† Electronic Supplementary Information (ESI):

Material or fuel: comparative cradle-to-grave climate and material footprint analysis for the use of methanol from recycled CO2

Sebastian Turnau*, Caroline Sophie Mignot, Clemens Mostert, Stefan Bringezu

University of Kassel, Center for Environmental Systems Research (CESR), Sustainable Resource Futures Group (SURF), 34117 Kassel, Germany;

*   E-Mail: Sebastian.turnau@uni-kassel.de

S1: Quantity of conventional products to be substituted with 100 kt methanol from recycled CO2

To provide absolute values for comparison a fictive production plant with a capacity of 100 kt of CO_2 based methanol per year is assumed as a common functional unit. The production of 100 kt of CO_2 based methanol requires approx. 1.03 TWh of renewable electricity for the electrolysis, hence the comparison provides additional information, which technology option reduces the climate footprint most with a fixed amount of renewable electricity. 100 kt of methanol provide a lower heating value of 553 GWh considering a relative lower heating value (LHV) of 19.9 MJ/kg methanol (1). The LHV values for other conventional (conv.) fuels are used to determine the amount of conv. fuel substitute with the LHV of 100 kt methanol from recycled CO_2. Conv. fuels consist of a mixture of several different compounds and may vary in quality between seasons and markets. The variation in quality may lead to a range of 5 -10% higher and lower than the provided values.

Table 1 lists the quantities of conventional product that can be substituted with the input of 100 kt methanol. Methanol directly substitutes HFO or petrol, while it must be processed partly to formaldehyde to form OME_1 as a conv. diesel substitute. Approximately 75 kt OME_1 can be generated from 100 kt methanol. The lower heating value provided by 1 kg conventional fuel is substituted with a mass of fuel from CO_2 recycling that provides the same lower heating value as the conventional fuel. The following equations 1 and 2 show the calculation for the change in the product climate or material footprint for the use of 100 kt methanol from recycled CO_2 to substitute conv. fuels (energetic use) or conv. polymers (material use):

$$\Delta FP_{energetic\ use} = \left(FP_{conv.\ fuel} - FP_{CCU\ fuel} \times \frac{LHV_{conv.fuel}}{LHV_{CCU\ fuel}} \right) \times m_{fuel} \tag{1}$$

$$\Delta FP_{material\ use} = (FP_{conv.\ material} - FP_{CCU\ material}) \times m_{material} \tag{2}$$

Where:

ΔFP:	Change in footprint
FP:	Footprint
LHV:	Lower heating value
m:	Substitutable amount of conventional product (see **Table 1**)

Table 1: Amount of conventional products that can be substituted by using products made from 100 kt methanol from recycled CO_2

Captured CO_2	Methanol from CO_2 recycling	Product from recycled CO_2	Conventional product	Substitutable amount	Basis for comparison	Reference for Conv. product	Reference for CCU substitute
137 [kt]	100 [kt]	100 [kt] methanol	HFO	51 [kt]	LHV	39 Mj/kg (2)	19.9 Mj/kg (1)
		100 [kt] methanol	Petrol	46 [kt]	LHV	43 Mj/kg (3)	19.9 Mj/kg (1)
		75 [kt] OME_1	Diesel	40 [kt]	LHV	42 Mj/kg (3)	22.5 Mj/kg (4)
		94 [kt] POM	POM	94 [kt]	Mass	1 kg (5)	1 kg (5)
		39 [kt] PP	PP	39 [kt]	Mass	1 kg (5)	1 kg (5)

S2: Description of the process model

Background system

The generation of electricity and heat, both necessary not only in conventional but also in CO_2-based production routes, is amongst others based on fossil resources. Renewable electricity is supplied by wind power and feeds the electrolysis. Electrolysis demands tab water and ultra-pure water, the supply is calculated with ecoinvent data. The Background system is modelled with data from ecoinvent database. All processes except the electrolysis use German grid electricity mix based on ecoinvent. Thermal energy, where required, uses heat generation for the chemical industry from ecoinvent database. For the calculation for section 3 the electricity and heat mix used is changed according to (S8).

Capturing of CO_2

The relevant input factors for the capture of CO_2 from a waste incineration plant, a cement factory and the atmosphere are illustrated in **Figure 1**, **Figure 2** and **Figure 3**. The input flows refer to 1 kg of captured CO_2. Cement plants and waste incineration plants are industrial point sources for the capture of the greenhouse gas, while air represents a diffuse CO_2 source. For all three sources, neither the process producing CO_2 nor the infrastructure and additional machinery or buildings necessary are taken into account as these may differ from case to case, depending on the available infrastructure and size of the capturing unit. Solely the direct input flows electricity and heat are therefore considered.

At a cement plant, the concentration of CO_2 in the flue gas resulting from the burning of clinker is relatively high with about 25 % (6). For the process of CO_2-capturing at a cement plant post-combustion amine scrubbing with monoethanolamine (MEA) is assumed (6). A specific electricity and heat supply and MEA-scrubbing liquid are necessary for the process (7). The MEA-scrubbing liquid can be regenerated after use, however, there is still an amount that is consumed and a resulting sludge that needs to be disposed (8,9). In this study the heat input of 0.763 kWh_{th} is the net heat demand that is received from the grid (10).
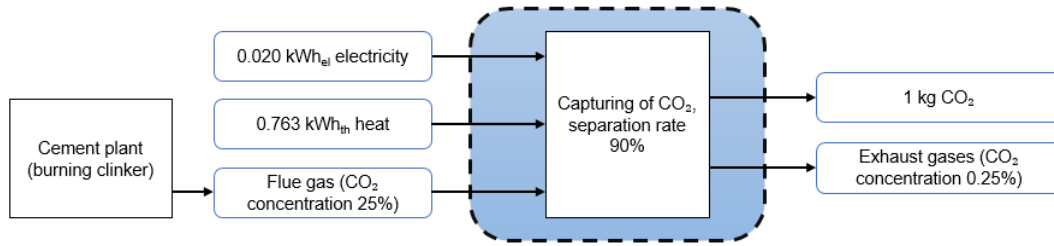
Figure 1: Illustration of carbon capture process from a cement plant (own illustration, data based on (7))

For the recovery of CO_2 from a waste incineration power plant, which is available in the flue gas with a concentration between 10 and 14 %, amine scrubbing with MEA is the chosen capture process (11). Electricity supply is considered from the grid based on (10), heat is assumed to be supplied from waste heat. As the facility itself produces heat and electricity, it can supply the required heat for the process of CO_2 recovery. Electricity is either fed into the grid or used for CO2 capture, while waste heat is assumed to be available. This may result in a slight efficiency loss of the plant as less heat and/or electricity can be fed into the respective grid (12) when considered. Here the waste incineration power plant, that supplies the CO_2, is not included in the process model.
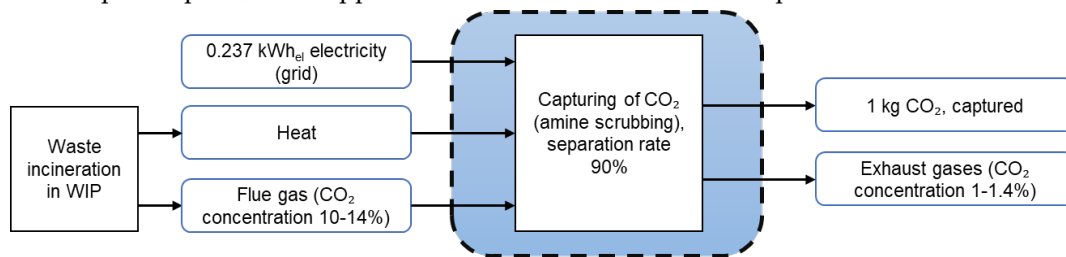

Figure 2: Illustration of carbon capture process from a waste incineration plant (own illustration, data based on (10))

Direct air capture (DAC) is used to capture CO_2 from the atmosphere. This technology has a higher demand for heat than the other CO_2 sources analyzed in this study (5). The net demand for heat provided from natural gas heating. However, when located next to an industrial facility, exhaust heat can be used for the process to increase efficiency (13).
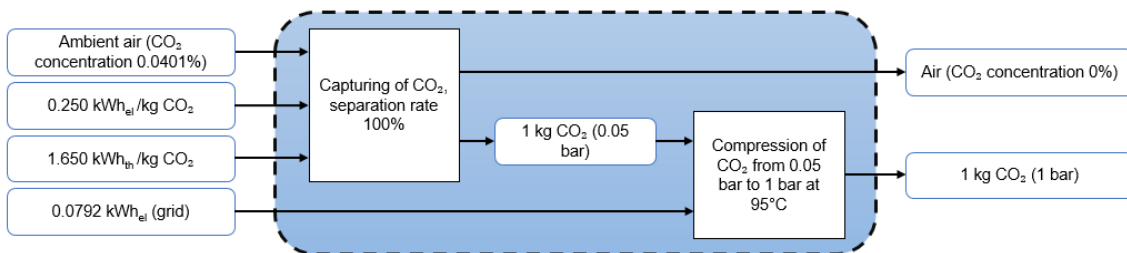

Figure 3: Illustration of carbon capture process from the atmosphere (own illustration, data based on (5))

Electrolysis

Via water electrolysis, hydrogen is produced from ultra-pure water and electricity. The technology is described and identified as a key driver for raw material input and costs for CO_2 based production in various literature (14–17). The three existing technologies are alkaline electrolysis (AE)

proton exchange membrane electrolysis (PEMEL) and high temperature electrolysis (HTEL) (15,18). For this the PEMEL is assumed since it represents a combination of dynamic production and high TRL without the need for additional heat. The electrolysis process is fed with renewable electricity from wind power, that is assumed to be available. The by-product oxygen is not further considered. The process used is depicted in **Figure 4**.
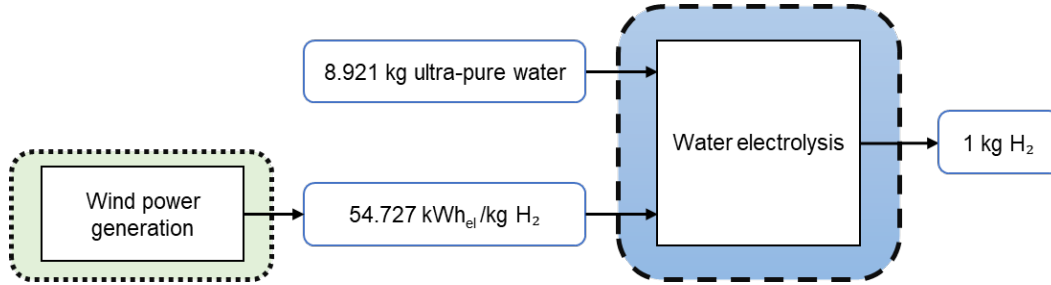

Figure 4: Illustration of electrolysis (own illustration, data based on (14))

Methanol synthesis

The methanol synthesis requires the recovered CO_2, hydrogen, electricity as well as a catalyst, resulting in methanol and water as a by-product, as shown in the following reaction (19).

$$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O \tag{1}$$

In general, several cycles are necessary to transform most of the CO_2. The reaction, which takes place at 50 bar pressure and 220°C, is exothermic, resulting in exhaust heat, which could be regenerated for the process of carbon capture (16) if the capturing is located close to methanol plant. The process scheme is shown in **Figure 5**. Water as a by-product of this reaction, which is removed from methanol via distillation.
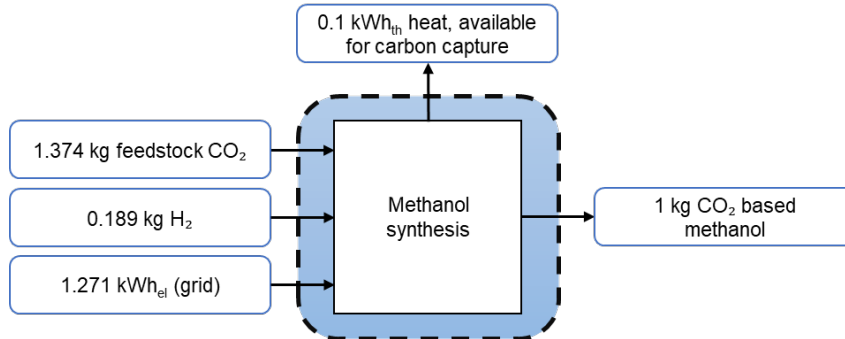

Figure 5: Illustration of methanol synthesis (own illustration, data based on (19))

Crude oil production

The production of diesel, petrol and HFO starts with the extraction of crude oil, which then undergoes the process of separation by fractional distillation in an oil refinery. In distillation towers, the crude oil is exposed to extreme heat, causing the separation into liquids and gases. After the process of conversion, where the processing of fuels is supported by catalysts, the final production step is the purification of the different crude oil-based products. Processes used for the LCA are taken from ecoinvent database (20). The refinery process is exothermic and supplies all electrical and thermal energy required (21), therefore it is assumed that the ecoinvent process is representative in the future.

