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1 Characterization of the chemical industry

The additional information regarding the first section of the study (i.e., the characterization of the chemical industry) can be found in this first section of the annex document.

Firstly, Table 1-1 shows the list of specific processes included in the study for each chemical. They were selected based on availability of information, production volume and environmental impact.

Secondly, the complete Sankey diagram showing all exchanges with the tecnosphere is presented. In the project report, the simplified diagram was used in order to show the relationships between chemical products and the application of each of them. For simplicity and to adjust to the section’s objective, the following fluxes were omitted, and can be seen in Fig. 1-1:

- Chemical factory (for organics)
- Electricity (medium voltage)
- Heat (district or industrial natural gas); heat (from steam, in chemical industry); heat (district or industrial, from fuels other than natural gas).
- Sulfuric acid
- Water, deionised (from tap water, at user); tap water; water, decarbonised (at user); water, completely softened (from decarbonised water, at user).
- Coconut oil (crude)
- Diethanolamine
- Nitrogen (liquid)
- Solvent (organic)
- Heavy fuel oil
- Natural gas (high pressure)
- Nickel (99,5%)
- Hard coal; hard coal from coke factory
- Iron sulfate
- Phosphoric acid (fertiliser grade without water in 70% solution state)
- Sodium hydroxide (without water in 50% solution state)
- Oxygen, average; oxygen (liquid)

- Aluminium oxide
- Copper oxide
- Methanol factory
- Molybdenum
- Zinc
- Chlorine (liquid); chlorine (gaseous)
- Acetic acid (without water, in 98% solution state)
- Steam (in chemical industry)
- Chemical (inorganic); chemical (organic)
- Chromium oxide (flakes)
- Compressed air (600 kPa gauge)
- Hydrogen (liquid)
- Titanium tetrachloride
- Hydrochloric acid (without water, in 30% solution state)
- Ethylene, dichloride

The chemicals represented in the simplified version are also included in Fig. 1-1, including:

- Ammonia (liquid)
- Ammonia, anhydrous (liquid)
- Benzene
- Ethylene oxide
- Ethylene (average)
- Propylene
- Xylene

Table 1-1: Included processes for each studied chemical.

Chemical	Processes
Acrylonitrile	Sohio process from polypropylene
Ammonia	Steam reforming
	Partial oxidation
	Cocamide diethanolamine production
Benzene	Catalytic reforming
	From coke oven
Cumene	Alkylation of benzene and propylene
Ethylene	Steam cracking out of naphtha
Ethylene glycol	Hydrolysis of ethylene oxide
Ethylene oxide	Direct oxidation from ethylene
Methanol	Steam reforming
Mixed xylene	Catalytic reforming
HDPE	Polymerization out of ethylene, gas phase
	Polymerization out of ethylene, Slurry
	Polymerization out of ethylene, solution
LDPE	Polymerization out of ethylene, autoclave
	Polymerization out of ethylene, tubular
LLDPE	Polymerization out of ethylene, autoclave
	Polymerization out of ethylene, tubular
	Polymerization out of ethylene, gas phase
	Polymerization out of ethylene, Slurry
	Polymerization out of ethylene, solution
Polypropylene	Polymerization out of propylene, bulk
	Polymerization out of propylene, gas phase
	Polymerization out of propylene, Slurry
Propylene	Steam cracking of naphtha
Propylene oxide	Chlorohydrin process
Styrene	Dehydrogenation of ethylbenzene
Terephthalic acid	Oxidation of p-xylene
Toluene	Catalytic reforming
Vinyl chloride	Direct chlorination and oxychlorination of ethylene

