe emissions	6.93E-04	6.93E-04	6.93E-04	
Reference: Crude Petrol Production				1.35E-04
Reference: Diesel distribution + desulphurisation				1.86E-05
Reference: Diesel refinery step				4.23E-05
Reference: Diesel utilization - exhaust pipe emissions				6.96E-04
Reference: Expanded system value conv. biomethane				1.80E-04

System Expansion Results for CO₂ cases [BM]: Human health, photochemical ozone creation



Table 29 - System Expansion Results for CO2 cases [AM]: GWP100a

System Expansion Results for CO ₂ cases [AM]: GWP100a				
CO2 Case Ammonia; FU = 1km+0.26kg NH ₃	OME 2018GR+RE, AM	OME 2050GR+RE, AM	OME 2018HY+RE, AM	Diesel Ref.
PtL: CO2 sourcing	0.432	0.425	0.432	
PtL: H2 production	0.402	0.079	0.025	
PtL: methanol step	0.098	0.052	0.040	
PtL: OME distribution	0.004	0.004	0.004	
PtL: OME step	0.151	0.057	0.027	
PtL: OME utilization - exhaust pipe emissions	0.200	0.200	0.200	
Reference: Crude Petrol Production				0.015
Reference: Diesel distribution + desulphurisation				0.004
Reference: Diesel refinery step				0.014
Reference: Diesel utilization - exhaust pipe emissions				0.176
Reference: Expanded system value conv. Ammonia				0.691



System Expansion Results for CO ₂ cases [AM]: CED - Renewable, TOTAL				
CO2 Case Ammonia; FU = 1 km+ 0.26 kg NH $_3$	OME 2018GR+RE, BM	OME 2050GR+RE, BM	OME 2018HY+RE, BM	Ref. Diesel
PtL: CO2 sourcing	0.106	0.136	0.106	
PtL: H2 production	2.995	3.839	4.461	
PtL: methanol step	0.136	0.766	0.782	
PtL: OME distribution	0.004	0.004	0.004	
PtL: OME step	0.290	2.019	2.061	
PtL: OME utilization - exhaust pipe emissions	0.000	0.000	0.000	
Reference: Crude Petrol Production				0.005
Reference: Diesel distribution + desulphurisation				0.005
Reference: Diesel refinery step				0.006
Reference: Diesel utilization - exhaust pipe emissions				0.000
Reference: Expanded system value conv. Ammonia				0.136



System Expansion Results for CO ₂ cases [AM]: CED - Fossil, TOTAL				
CO2 Case Ammonia; FU = 1 km+0.26kg NH ₃	OME 2018GR+RE, BM	OME 2050GR+RE, BM	OME 2018HY+RE, BM	Ref. Diesel
PtL: CO2 sourcing	8.815	8.712	8.815	
PtL: H2 production	5.519	0.726	0.283	
PtL: methanol step	0.888	0.145	0.050	
PtL: OME distribution	0.059	0.059	0.059	
PtL: OME step	1.936	0.390	0.139	
PtL: OME utilization - exhaust pipe emissions	0.000	0.000	0.000	
Reference: Crude Petrol Production				2.938
Reference: Diesel distribution + desulphurisation				0.059
Reference: Diesel refinery step				0.203
Reference: Diesel utilization - exhaust pipe emissions				0.000
Reference: Expanded system value conv. Ammonia				8.712



System Expansion Results for CO ₂ cases [AM]: ecosystem quality, freshwater and terrestrial acidification				
CO2 Case Ammonia; FU = 1km+0.26kg NH ₃	OME 2018GR+RE, BM	OME 2050GR+RE, BM	OME 2018HY+RE, BM	Ref. Diesel
PtL: CO2 sourcing	1.26E-03	1.26E-03	1.26E-03	
PtL: H2 production	8.81E-04	4.78E-04	1.49E-04	
PtL: methanol step	2.29E-04	9.68E-05	2.77E-05	
PtL: OME distribution	2.52E-05	2.52E-05	2.52E-05	
PtL: OME step	4.99E-04	2.54E-04	7.15E-05	
PtL: OME utilization - exhaust pipe emissions	5.01E-04	5.01E-04	5.01E-04	
Reference: Crude Petrol Production				2.28E-04
Reference: Diesel distribution + desulphurisation				2.76E-05
Reference: Diesel refinery step				1.22E-04
Reference: Diesel utilization - exhaust pipe emissions				5.05E-04
Reference: Expanded system value conv. Ammonia				1.26E-03



System Expansion Results for CO ₂ cases [AM]: ecosystem quality, freshwater eutrophication				
CO2 Case Ammonia; FU = 1 km+ 0.26 kg NH $_3$	OME 2018GR+RE, BM	OME 2050GR+RE, BM	OME 2018HY+RE, BM	Ref. Diesel
PtL: CO2 sourcing	5.62E-05	4.56E-05	5.62E-05	
PtL: H2 production	5.32E-04	4.39E-05	1.47E-05	
PtL: methanol step	2.83E-05	9.06E-06	2.88E-06	
PtL: OME distribution	1.49E-06	1.49E-06	1.49E-06	
PtL: OME step	5.99E-05	2.34E-05	7.17E-06	
PtL: OME utilization - exhaust pipe emissions	0.00E+00	0.00E+00	0.00E+00	
Reference: Crude Petrol Production				2.11E-06
Reference: Diesel distribution + desulphurisation				1.42E-06
Reference: Diesel refinery step				5.85E-07
Reference: Diesel utilization - exhaust pipe emissions				0.00E+00
Reference: Expanded system value conv. Ammonia				4.56E-05



Table 34 - System Expansion Results for $\rm CO_2$ cases [AM]: ecosystem quality, marine eutrophication

System Expansion Results for CO₂ cases [AM]: ecosystem quality, marine eutrophication