OME₁ production

After the methanol synthesis distillation clears the methanol from water and methanol can be used as a synthetic fuel directly (19) or further processed to OME_1. Deutz. et al. (22) analyzed the blending of OME_1 and conventional diesel, where OME_1 replaces 24 mass % of the conventional fuel. To produce OME_1 in the given process, formaldehyde is required in addition to CO_2-based methanol and electricity (23). Formaldehyde forms via catalytic oxidation of methanol. Silver is used as a catalyst, air and steam are present and formaldehyde is extracted from the resulting gases by absorption in water resulting in an aqueous formaldehyde solution (24). OME_1 forms from a condensation reaction from methanol and formaldehyde. The heterogeneously catalyzed reaction happens over an acid catalyst in a two-pressure distillation (25). **Figure 6** depicts the production of formaldehyde and OME_1 production.
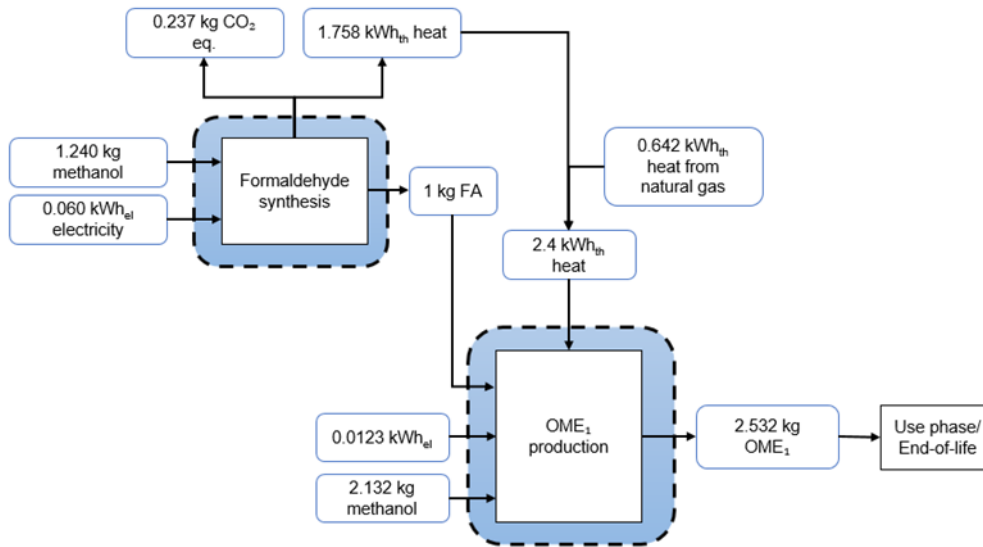

Figure 6: Illustration of processes for OME1 production (own illustration, data based on (22))

Direct use of renewable electricity as a fuel

Direct use of renewable electricity as a fuel for battery electric vehicles is part of the products system. It is compared to the analyzed carbon based fuels if used for mobility based on the lower heating value provided by 100 kt of methanol from recycled CO_2. It is comparable to fuels as production of cars and traffic infrastructure are not included in the analysis. Electricity production from wind is used.

Use phase and end-of-life for fuels

The use phase and the end-of-life phase of the fuels occur at the same time during combustion in a marine turbine or combustion engine. A transport of the produced fuels to a harbor (100 km) or gas station (300 km) is included. The energy resulting from combustion of fuels is utilized to move the vehicle, while CO_2 is emitted to the atmosphere. Direct electricity as fuel does not generate emissions in the use phase. Input and output flows for the combustion are depicted based on emission factors in **Figure 7**. HFO is calculated using an ecoinvent process instead of emission factors, therefor no values are depicted for HFO:
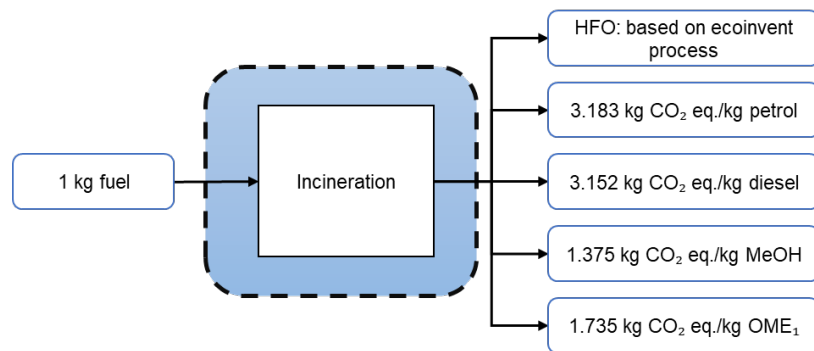
Figure 7: Simplified illustration of incineration process of all analyzed fuels (own illustration, data based on (1–3,26)

Conventional polypropylene production

Polypropylene (PP) is a polymer with a wide range of application possibilities in packaging and other sectors like the automobile industry. It is one of the two most demanded polymers in Europe, next to polyethylene (27). It is produced via the polymerization of the monomer propylene. The production routes of conventional and CO_2-based PP differ only in the generation of propylene, whereas the following process of polymerization to form PP is the same for both routes. Conventionally produced PP is mostly based on crude oil, which serves as the carbon supplier for the polymer.. For polymerization of the analyzed olefins, the gas phase cascading process is chosen (28). This is a stable process and is less susceptible to faults than other options. The reaction temperature lies between 60 and 85°C, the pressure between 20 and 35 bar. A titan catalyst is used for the reaction (28). A scheme for the conventional production and polymerization of PP is procided in **Figure 8.**
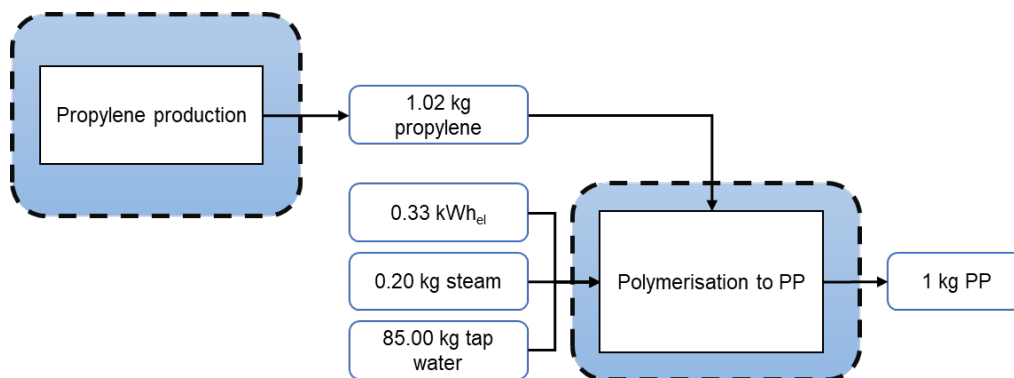

Figure 8: Illustration of conventional PP production (own illustration, data based on (20,28)

Conventional polyoxymethylene production

Polyoxymethylene (POM), is a special polymer, with production volumes much smaller than PP and applications in the industrial, automotive or consumer industry with injection-molded mechanical or electrical parts (29). POM is available as a homopolymer (POM-h) and as a copolymer (POM-c). POM-h is generated through the polymerization of formaldehyde, which is formed via oxidation of methanol, which, in turn, is generated from natural gas. To gain POM-c, trioxane, which results from the trimerization of formaldehyde, and a smaller quantity of a copolymer are polymerized (29). As the difference between POM-h and POM-c concerning the environmental impacts their production causes is small, only the production of POM-h is considered in this study. Data for POM production are mostly adopted from (29,30) similar to the process used in (5), where

POM was produced from natural gas via methanol and formaldehyde based on (31). A scheme for the process is depicted in **Figure 9.**
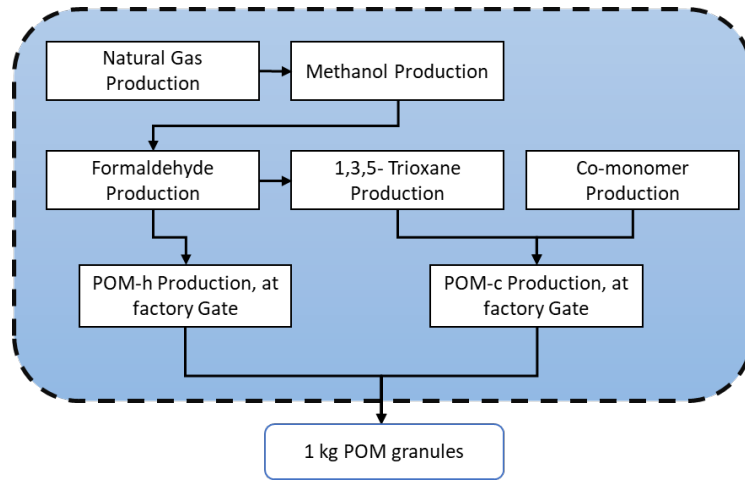

Figure 9: Illustration of conventional POM production (own illustration, data based on (29,31)

Polypropylene production from methanol from CO₂ recycling

As mentioned before, the production of PP based on recovered CO$_2$ differs from the conventional production route only in the generation of propylene. CO$_2$-based propylene is based on methanol and generated via the methanol-to-olefins (MTO) process as described in (32,33). Here, gaseous methanol is being cooled in a quenching tower and cleaned from H$_2$S and CO$_2$ in an alkaline tower with the help of sodium hydroxide solution (32). The relevant reaction is the following:

$$3CH_3OH \rightarrow C_3H_6 + 3H_2O \tag{2}$$

Polypropylene is generated from propylene in the following process of polymerization to PP as depicted in **Figure 10**.
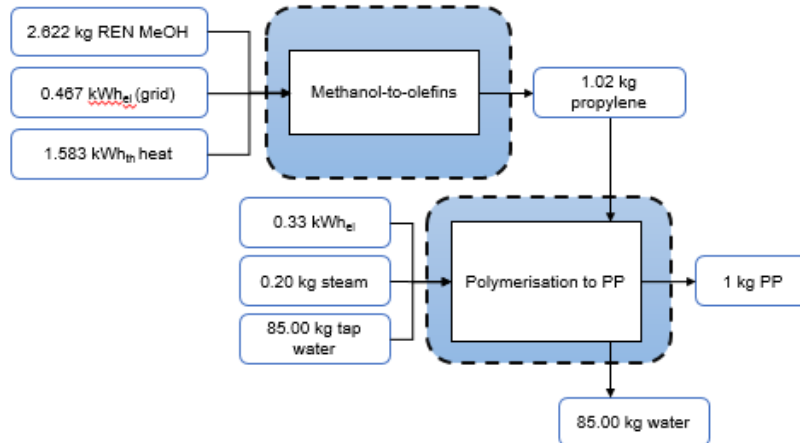
Figure 10: Illustration of methanol PP production for methanol from CO₂ (own illustration, data based on (28) for polymerization; (32) for Methanol-to-olefins)

Polyoxymethylene production from methanol from recycled CO₂

The process for the CO$_2$-based production of POM is adapted to ecoinvent from the conventional production process available in the data basis GaBi plastics (30). The elementary flow data from GaBi is transferred to model a unit process in ecoinvent 3.1. considering ecoinvent elementary flows that

are comparable to GaBi elementary flows. The process was tested and delivered the same impacts for the considered footprints as the original GaBi process. The conventional process of POM production uses methane from natural gas to produce methanol as raw material. Methane serves as the carbon molecule supplier for POM. When producing POM based on methanol from CO_2, the step of generating methanol from natural gas becomes redundant as methanol can directly be synthesized from CO_2 and H_2. A scheme is provided in **Figure 11**.
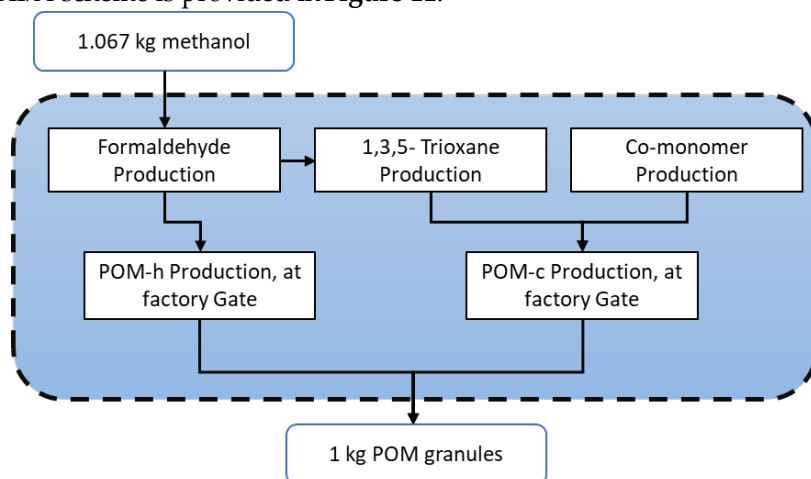

Figure 11: Illustration of POM production using methanol from CO2 (own illustration, data based on black box model from (30) and process data from (29,31))

Only the methane-based methanol required to supply carbon as a raw material is replaced with methanol from CO_2. It is calculated that the methanol required to deliver the carbon molecules to produce 1 kg of POM provides 24.2 MJ of energy. The conventional process via methane provides 17.2 MJ of energy from the amount of methane that is required to provide the carbon molecules for 1 kg of POM. Assuming that only 17.2 MJ of energy are required for the process, the CO_2 based process provides additional 7 MJ of energy that are not required for the production of POM and can be used as waste heat or for heat integration. Only carbon molecule feedstock is considered, other thermal energy demand for e.g. heating is not considered. The calculation is shown in Table 2 as follows:

Table 2: Calculation of methanol demand of CO_2 based POM

	Unit	Value / Calculation
Required Formaldehyde	kg/kg POM	1
Required Formaldehyde	mol/kg POM	= 1 kg/kg POM / (30.03 g/mol *1000) = **33.30**
Required Methanol	kg/kg POM	= 33.30 mol/kg POM * 32.04 g/mol / 1000 = **1.067**
Methanol Feedstock Calorific Value	MJ/kg POM	= 1.067 mol/kg POM * 22.7 MJ/kg = **24.221**
Feedstock methane conventional process	MJ/kg POM	17.166 (29,34)
Usable exhaust energy (heat)	MJ/kg POM	24.221MJ/kg POM – 17.166 MJ/kg POM = **7.04**
Methanol gross calorific value	MJ/kg methanol	22.7 (1)
Formaldehyde molar mass	g/mol FA	30.03
Methanol molar mass	g/mol methanol	32.042

Road transportation for polymer use and EoL phase

The use of Polymers is assumed to require road transportation in a 16 to 23 t lorry with a demand of 0.000029 l diesel fuel per kg of transported product in this study. (35)

Use phase of polymers

After leaving the first production facility in the form of granulate, the polymer is further processed via injection molding, which is a common processing method for polymers, where melted plastic granulate is injected into a mold to form plastic products (36). Injection molding is assumed the only form of processing to ensure comparability. It is assumed that the polymer granulate leave the industrial cluster at the production gate, hence a road transport of 300 km are assumed (35). A scheme is provided in **Figure 12**.
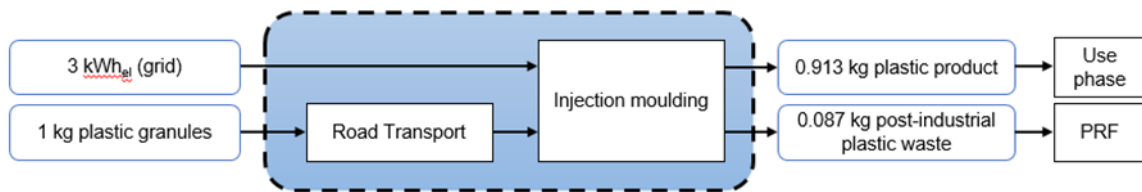
Figure 12: Illustration of industrial processing of polymers via injection molding (own illustration, data based on (36,37))

Resulting from this process are final products, which can be used directly or can be integrated into other products such as packaging of consumer product or cars, as well as post-industrial waste. Post-industrial waste can be defined as production waste from industrial processing. It directly enters the process of recycling without entering the use phase, as it is pure and not contaminated (37). The final products are used for a certain amount of time by the technology user and become anthropogenic stock (38).

End-of-life (EoL) phase of polymers

Subsequent to the use phase the plastic becomes plastic waste. The plastic waste is collected and transported to a material recovery facility, assuming a transport distance of 300 km (35). At the MRF, the waste is sorted as depicted in **Figure 13**. The MRF requires 0.0057 kWh$_{el}$ and 0.0084 kg diesel per kg sorted plastic waste (39).
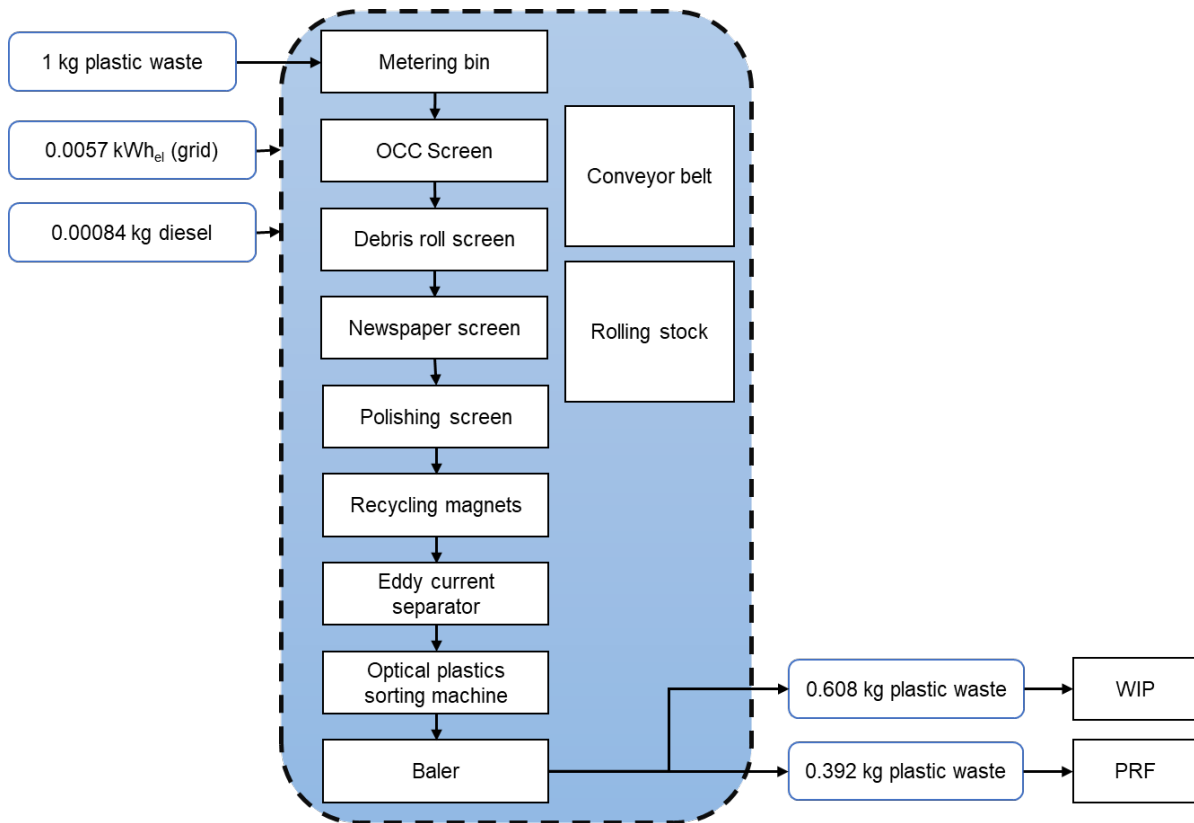
Figure 13: Illustration of a material recovery facility (MRF) (own illustration, data based on (39))

Depending on its purity or grade of contamination, it is either further transported to a plastics recycling facility (PRF) or brought to a waste incineration plant (WIP). At the PRF, the flow of plastic waste from the MRF eligible for recycling comes together with the stream of post-industrial waste, which has a high varietal purity (37). At a PRF, the waste is washed, shredded and extruded into scrap polymer granulate, which then enters the next cycle of processing and usage as depicted in **Figure 14.** Per kg sorted plastic waste, the PRF requires 0.685 kWh$_{el}$ electricity, 0.008 kg diesel and 0.002 kg water for the different sub-processes.
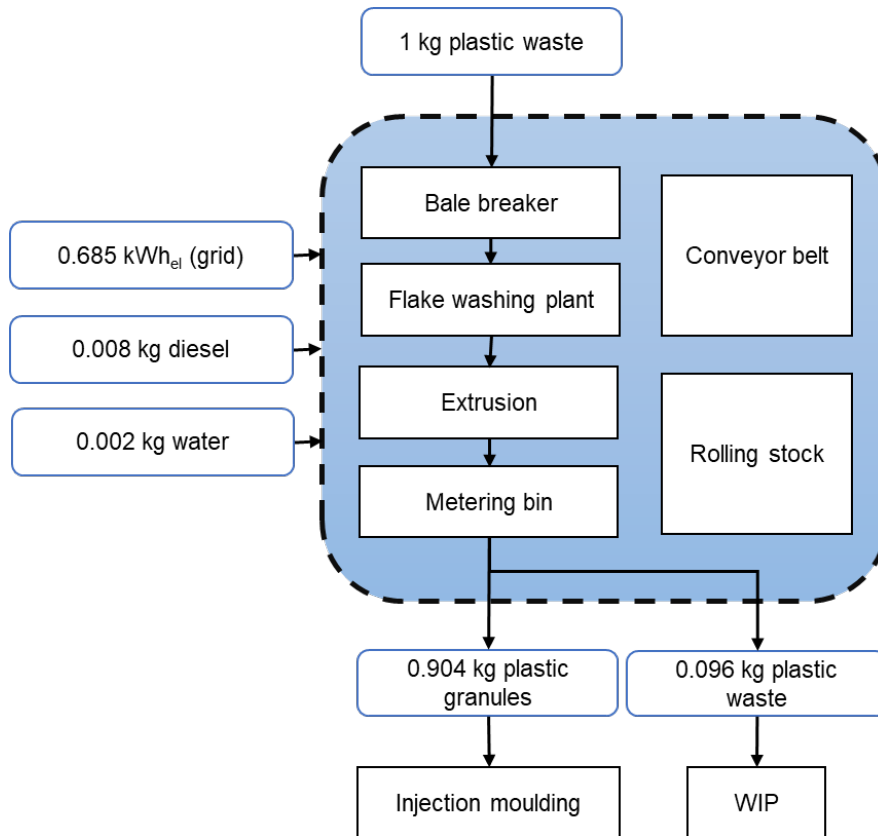
Figure 14: Illustration of a plastics recycling facility (PRF) (own illustration, data based on (39))

At the PRF there is a small amount of process waste, leaving the facility to be thermally disposed in a WIP instead of being recycled (37). This cycle of processing, use and recycling can be repeated several times, but due to chemical degradation of the polymers, recycling has its limit after a maximum of four to six cycles (40–42).

In the WIP plastic waste is incinerated to generate energy, for district heating and the generation of electricity, which can then be fed into the grid (39). The WIP is depicted in **Figure 15**. Since PP and POM have different lower heating values, the respective amounts of usable energy and emitted CO_2 are depicted for both polymers. A detailed calculation can be found in **Table 3** and the factors for the final emission are shown in **Table 4**.
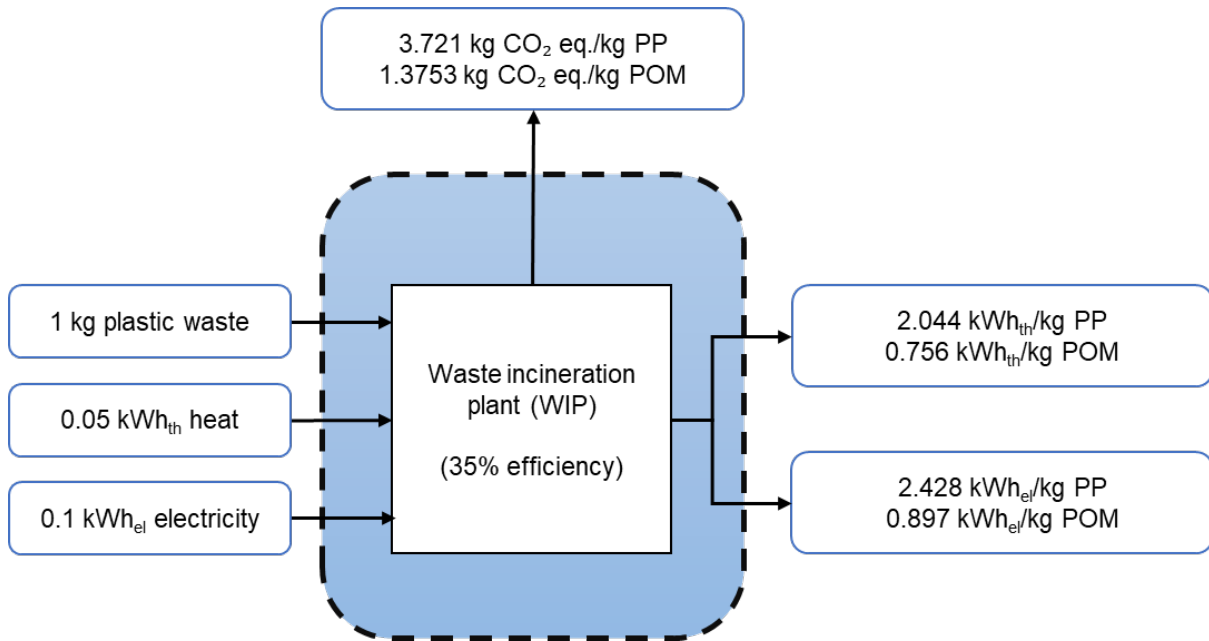
Figure 15: Illustration of waste incineration plant (own illustration, data based on (39,43–45))

Table 3: Calculation of usable energy in waste incineration power plant

	Unit	Calculation / Value
WIP efficiency: Waste to thermal energy: Waste to electrical energy:	%	35 (44) 16 (44) 19 (44)
LHV PP	MJ/kg PP	46 (45)
LHV POM	MJ/kg PP	17 (45)
Usable thermal energy from PP	kWh$_{th}$/kg PP	LHV: 46 MJ/kg → 12.778 kWh/kg 12.778 kWh/kg * 0.16 **= 2.044**
Usable electrical energy from PP	kWh$_{el}$/kg PP	LHV: 46 MJ/kg → 12.778 kWh/kg 12.778 kWh/kg * 0.19 **= 2.428**
Usable thermal energy from POM	kWh$_{th}$/kg POM	LHV: 17 MJ/kg → 4.722 kWh/kg 4.722 kWh/kg * 0.16 **= 0.756**
Usable electrical energy from POM	kWh$_{el}$/kg POM	LHV: 17 MJ/kg → 4.722 kWh/kg 4.722 kWh/kg * 0.19 **= 0.897**