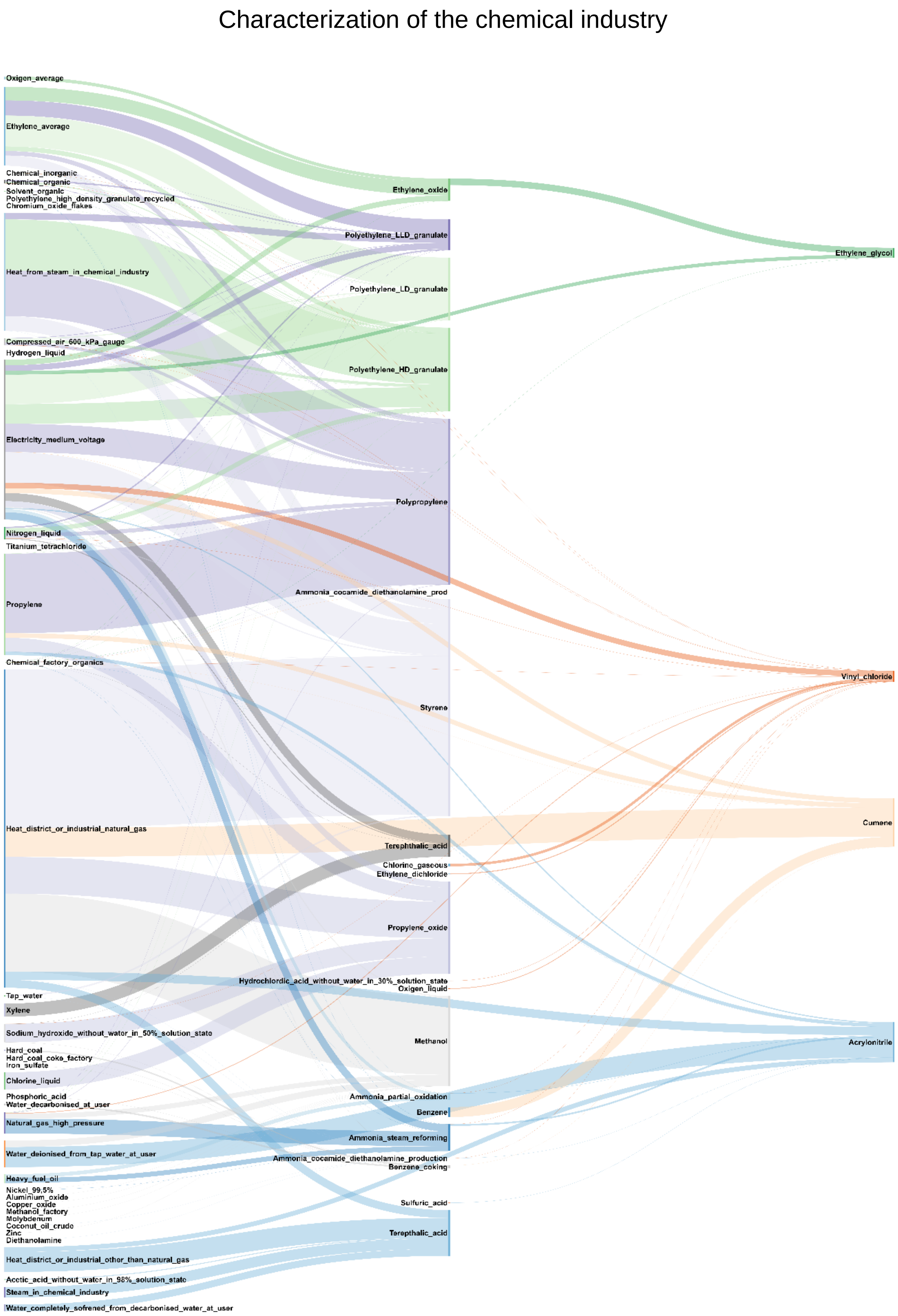


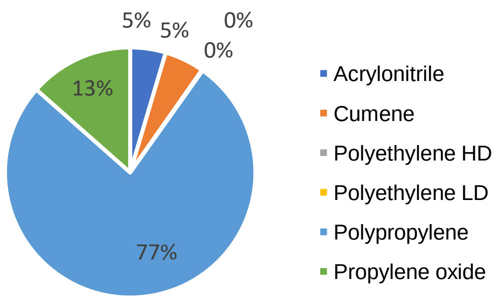
Fig. 1-1: Sankey diagram showing the total exchange of fluxes between the chemicals and the technosphere.