CO2 Case Ammonia; FU = 1 km+ 0.26 kg NH $_3$	OME 2018GR+RE, BM	OME 2050GR+RE, BM	OME 2018HY+RE, BM	Ref. Diesel
PtL: CO2 sourcing	2.01E-04	1.98E-04	2.01E-04	
PtL: H2 production	2.58E-04	7.21E-05	2.69E-05	
PtL: methanol step	3.70E-05	1.62E-05	6.53E-06	
PtL: OME distribution	6.49E-06	6.49E-06	6.49E-06	
PtL: OME step	7.69E-05	3.85E-05	1.31E-05	
PtL: OME utilization - exhaust pipe emissions	2.63E-04	2.63E-04	2.63E-04	
Reference: Crude Petrol Production				2.71E-05
Reference: Diesel distribution + desulphurisation				6.15E-06
Reference: Diesel refinery step				8.69E-06
Reference: Diesel utilization - exhaust pipe emissions				2.64E-04
Reference: Expanded system value conv. Ammonia				1.98E-04



System Expansion Results for CO ₂ cases [AM]: ecosystem quality, terrestrial eutrophication				
CO2 Case Ammonia; FU = 1 km+ 0.26 kg NH $_3$	OME 2018GR+RE, BM	OME 2050GR+RE, BM	OME 2018HY+RE, BM	Ref. Diesel
PtL: CO2 sourcing	1.89E-03	1.87E-03	1.89E-03	
PtL: H2 production	1.81E-03	8.23E-04	2.62E-04	
PtL: methanol step	3.33E-04	1.66E-04	4.77E-05	
PtL: OME distribution	7.18E-05	7.18E-05	7.18E-05	
PtL: OME step	7.23E-04	4.36E-04	1.24E-04	
PtL: OME utilization - exhaust pipe emissions	2.89E-03	2.89E-03	2.89E-03	
Reference: Crude Petrol Production				2.94E-04
Reference: Diesel distribution + desulphurisation				6.50E-05
Reference: Diesel refinery step				9.10E-05
Reference: Diesel utilization - exhaust pipe emissions				2.90E-03
Reference: Expanded system value conv. Ammonia				1.87E-03



System Expansion Results for CO ₂ cases [AM]: human health, ozone layer depletion				
CO2 Case Ammonia; FU = 1 km+ 0.26 kg NH $_3$	OME 2018GR+RE, BM	OME 2050GR+RE, BM	OME 2018HY+RE, BM	Ref. Diesel
PtL: CO2 sourcing	8.30E-08	8.27E-08	8.30E-08	
PtL: H2 production	2.04E-08	6.94E-09	2.60E-09	
PtL: methanol step	6.06E-09	1.38E-09	4.53E-10	
PtL: OME distribution	4.64E-10	4.64E-10	4.64E-10	
PtL: OME step	1.33E-08	3.68E-09	1.23E-09	
PtL: OME utilization - exhaust pipe emissions	0.00E+00	0.00E+00	0.00E+00	
Reference: Crude Petrol Production				3.57E-08
Reference: Diesel distribution + desulphurisation				4.61E-10
Reference: Diesel refinery step				2.41E-09
Reference: Diesel utilization - exhaust pipe emissions				0.00E+00
Reference: Expanded system value conv. Ammonia				8.27E-08



Table 37 - System Expansion Results for CO₂ cases [AM]: Human health, respiratory effects, inorganics

System Expansion Results for CO ₂ cases [AM]: Human health, respiratory effects, inorganics				
CO₂ Case Ammonia: FU = 1km+0.26kg NH₂	OME	OME	OME	Ref. Diesel
	2018GR+RE, BM	2050GR+RE, BM	2018HY+RE, BM	
PtL: CO2 sourcing	2.98E-04	2.98E-04	2.98E-04	
PtL: H2 production	7.54E-05	6.51E-05	2.42E-05	
PtL: methanol step	2.24E-05	1.31E-05	4.34E-06	
PtL: OME distribution	2.92E-06	2.92E-06	2.92E-06	
PtL: OME step	4.88E-05	3.44E-05	1.13E-05	
PtL: OME utilization - exhaust pipe emissions	5.27E-06	5.27E-06	5.27E-06	
Reference: Crude Petrol Production				1.37E-05
Reference: Diesel distribution + desulphurisation				3.30E-06
Reference: Diesel refinery step				1.43E-05
Reference: Diesel utilization - exhaust pipe emissions				1.18E-05
Reference: Expanded system value conv. Ammonia				2.98E-04



Table 38 - System Expansion Results for \mbox{CO}_2 cases [AM]: Human health, photochemical ozone

System Expansion Results for CO₂ cases [AM]: Human health, photochemical ozone creation

CO2 Case Ammonia; FU = 1km+0.26kg NH ₃	OME	OME		Ref. Diesel
	2010GR+RE, DIVI	2030GR+RE, DIVI	2010HT+RE, DIVI	
PtL: CO2 sourcing	6.69E-04	6.65E-04	6.69E-04	
PtL: H2 production	4.57E-04	2.13E-04	8.57E-05	
PtL: methanol step	1.00E-04	4.29E-05	1.54E-05	
PtL: OME distribution	1.94E-05	1.94E-05	1.94E-05	
PtL: OME step	2.18E-04	1.13E-04	4.05E-05	
PtL: OME utilization - exhaust pipe emissions	6.93E-04	6.93E-04	6.93E-04	
Reference: Crude Petrol Production				1.35E-04
Reference: Diesel distribution + desulphurisation				1.86E-05
Reference: Diesel refinery step				4.23E-05
Reference: Diesel utilization - exhaust pipe emissions				6.96E-04
Reference: Expanded system value conv. Ammonia				6.65E-04



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