S3: Recycling system for the process model

The amount of generated waste in the industrial processing, MRF and PRF are calculated using the following equations. The equations use values based on the German recovery rates for plastic waste in 2017 as illustrated in **Figure 16** based on (37). No imports and exports were taken into account. The percentage rates are used as a basis for the calculation of the relative material flows for 1 kg of virgin polymer as depicted in **Figure 17**. While the differently colored rows show the different use phases, the boxes on the right show the amount of plastic incinerated after each use phase and the amount of primary material that is replaced by recycled plastic material assuming functional

equivalence. The first line, which is marked in yellow, depicts the processing, use and waste management of polymers without recycling. The next line shows the first use phase if recycling is available. After three recycling cycles and four use phases, 1.481 kg of primary material is substituted by recycled material as secondary input as depicted right at the bottom of **Figure 17**. The overall recycling rate for the recycling system in this study after 4 use phases is 33 %.

$$Material\ efficiency_{IP_{PIW\ to\ PRF}} = \frac{m_{PIW}}{m_{VPP}} = \frac{953\frac{kt}{a}}{11015\frac{kt}{a}} = 8.7\% \tag{3}$$

$$Separation\ Efficiency_{MRF_{PWC\ to\ PRF}} = \frac{m_{MR\ of\ PCW}}{m_{PCW} - m_{PCW\ to\ landfill}} = \frac{2024\ kt/a}{5166\ kt/a} = 39.2\% \tag{4}$$

$$Material\ efficiency_{PRF_{PIW\ to\ re-granulate}} = \frac{m_{MR\ of\ PIW}}{m_{PIW} - m_{PIW\ to\ landfill}} = \frac{849\ kt/a}{949\ kt/a} = 89.5\% \tag{5}$$

$$Material\ efficiency_{PRF_{PCW\ to\ re-granulate}} = \frac{m_{recycled\ material}}{m_{Material\ recycling}} = \frac{1411\ kt/a}{1975\ kt/a} = 71.4\% \tag{6}$$

Where:
m   = Weight of material
IP   = Industrial Processing (Injection Molding)
PIW   = Post-industrial Waste
VPP   = Virgin Polymer Production for Germany in 2017 (37)
MRF   = Material Recovery Facility
MR   = Material Recycling
PCW   = Post-consumer Waste
PRF   = Plastics Recycling Facility
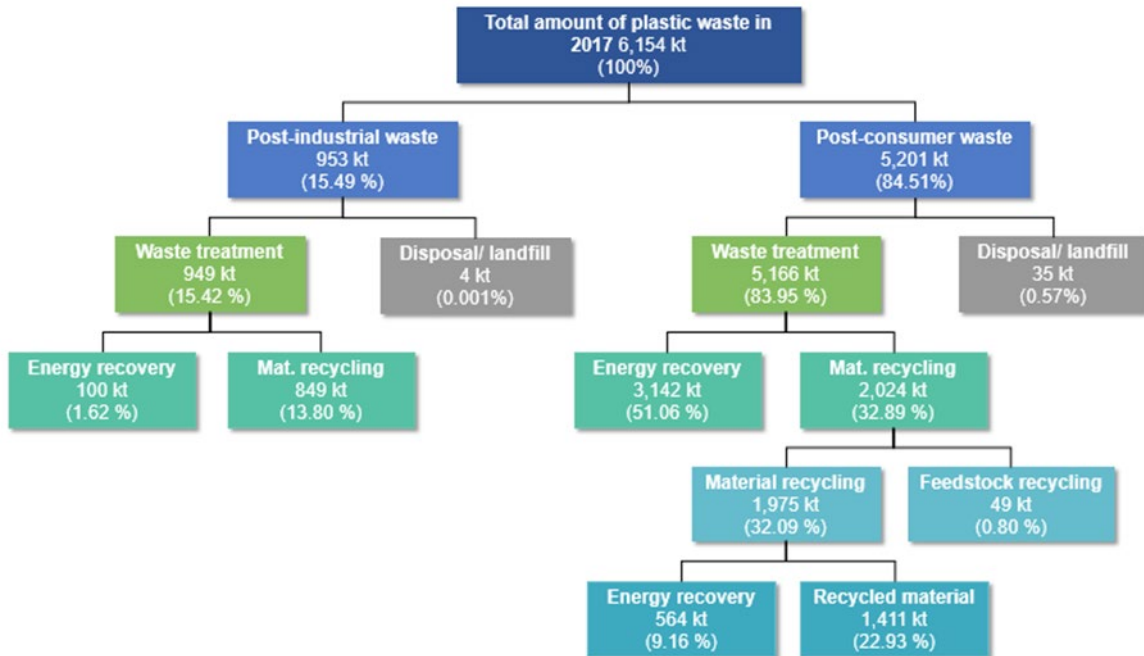
Figure 16: Plastic waste recovery rates in Germany in 2017 (own illustration based on Conversio (37))
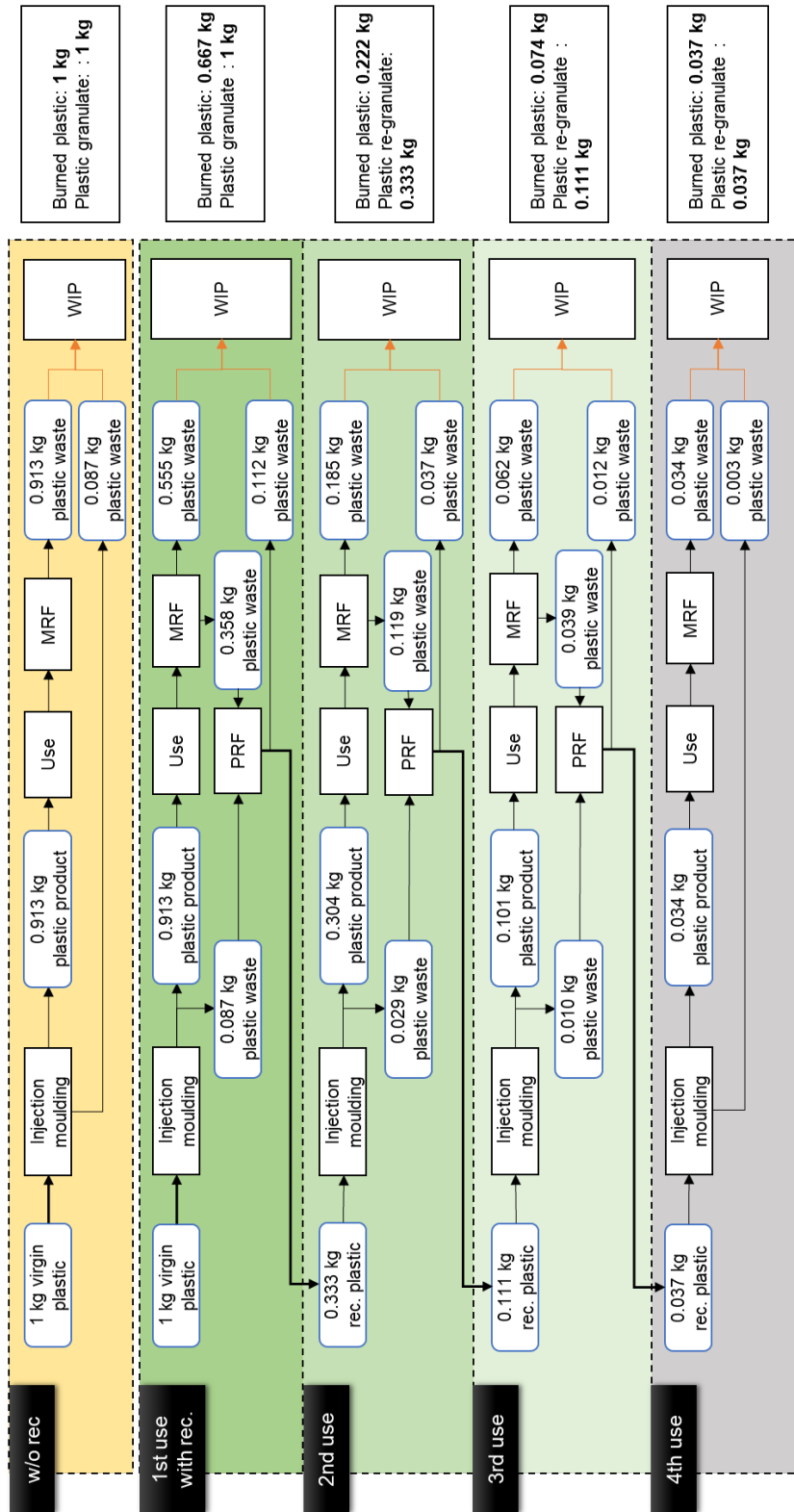
Figure 17: Flows for plastic waste in Germany considered by the recycling system in the process model, without imports and exports (own illustration, data based on Conversio (37)). (w/o rec – without consideration of recycling; with rec – with consideration of recycling; MRF – Material Recovery Facility; PRF – Plastics Recycling Facility; WIP – Waste Incineration Plant)

S4: Emission Factors for end-of-life

Table 4: Calculation of emission factors for end-of-life of studied fuels and polymers. The value shown for HFO is a reference value from literature for comparison. The process modell calculates emissions based on HFO production and HFO incineration from ecoinvent 3.1, which causes an overall climate footprint of 2.8 kg CO_2 eq./ kg HFO if IPCC factors re considered. The Emission factor from literature shows that CO_2 emissions from incineration are 3.2 kg CO_2 per kg of HFO.

| Emission factor	Calculation	Source
(ecoinvent process used in process model, calculation plotted for comparison only)	Emissions from HFO in Germany, 2016: 81.6 t CO_2/TJ LHV: 40 GJ/t → 0.040 TJ/t 0.04 TJ/t * 81.6 t CO_2/TJ = **3.264 t CO_2/t**	(2,3)
3.183 kg CO_2 /kg petrol	No calculation necessary	(3)
3.152 kg CO_2 /kg diesel	Emissions from diesel fuel in Germany, 2016: 74.0 t CO_2/TJ LHV: 42.6 GJ/t → 0.043 TJ/t 0.043 TJ/t * 74.0 t CO_2/TJ = **3.152 t CO_2/t**	(2,3)
1.373 kg CO_2 /kg MeOH	Calculation via molar mass: MeOH: 32.05 g/mol 1000g / 32.05 g/mol * 1 C-atom /mol = 31.201 C-atoms 31.201 C-atoms * 44 g/mol CO_2 /1000 = **1.373 t CO2/t**	
1.735 kg CO_2 /kg OME_1	Calculation via molar mass: OME_1: 76.1 g/mol 1000g / 76.1 g/mol * 3 C-atoms /mol = 39.42 C-atoms 39.42 C-atoms* 44 g/mol CO_2 = **1.735 t CO_2/t**	
3.721 kg CO2 /kg PP	Emissions from plastic waste in Germany, 2016: 80.9 t CO_2/TJ LHV: 46 GJ/t → 0.046 TJ/t 0.046 TJ/t * 80.9 t CO_2/TJ = **3.721 t CO_2/t**	(3,45)
1.375 kg CO_2 /kg POM	Emissions from plastic waste in Germany, 2016: 80.9 t CO_2/TJ LHV: 17 GJ/t → 0.017 TJ/t 0.017 TJ/t * 80.9 t CO_2/TJ = **1.375 t CO_2/t**	(3,45)

S5: LCI – Lifecycle Inventory

Table 5 shows input and output flows of the analysed processes considered in the foreground system. POM production from CO_2 is not included in this table, the process is mainly based on (30) and considered as a system process based on elementary flows, which is explained in S3. Positive numbers symbolize an input flow, while negative numbers show an output flow.