1.1 Uses of propylene as market shares

Table 1-2: Breakdown of the uses of propylene according by different sources compared to obtained results (World).

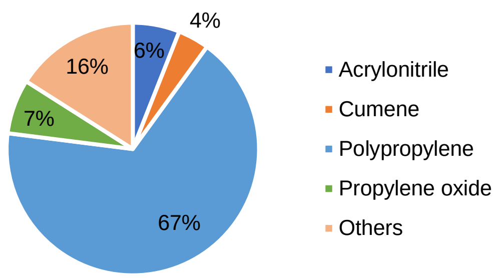
Calculated (Europe, 2018)

Used for	**% total volume propylene**
Acrylonitrile	4.9
Cumene	5.5
Polyethylene HD	0.0
Polyethylene LD	0.1
Polypropylene	82.6
Propylene oxide	14.5
	107.7



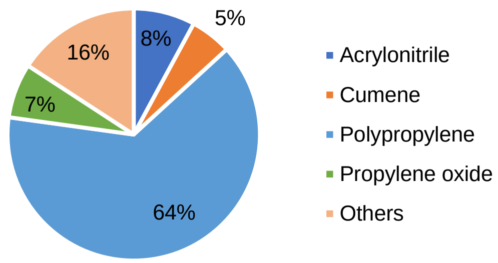
Plotkin (World, 2016)

Used for	**% total volume propylene**
Acrylonitrile	6.0
Cumene	4.0
Polypropylene	67.0
Propylene oxide	7.0
Others	16.0
	butanol, acrylic acid, others
	100



Sawyer (World, 2015)

Used for	**% total volume propylene**
Acrylonitrile	7.9
Cumene	5.3
Polypropylene	64.0
Propylene oxide	7.0
Others	15.8
	isopropanol, butyraldehyde, acrylic acid
	100



Carr (World 2020)

Used for	**% total volume propylene**
Acrylonitrile	6.0
Cumene	4.0
Polypropylene	69.0
Propylene oxide	8.0
Others	13.0
	Acrylic acid (4), butanols (3), isopropanol (1%), 2-ethyl hexanol (3%), others (2%)
	100

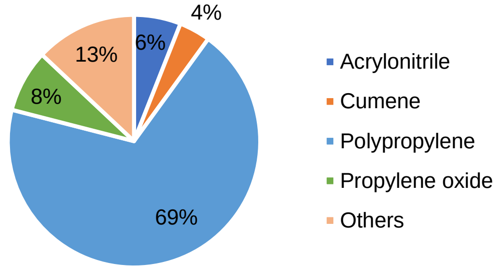
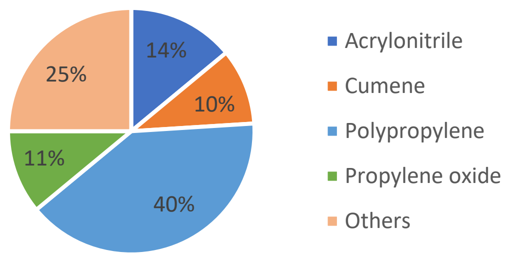


Table 1-3: Breakdown of the uses of propylene according by different sources compared to obtained results (USA)

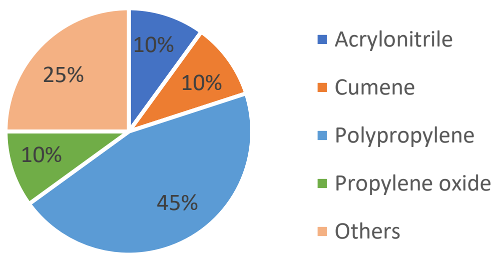
Kolb & Field
(USA, n.d.)