Table 5: Overview of input and output flows for analysed production processes

Process	Stream	Amount	Unit	Data Source
CO_2 capture				
CO_2 capture from waste incineration (MEA)	Electricity	0.237	kWh$_{el}$/kg CO_2	(10)
	Captured CO_2	-1.000	kg CO_2	
CO_2 capture from cement factory (MEA)	Electricity	0.020	kWh$_{el}$/kg CO_2	(7)
	Heat	0.763	kWh$_{th}$/kg CO_2	(7)
	Captured CO_2	-1.000	kg CO_2	

CO_2 capture from air (direct air capture)	Electricity	0.250	kWh$_{el}$/kg CO_2	(5,46)
	Heat	1.650	kWh$_{th}$/kg CO_2	(5,46)
	Captured CO_2	-1.000	kg CO_2	
Electrolysis				
Electrolysis for hydrogen production	Electricity	54.727	kWh$_{el}$/kg H_2	(14)
	Ultra-pure water	8.921	kg/kg H_2	(14)
	Hydrogen	-1.000	kg H_2	
Methanol synthesis				
Methanol synthesis for transport and plastic sector	Captured CO_2	1.374	kg/kg methanol	(19)
	Hydrogen	0.189	kg/kg methanol	(19)
	Electricity	1.271	kWh$_{el}$/kg methanol	(19)
	Methanol	-1.000	kg methanol	
Formaldehyde synthesis (from methanol)				
Formaldehyde synthesis for OME$_1$ production	Methanol	1.240	kg/kg FA	(22)
	Electricity	0.060	kWh$_{el}$/kg FA	(22,24)
	Formaldehyde	-1.000	kg FA	
	CO_2 emissions	-0.237	kg/kg FA	(22)
	Heat	-1.758	kWh$_{th}$/kg FA	(22)
OME$_1$ production				
OME$_1$ production from methanol and formaldehyde	Methanol	0.842	kg / kg OME$_1$	(22)
	Formaldehyde	0.395	Kg/kg OME$_1$	(22)
	Electricity	0.005	kWh$_{el}$ /kg OME$_1$	(22)
	Heat	2.400	kWh$_{th}$ /kg OME$_1$	(22)
	Heat (excess heat is used for OME1 production to reduce actual heat demand to 0.642	-1.758	kWh$_{th}$ /kg OME$_1$	(22)
	OME$_1$	-1.000	kg OME$_1$	
Propylene production via MTO				
MTO	Methanol	2.571	kg/kg propylene	(32)
	Electricity	0.458	kWh$_{el}$ /kg propylene	(32)

	Heat	1.552	kWh$_{th}$ /kg propylene	(32)
	Propylene	-1.000	kg propylene	

Polymerisation of propylene to PP				
Polymerisation of propylene	Propylene	1.020	kg /kg PP	(28)
	Tap water	85.000	kg /kg PP	(28)
	Electricity	0.330	kWh$_{el}$ /kg PP	(28)
	Steam	0.200	kg steam/kg PP	(28)
	PP granules	-1.000	kg PP	

Industrial plastics processing				
Injection moulding	PP or POM granules	1.000	kg PP or POM granules	
	Road Transport	300.000	km/kg PP or POM granules	Distance is based on (35)
	Electricity	3.000	kWh$_{el}$ / kg PP or POM granules	(36)
	Plastic products	-0.913	kg plastic products / kg PP or POM plastic granules	(37)
	Plastic waste to PRF	-0.087	kg waste plastic / kg PP or POM plastic granules	(37)

Plastic waste collection and sorting				
Waste collection and sorting in material recovery facility (MRF)	Plastic waste (unsorted)	1.000	kg plastic waste	
	Road Transport	300.000	km/kg plastic waste	Distance is based on (35)
	Electricity	0.006	kWh$_{el}$ /kg plastic waste	(39)
	Diesel	0.008	kg/kg plastic waste	(39)
	Plastic waste to PRF (sorted)	-0.387	kg plastic waste / kg plastic waste	(37)
	Plastic waste to WIPP	-0.613	kg plastic waste / kg plastic waste	(37)

Plastic recycling				

Transport from industrial processing facility or MRF to PRF and plastic material recycling incl. extrusion (PRF)	Plastic waste to PRF (sorted)	1.000	kg plastic waste to PRF	
	Road Transport	300.000	km/kg plastic waste to PRF	Distance is based on (35)
	Electricity	0.685	kWh_{el} /kg plastic waste to PRF	(39)
	Tap water	0.002	kg/kg plastic waste to PRF	(39)
	Diesel	0.008	kg/kg plastic waste to PRF	(39)
	Recycled plastic granules	-0.904	kg recycled plastic/kg plastic waste to PRF	(37)
	Plastic waste to WIPP	-0.096	kg waste plastic/kg plastic waste to PRF	(37)
Fuel combustion				
Combustion of HFO	HFO fuel	1.000	kg HFO	
	Direct CO2 emissions		kg CO_2 eq./kg HFO	Calculated using ecoinvent data: "heavy fuel oil, burned in refinery furnace, cut-off, U" (20) to include all GHG affecting substances
Combustion of petrol	Petrol	1.000	kg petrol	
	Direct CO2 emissions	-3,152	kg CO_2 eq./kg petrol	
Combustion of diesel	Diesel	1.000	kg diesel	
	Direct CO2 emissions	-3,183	kg CO_2 eq./kg diesel	
Combustion of methanol	Methanol	1.000	kg methanol	
	Direct CO2 emissions	-1.373	kg CO_2 eq./kg methanol	Calculated based on molar mass, see ESI (S4)
Combustion of OME_1	OME_1	1.000	kg OME_1	
	Direct CO2 emissions	-1.732	kg CO_2 eq./kg OME_1	Calculated based on molar mass ESI (S4)
Waste incineration				
Incineration of PP waste in WIPP	Electricity	0.100	kWh_{el} /kg plastic waste	(39)
	Heat	0.050	kWh_{th} /kg plastic waste	(39)

	Usable energy	-2.044	kWh$_{th}$ /kg PP	(44,45)
	Usable energy	-2.428	kWh$_{el}$ /kg PP	(44,45)
	Direct CO2 emissions	-3.721	kg CO2eq/kg PP	(3) ESI (S4)
Incineration of POM waste in WIPP	Electricity	0.100	kWh$_{el}$ /kg plastic waste	(39)
	Heat	0.050	kWh$_{th}$ /kg plastic waste	(39)
	Usable energy	-0.756	kWh$_{th}$/kg POM	(44,45)
	Usable energy	-0.897	kWh$_{el}$ /kg POM	(44,45)
	Direct CO2 emissions	-1.375	Kg CO2eq/kg POM	(3) ESI (S4)

S6: LCIA –Lifecycle Impact Assessment

This chapter shows the results for the product climate and material footprint. These charts are intermediate results that may help to comprehend the aggregation steps that were necessary to present the key findings of the LCA for the paper. A grouping of the results as described in (47,48) to correspond to the functional unit is considered necessary.

- **Figure 18**, **Figure 19** and **Figure 20** show results for 1 kg of the specific product and 1 kg of CO_2 based substitute.
- **Figure 21**, **Figure 22** and **Figure 23** show results with fuel products levelled to substitute the conventional fuel based on the specific lower heating value.
- **Figure 24** illustrates the change in climate and material footprints for the substitution of 1 kg conventional product with products based on CO_2 from recycling considering results of **Figure 21**, **Figure 22** and **Figure 23**.

The CO_2 sources cement plant and waste incineration power plant are aggregated to only show industrial point sources ("point"). In addition direct air capture (DAC) is shown to point out the effect of waste heat utilization for CO_2 capturing when comparing "point" to "DAC":
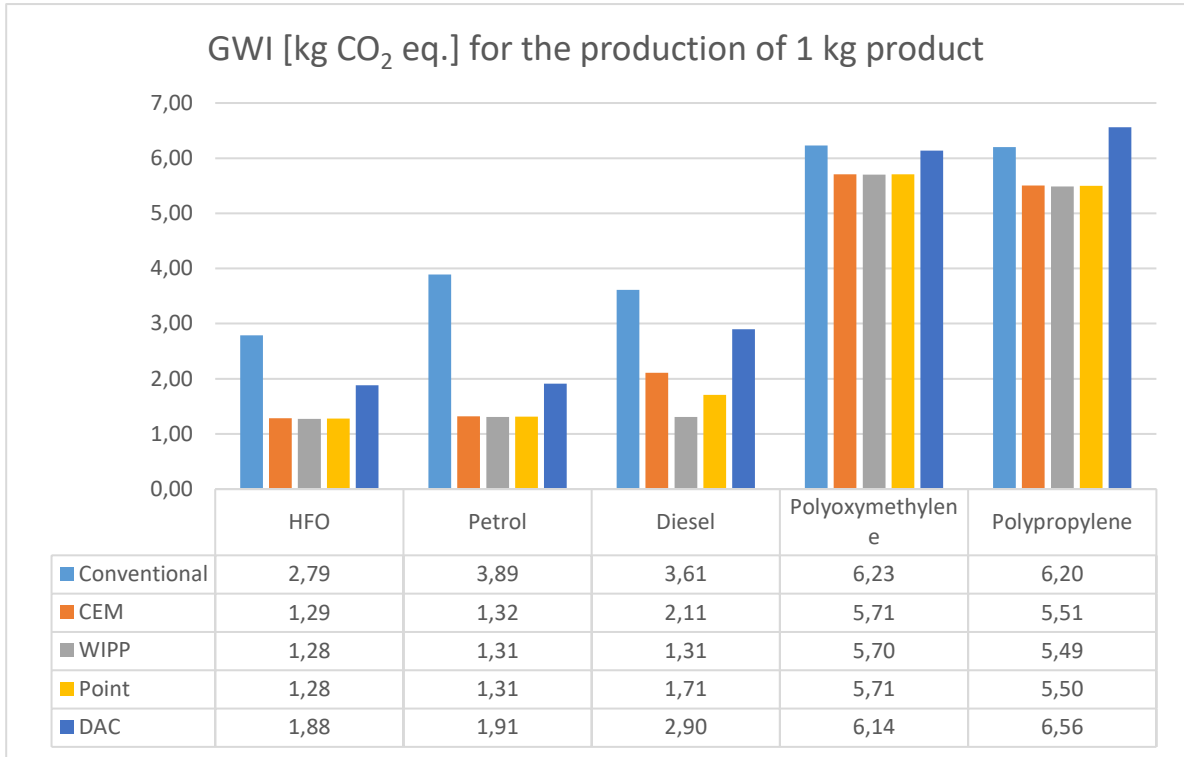
GWI [kg CO$_2$ eq.] for the production of 1 kg product

	HFO	Petrol	Diesel	Polyoxymethylene	Polypropylene
Conventional	2,79	3,89	3,61	6,23	6,20
CEM	1,29	1,32	2,11	5,71	5,51
WIPP	1,28	1,31	1,31	5,70	5,49
Point	1,28	1,31	1,71	5,71	5,50
DAC	1,88	1,91	2,90	6,14	6,56

Figure 18: GWI for the production of 1 kg product

RMI [kg material] for the production of 1 kg product

	HFO	Petrol	Diesel	Polyoxymethylene	Polypropylene
Conventional	2,36	1,57	1,47	6,07	3,84
CEM	1,55	1,58	2,34	6,67	5,89
WIPP	1,63	1,65	2,45	6,73	6,02
Point	1,59	1,62	2,39	6,70	5,96
DAC	1,90	1,92	2,81	6,92	6,50
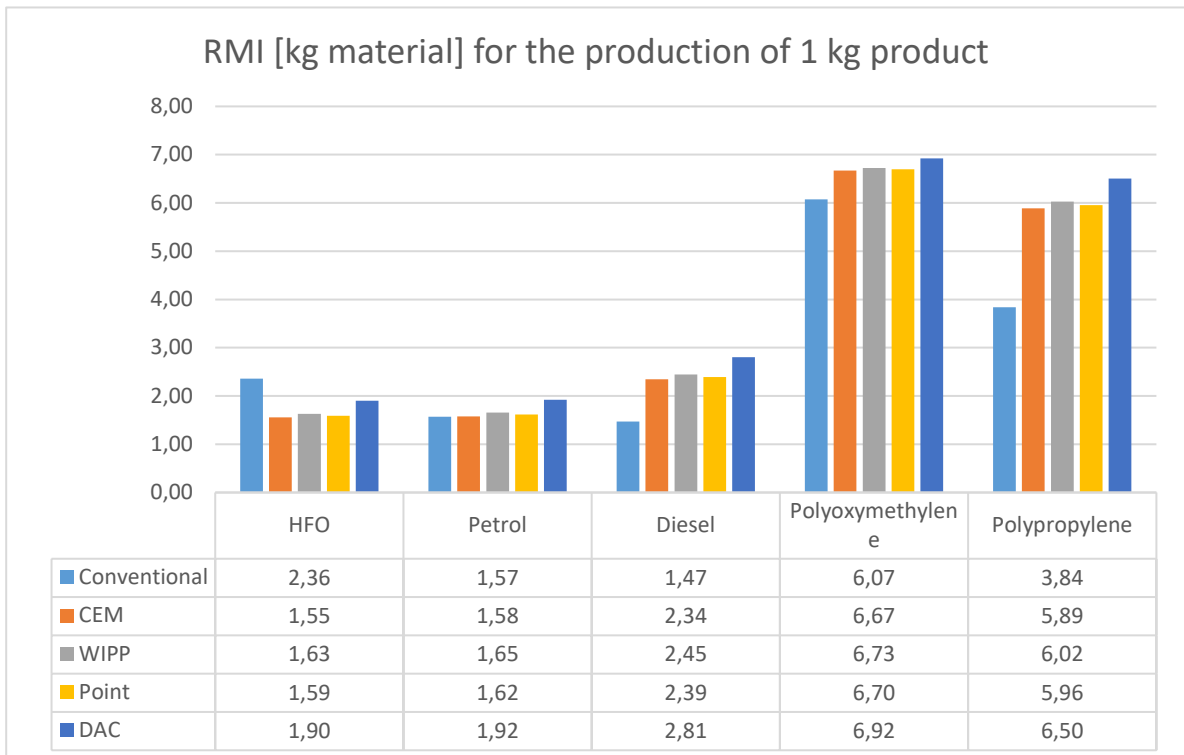
Figure 19: RMI for the production of 1 kg product

TMR [kg raw material] for the production of 1 kg product

	HFO	Petrol	Diesel	Polyoxymethylene	Polypropylene
Conventional	3,19	2,26	2,07	13,36	11,91
CEM	4,47	4,47	6,39	15,68	19,36
WIPP	5,02	5,02	7,12	16,07	20,33
Point	4,75	4,75	6,76	15,88	19,84
DAC	5,46	5,46	7,70	16,39	21,10
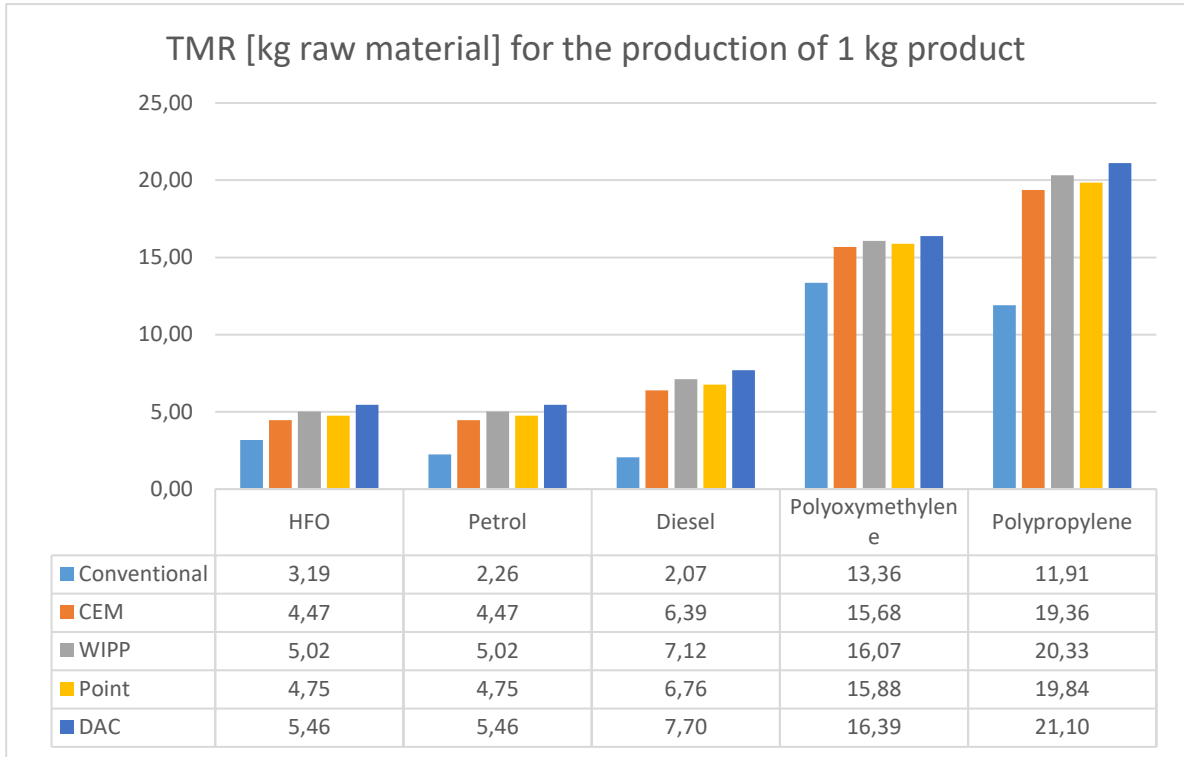
Figure 20: TMR for the production of 1 kg product

GWI [kg CO_2 eq.] for the substitution of 1 kg conventional product

	HFO	Petrol	Diesel	Polyoxymethylene	Polypropylene
Conventional	2,79	3,89	3,61	6,23	6,20
CEM	2,52	2,89	3,99	5,71	5,51
WIPP	2,50	2,86	3,96	5,70	5,49
Point	2,51	2,87	3,97	5,71	5,50
DAC	3,68	4,19	5,48	6,14	6,56

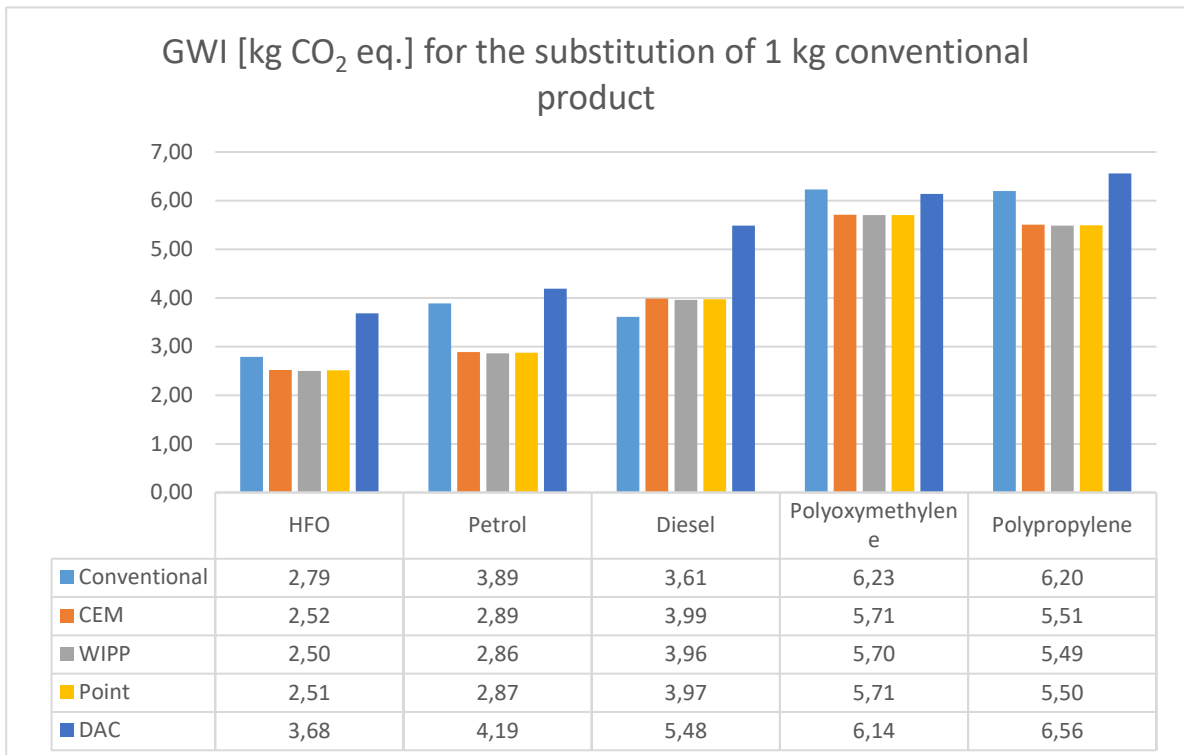Figure 21: GWI for the substitution of 1 kg conventional product

RMI [kg material] for the substitution of 1 kg conventional product

	HFO	Petrol	Diesel	Polyoxymethylene	Polypropylene
Conventional	2,36	1,57	1,47	6,07	3,84
CEM	3,05	6,20	4,44	6,67	5,89
WIPP	3,20	5,51	4,63	6,73	6,02
Point	3,12	5,49	4,53	6,70	5,96
DAC	3,73	5,50	5,31	6,92	6,50
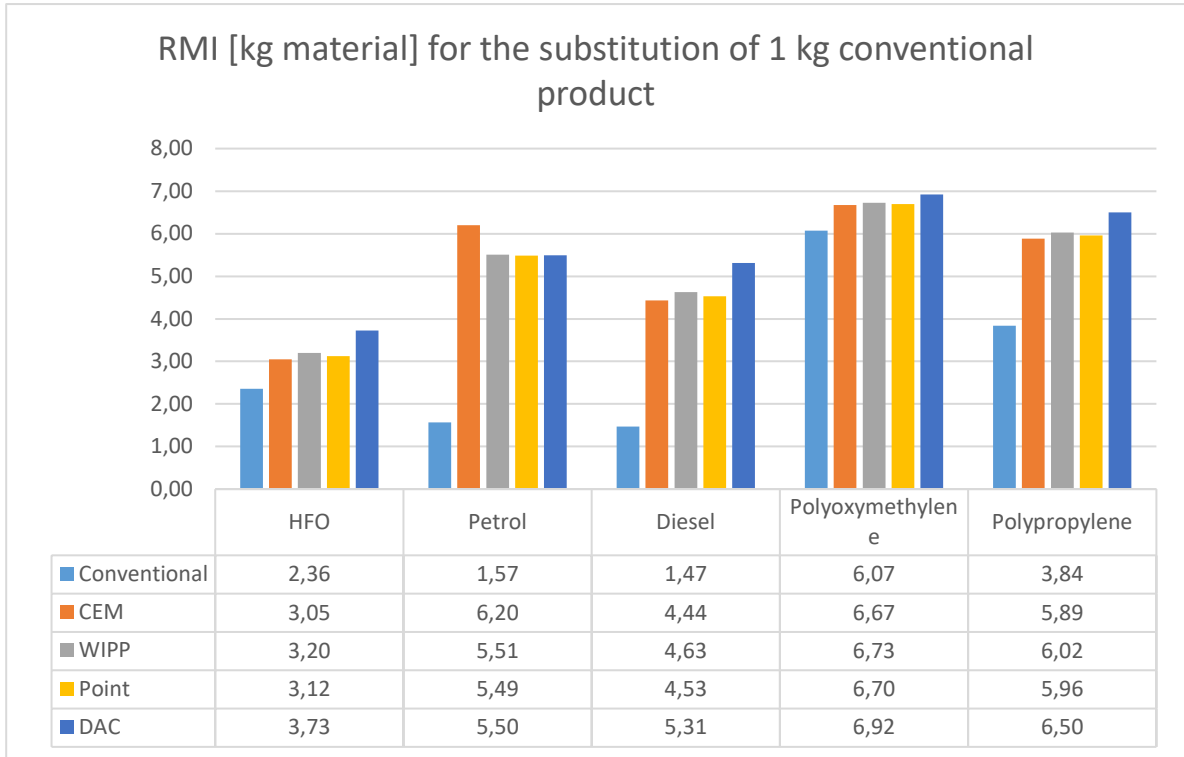
Figure 22: RMI for the substitution of 1 kg conventional product

TMR [kg raw material] for the substitution of 1 kg conventional product

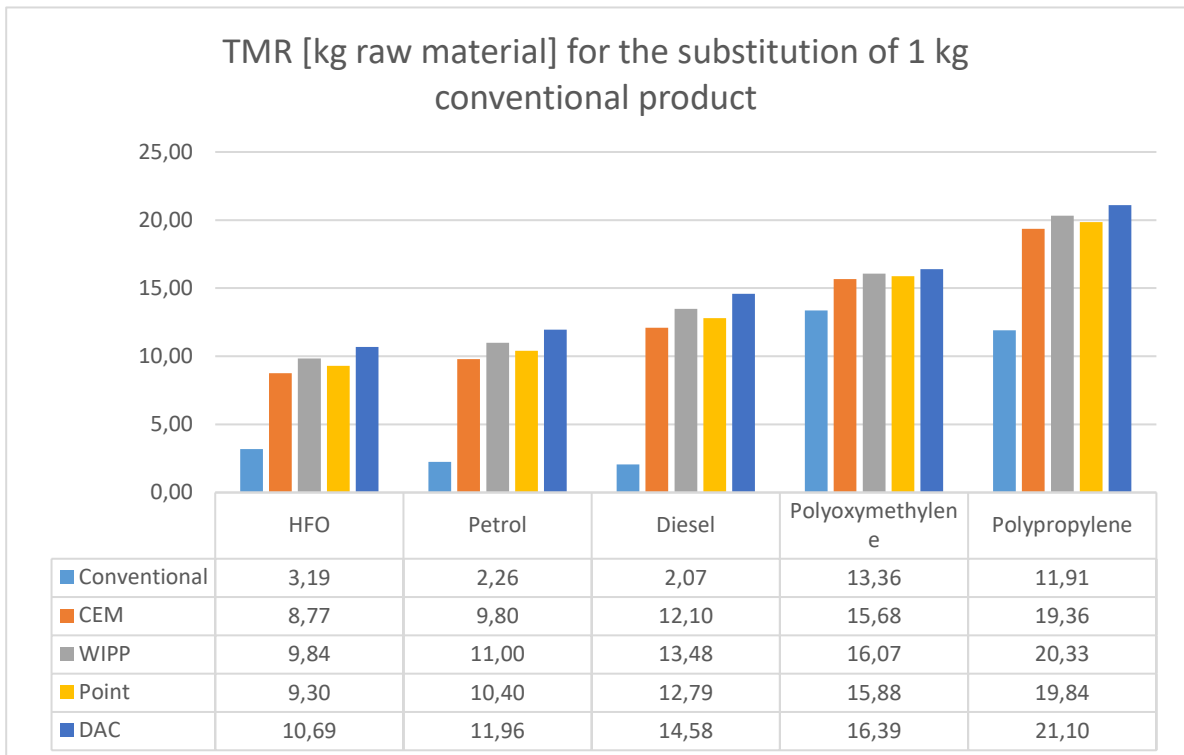|	HFO	Petrol	Diesel	Polyoxymethylene	Polypropylene
Conventional	3,19	2,26	2,07	13,36	11,91
CEM	8,77	9,80	12,10	15,68	19,36
WIPP	9,84	11,00	13,48	16,07	20,33
Point	9,30	10,40	12,79	15,88	19,84
DAC	10,69	11,96	14,58	16,39	21,10