Used for	**% total volume propylene**
Acrylonitrile	14.0
Cumene	10.0
Polypropylene	40.0
Propylene oxide	11.0
Others	25.0
	(butanal 8%, isopropyl alcohol 7%, miscellaneous 10%)
	100



Hocking
(USA, 2005)

Used for	**% total volume propylene**
Acrylonitrile	10.0
Cumene	10.0
Polypropylene	45.0
Propylene oxide	10.0
Others	25.0
	exoalochols and others
	100



2 LCI boundaries

In the study, the boundaries for the LCA are established at a cradle-to-gate approach according to the LCA's aims. The *ecoinvent* database occasionally does not provide information on specific fluxes for a database. The study acknowledges the exclusion of these LCI entries. Table 2-1 shows the included fluxes from the raw material extraction stage until these feedstocks are delivered at the production plant, and the LCIs that *ecoinvent* could not determine and are therefore excluded from each dataset.

Table 2-1: Dataset boundaries for the LCA (cradle-to-gate); specifications of excluded fluxes.

Ecoinvent activity name	**Database includes**	**Database does not include**
methanol//[GLO] methanol production	Raw materials and energy consumption, emissions to air and water from the process and infrastructure use	Use of CO2
ethylene, average//[RER] ethylene production, average	RM extraction until delivery at plant	Recyclable wastes, amount of air/N2/O2 consumed, unspecified metal emission to air and to water, mercaptan emission to air, CFC/HCFC emission to air, dioxin to water
propylene//[RER] propylene production	RM extraction until delivery at plant	Recyclable wastes, amount of air/N2/O2 consumed, unspecified metal emission to air and to water, mercaptan emission to air, CFC/HCFC emission to air, dioxin to water
cumene//[RER] cumene production	RM, transport of materials to manufacturing plant	Solid wastes
ethylene glycol//[RER] ethylene glycol production	RM and energy consumption, emissions to air and water from the process and infrastructure use	
styrene//[RER] styrene production	RM and energy consumption, emissions to air and water from the process and infrastructure use, waste treatment process	
purified terephthalic acid//[RER] purified terephthalic acid production	RM and energy input, waste as well as air and water emissions. Transport and infrastructure estimated	Sum parameters to water (DOC, TOC, COD)

Table 2-1 (continued).

propylene oxide, liquid//[RER] propylene oxide production, liquid	RM, transport, estimated emissions to air and water (incomplete), estimation of energy demand and infrastructure (approx), treatment of wastewater	Solid wastes
vinyl chloride//[RER] vinyl chloride production	RM extraction until delivery at plant	Recyclable wastes, amount of air/N2/O2 consumed, unspecified metal emission to air and to water, mercaptan emission to air, CFC/HCFC emission to air, dioxin to water
acrylonitrile//[RER] Sohio process	RM and energy consumption, emissions, and infrastructure use	
ammonia, liquid//[RER] ammonia production, partial oxidation, liquid	RM, fuel and energy consumption, emissions, wastes and infrastructure use	
ammonia, liquid//[RER] cocamide diethanolamine production	RM, fuel and energy consumption, emissions, and infrastructure use	
ammonia, liquid//[RER] ammonia production, steam reforming, liquid	RM, energy consumption & auxiliaries, emissions, wastes and infrastructure/land use	
polyethylene, high density, granulate//[RER] polyethylene production, high density, granulate	RM extraction until delivery at plant	Recyclable wastes, amount of air/N2/O2 consumed, unspecified metal emission to air and to water, mercaptan emission to air, CFC/HCFC emission to air, dioxin to water
polyethylene, high density, granulate//[Europe without Switzerland] polyethylene, high density, granulate, recycled to generic market for high density PE granulate	Transport	
polyethylene, low density, granulate//[RER] polyethylene production, low density, granulate	RM extraction until delivery at plant	Recyclable wastes, amount of air/N2/O2 consumed, unspecified metal emission to air and to water, mercaptan emission to air, CFC/HCFC emission to air, dioxin to water