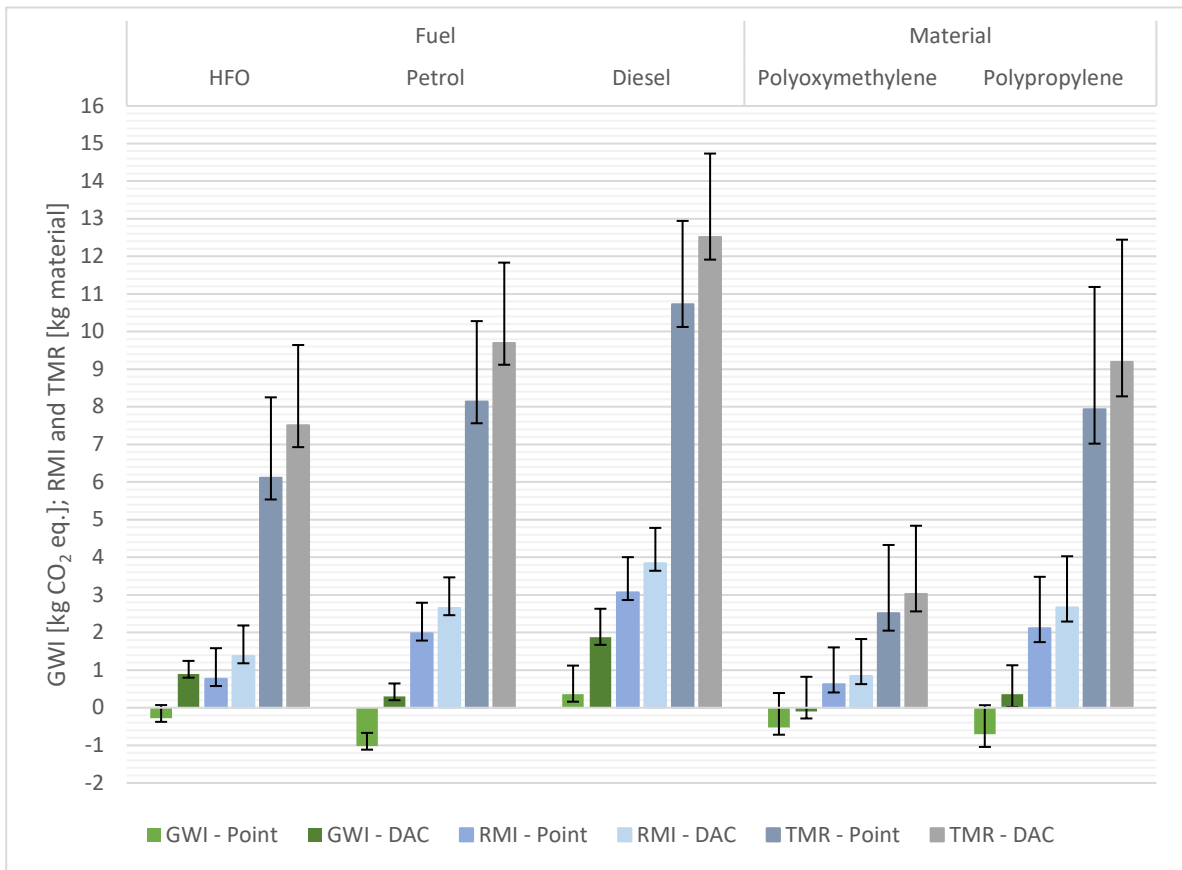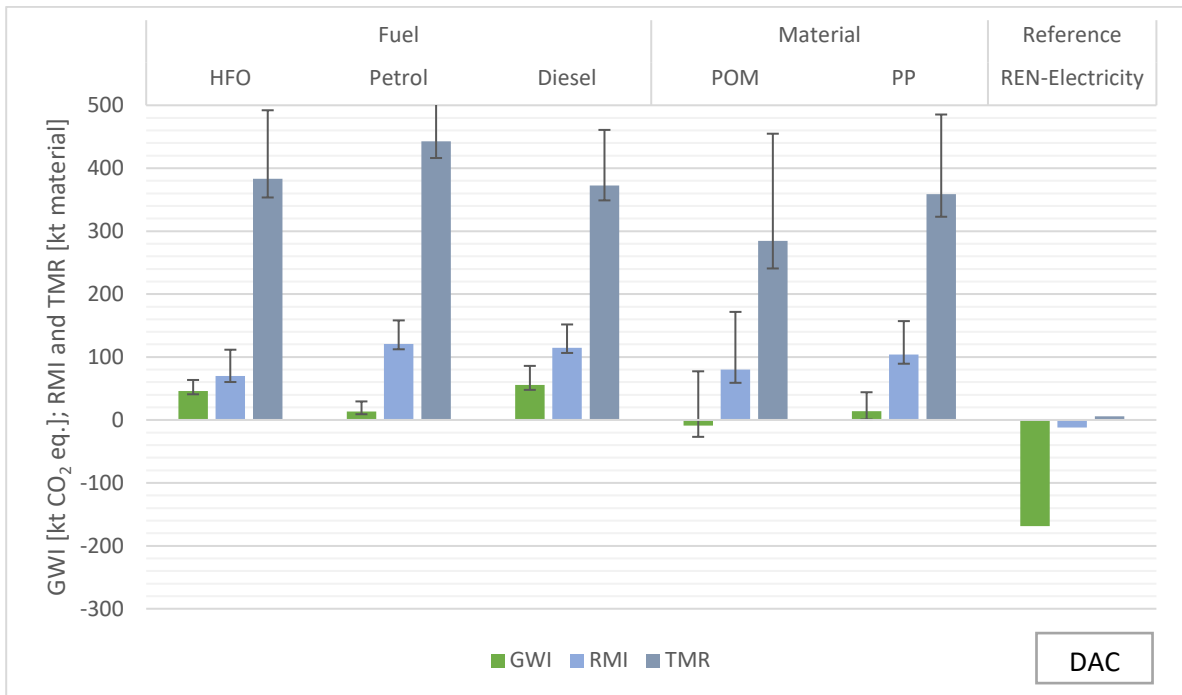Figure 23: TMR for the substitution of 1 kg conventional product

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Figure 24: Comparison of changes in the product climate and material footprint measured by respective impact indicators (GWI, RMI, TMR) if 1 kg conventional product as FU is substituted by products from recycled CO_2 from industrial point sources (Point) or direct air capture (DAC). ("HFO" – Heavy fuel oil; "GWI" – global warming impact; "RMI" – raw material input; "TMR" - total material requirement)

Figure 25: Comparison of changes in the product climate and material footprint measured by respective impact indicator (GWI, RMI, TMR) if conventional products are substituted by products from recycled CO_2 from direct air capture (DAC) based on the use of 100 kt methanol and considering overall energy efficiency for passenger cars (67 % for electric cars and 27 % for cars with combustion engines (49)) are provided as a reference. ("HFO" – Heavy fuel oil; "POM" – Polyoxymethylene; "PP" – Polypropylene; "GWI" – global warming impact; "RMI" – raw material input; "TMR" - total material requirement; "REN"- Electricity from renewable sources)

S7: Normalization against national reference values

CO_2 recycling technologies often require additional energy input and infrastructure to produce renewable electricity, which in turn requires materials (5,17,50). A normalization and weighting of results as described in (48) helps assessing the resulting target conflict between climate and resource protection. The German government already identified and addressed that tradeoffs in reduction of climate footprint and raw material consumption may be analyzed by normalization against national reference values (51). The following **Table 6** lists the national reference values for GWI, RMI and TMR for Germany GRI and TMR for the European Union, **Figure 26** shows the normalized results of the LCA for EU reference values:

Table 6: German and EU reference values for the normalization of indicators on national level

Indicator	Unit	Value	Source
$GWI_{Germany}$	kg CO_2 eq.	$909*10^9$	(52)
$RMI_{Germany}$	kg	$2,643*10^9$	(17)
$TMR_{Germany}$	kg	$7,853*10^9$	(43)

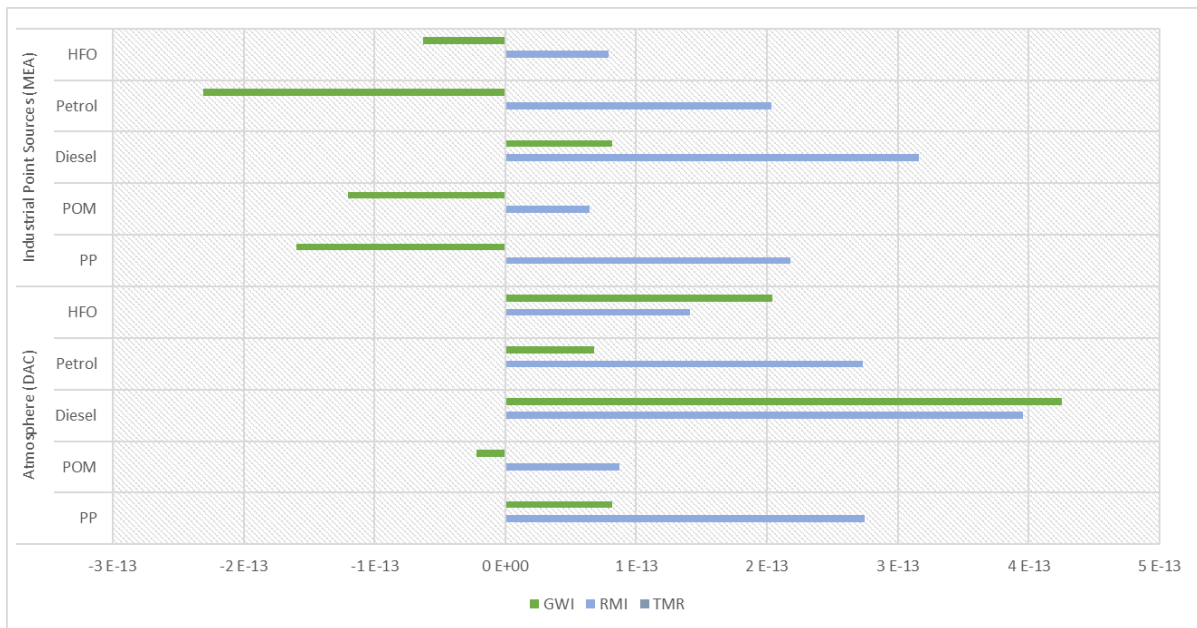| Indicator	Unit	Value	Source
GWI_{EU}	kg CO_2 eq.	$4,400*10^9$	(50)
RMI_{EU}	kg	$9,700*10^9$	(50)

Figure 26 - Normalized results for change in the values of impact indicators (GWI, RMI, TMR) for the product climate and material footprint compared to the national reference values for the European Union. ("MEA" – Amine scrubbing; "DAC" – direct air capture; "HFO" – heavy fuel oil; "POM" – polyoxymethylene; "PP" - polypropylene; "GWI" – global warming impact; "RMI" – raw material input; "TMR" - total material input; "Industrial Point sources" - indicates that CO_2 is captured using amine scrubbing, an average values for capturing from cement plant and from waste incineration plant is depicted, assuming that waste heat can be utilized at the source; "Atmosphere" - CO_2 is captured using DAC, assuming that no waste heat is used).

S8: Development of the German grid mix for Section 3.

The electricity grid mix for the analysis in chapter 3.3. is assumed to develop as described for the long-term scenarios "basis" for the transformation of the German energy system in 2020, 2030 and 2050 as described by Fraunhofer (53). The basis scenario implies the accomplishment of Germany's goals in energy and climate policy until 2050. For the calculation in ecoinvent a small share of energy provided from "other conventional" or "other renewable sources" as described by Fraunhofer is distributed to the other fossil based or renewable based power generation technologies based on the share that each technology has on the total fossil or renewable energy production in the respective year. In addition to the 2020, 2030 and 2050 grid mixes the "Defossilized" state depicts a rather ideal change of the current grid mix. The assumed 100% renewable electricity mix has the composition of renewables described in the 85% scenario by (54). **Figure 27** illustrates the grid mix compositions for 2020, 2030, 2050 and the defossilized state:
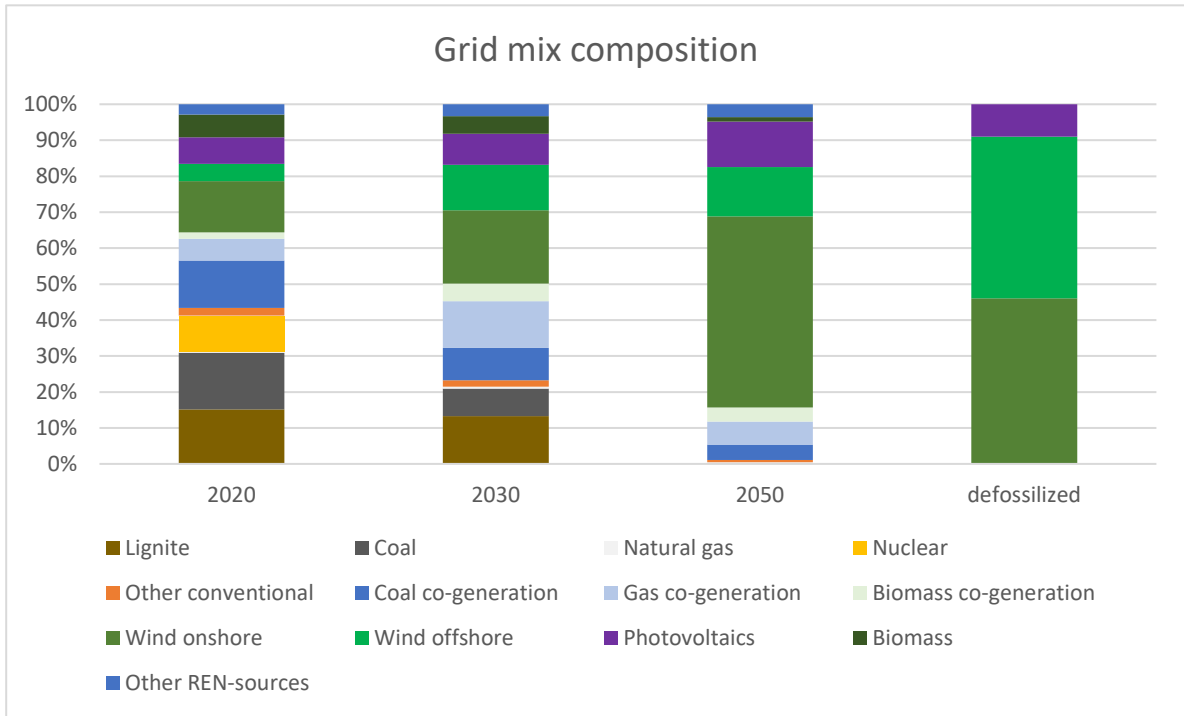
Figure 27: Composition for the grid mix considered in the defossilized state

The heat grid is assumed to solely use natural gas to supply thermal energy in 2020, 2030 and 2050. In the defossilized state thermal energy is provided by renewable electricity, which is used to generate thermal energy in electrode vessels with a 99% heating efficiency. Development of the German heat grid from 2015 to 2050 is described in a study by Agora Energiewende (55), where natural gas plays a major role in 2015 (55% share) and 2030 (75% share), but reduces importance in 2050 (25% share) due to the use of renewable heating technologies. Overall natural gas will be the dominant fuel for district heating until 2030 and remain a large fraction of the heating mix in 2050. In the defossilized state heat is solely supplied by renewable electricity instead of natural gas. **Figure 28** shows the product climate and material footprint for 1 kWh of supplied energy (electricity and heat) as FU:
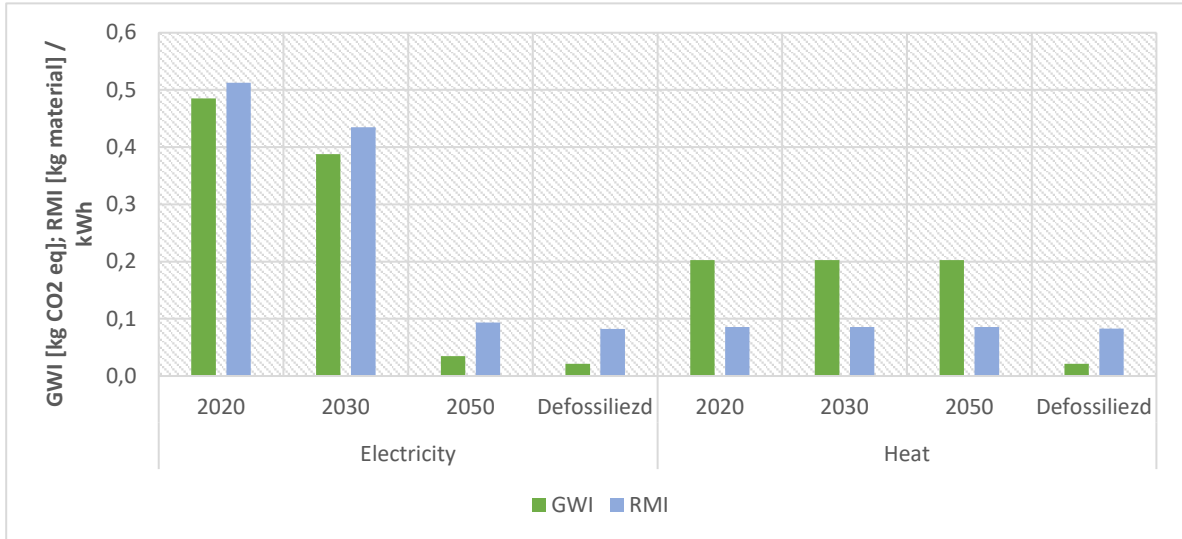
Figure 28: Climate and material footprint for the provision of 1 kWh of electrical or thermal energy as FU from the German grid in 2020, 2030, 2050 and in the defossilized state

S9: Schemes for the "substitution by system expansion" approach used in section 3.

The approaches for the two system expansions to evaluate the additional benefits from the EoL phase of PP from CO_2 (CCU PP) are depicted in the following in the way described by Walter Klöpffer & Birgit Grahl in their book on LCA (56). **Figure 29** shows the scheme for the system expansion for the process model to determine the additional benefit of 0.48 kg available PP re-granulate per kg virgin PP from material recycling and **Figure 30** shows the scheme for the system expansion to determine the additional benefits from substitution of 2.428 kWh electrical and 2.044 kWh thermal energy per kg of incinerated PP, both calculated and rounded for the functional unit of 100 kt of methanol from CO_2:
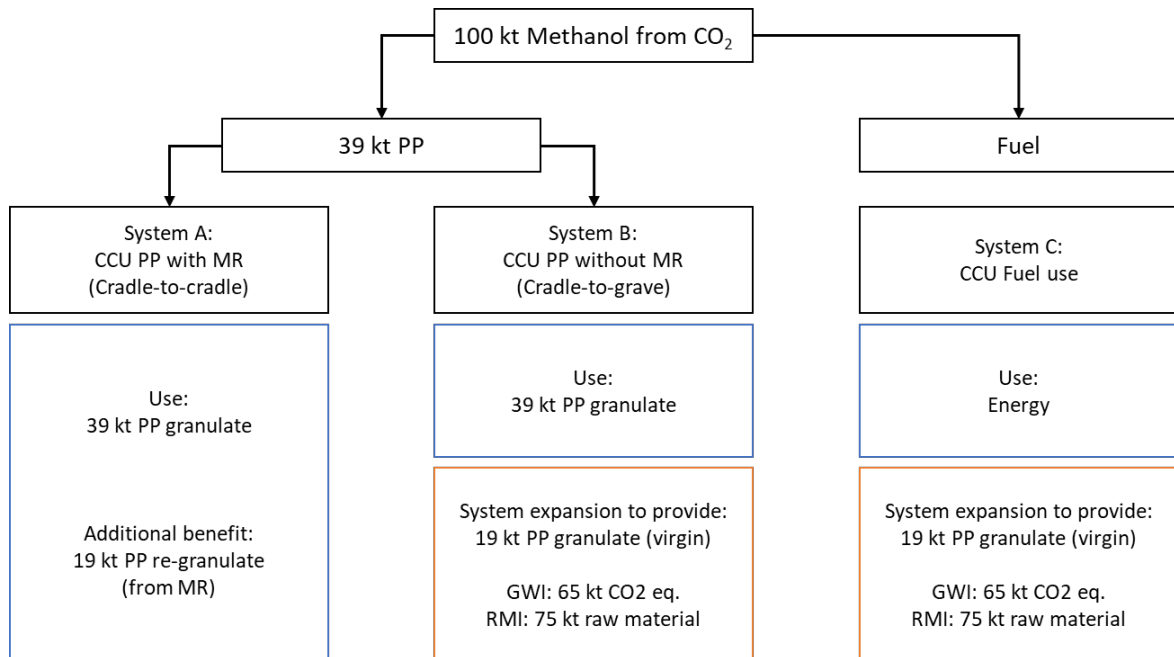

Figure 29: Substitution via system expansion to consider additional benefits from material recycling (MR) of polypropylene (PP)
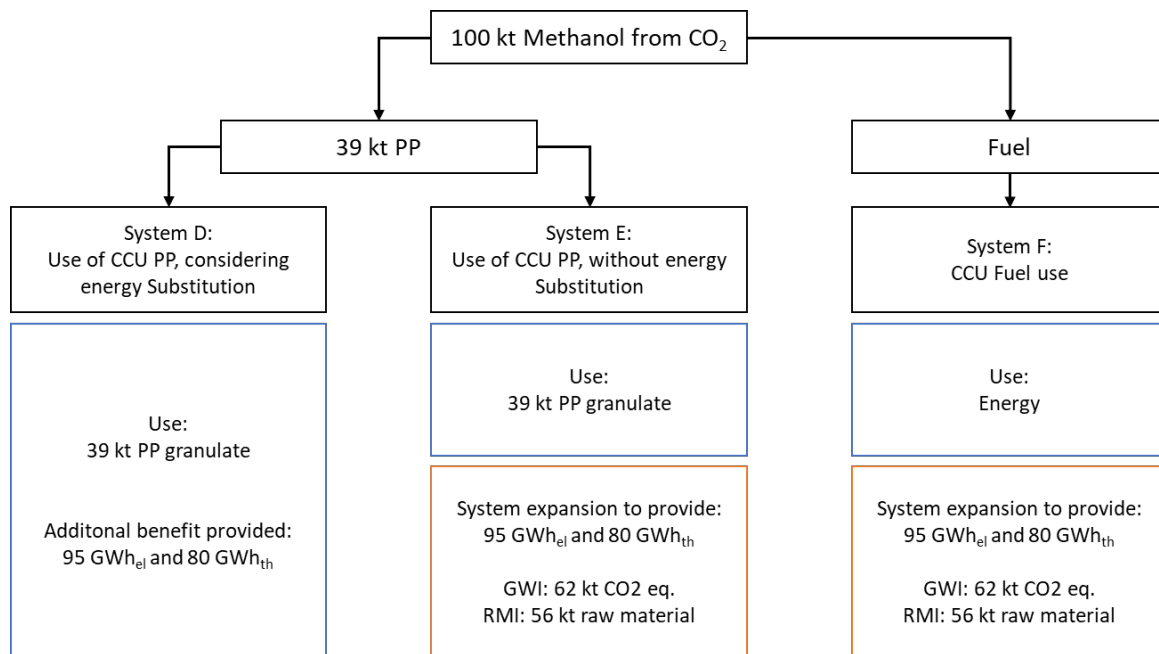
Figure 30: Substitution via system expansion to consider additional benefits from polypropylene (PP) incineration

S10: Technical summary table

The provision of a technical summary for life cycle assessments (LCA) is suggested by the guidelines for life cycle and techno-economic assessment (57). **Table 7** shows an adapted version of the technical summary for this study containing respective data and results:

Table 7: Technical summary for the LCA

Goal	**CCU product**	MeOH (as HFO and petrol substitute), OME_1 (as diesel substitute), POM, PP
	Goal	Process selection for highest climate footprint reduction potential without tradeoff in material footprint
	Brief description	The analysis compares CCU production routes for representative fuels and polymers based on the footprint reduction potential from the use of 100 kt methanol from CO_2. Results are normalized to German reference values. PP use is analyzed in detail for 2020, 2030, 2050 and a defossilized state to show the effect of additional benefits from material recycling and polymer incineration in a comparison of CCU PP as material to CCU fuels.
	Intended audience	Policy, Decision support (Situation B (48)), Strategy
	Functional unit	Use of 100 kt methanol from CO_2 to substitute conventional products
	Limitations & assumptions	Recycling rate of 33% for polymers,
Scope	**Boundary**	Life cycle wide; incl. cascading closed loop material recycling for polymers
	Location	Germany

	Time frames	present; 2030 and 2050 and ideal defossilized state
	Multi-functional approach	Sub-division
Inventory	Data source	Mixed sources
	Energy sources	Ecoinvent German grid mix, actual German grid mix for 2020, 2030 and 2050, renewable grid mix, solely wind power for electrolysis process.
	Main sub-processes and TRLS	**Sub-process** Electrolysis Methanol synthesis Methanol-to-olefins Other **TRL** 8 8 8 9+
	Database & software	Ecoinvent 3.1, GaBi database, openLCA 1.9
Assessment	LCIA method	**Methods:** Climate footprint Material footprint **Single categories:** Global warming impact (GWI, acc. to IPCC 2013) Raw material input (RMI) Total material requirement (TMR)
	Highlighted results	POM and Petrol substitution show highest potential to reduce GWI. HFO and PP show GWI reduction. Diesel does not show GWI reduction. All studied products show a tradeoff in product climate and material footprint. A more detailed analysis of PP and CCU fuel substitution shows high potential to overcome tradeoff for all studied technologies. Material recycling and incineration of polymers provide additional benefits that are by a factor of three higher than the GWI reduction from the substitution alone. CCU PP shows highest potential to reduce GWI until 2050, when EoL is considered and if compared to the studied fuels. All studied CCU technologies show significantly improved potential to reduce GWI in the defossilized state compared to 2020.
Interpretation	Main conclusions	CCU reduces GWI if renewable electricity is used for H_2 production. Additional benefits from PP EoL phase are three times higher than GWI reduction from the substitution of conventional PP with CO_2. The additional material demand for the substitution is reduced, while the GWI reduction increases due to the defossilization of the German electricity grid in the future. CCU production provides significantly improved GHG reduction compared to fossil production if REN-electricity is used instead of grid electricity on a lifecycle wide basis.
	Sensitivity analysis	Electrolysis, CO capture and transportation distances are varied.

Nomenclature

CCU	Carbon capture and utilisation
CO_2 eq.	Carbon dioxide equivalent units
DAC	Direct air capture
EoL	End-of-life
FA	Formaldehyde
FP	Footprint
GaBi	Ganzheitliche Bilanzierung (holistic accounting)
GHG	Greenhouse gas
GWI	Global warming impact
GWP	Global warming potential
HFO	Heavy fuel oil
kWh_{el}	Kilowatt-hour electrical energy
kWh_{th}	Kilowatt-hour thermal energy
LCA	Life cycle assessment
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
LHV	Lower heating value
MeOH	Methanol
MR	Material recycling
MRF	Material recovery facility
MTO	Methanol-to-Olefins
OME_1	Dimethoxymethane
PEMEL	Polymer electrolyte membrane electrolysis
POM	Polyoxymethylene
PP	Polypropylene
PRF	Plastic recycling facility
Re-granulate	Plastic granulate from material recycling
REN-electricity	Electricity from renewable energies
RMI	Raw material input
TMR	Total material requirement
WIP	Waste incineration plant

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