Table 2-1 (continued).

polyethylene, high density, granulate//[Europe without Switzerland] polyethylene, high density, granulate, recycled to generic market for high density PE granulate	Transport	
polyethylene, low density, granulate//[RER] polyethylene production, low density, granulate	RM extraction until delivery at plant	Recyclable wastes, amount of air/N2/O2 consumed, unspecified metal emission to air and to water, mercaptan emission to air, CFC/HCFC emission to air, dioxin to water
polyethylene, linear low density, granulate//[RER] polyethylene production, linear low density, granulate	RM extraction until delivery at plant	Recyclable wastes, amount of air/N2/O2 consumed, unspecified metal emission to air and to water, mercaptan emission to air, CFC/HCFC emission to air, dioxin to water
polypropylene, granulate//[RER] polypropylene production, granulate	RM extraction until delivery at plant	Recyclable wastes, amount of air/N2/O2 consumed, unspecified metal emission to air and to water, mercaptan emission to air, CFC/HCFC emission to air, dioxin to water
benzene//[RER] benzene production	RM extraction until delivery at plant	Recyclable wastes, amount of air/N2/O2 consumed, unspecified metal emission to air and to water, mercaptan emission to air, CFC/HCFC emission to air, dioxin to water
benzene//[DE] coking	RM, energy, transport, total emissions to air and water	
toluene, liquid//[RER] toluene production, liquid	RM extraction until delivery at plant	Recyclable wastes, amount of air/N2/O2 consumed, unspecified metal emission to air and to water, mercaptan emission to air, CFC/HCFC emission to air, dioxin to water
xylene//[RER] xylene production	RM extraction until delivery at plant	

3 Data Quality Analysis: Assigned scores for all datasets

For the categories of geographical and temporal coverage, repetitive reasoning has been applied because the same information is provided for most datasets in the database. Therefore, the scores for these categories are explained first, while the scores for the technological coverage, completeness and reliability are presented later for each chemical individually.

1.1.1 Geographical and temporal coverage

The aim of the geographical coverage category is to consider potential technological differences between areas (Weidema & Wesnaes, 1996). Therefore, a score of 2 is assigned to those LCI sets which are defined for the RER area, since the EU-28 aggregate is within continental Europe. For the HDPE dataset that includes all Europe without Switzerland, a score of 2 is assigned as well. For methanol, a score of 5 is defined since the data are provided in a global scale, and major technological differences can derivate from it. In the case of the dataset for the coking of benzene specific to Germany, the score is 3 since currency is the same and cost conditions can be considered similar to those of the rest of the EU-28.

As for temporal coverage, it is important to recall that the temporal frame studied ends at 2018. On the other hand, the database used to match CFs for the PB-LCIA method (Ryberg et al., 2018b) is *ecoinvent* v3.5 (2018), which was released in 2018 and is based on data published for the same year. Therefore, the time period of the database ends at the same year as the study and, consequently, all scores in the pedigree matrix for this category are 1. There are only two cases (styrene, production and ammonia from cocamide DEA production) where inputs are taken as industrial data based on 5-year averages, but since this time window starts in 2015, data are considered valid until 2020 and therefore includes the year of the study (Ziel et al., 2016). It must be taken into account that part of data collected from *ecoinvent* v3.5 was already in version v2 and has been updated, however the start date for data collection can still range from years ago.

1.1.2 Technological coverage, completeness, and reliability

1.1.2.1 Methanol

The score for the reliability category is 2 since data are collected from literature and reports that used measurements made at chemical plants and reviewed, but catalyst use is only estimated (not measured). Regarding the completeness category, according to *ecoinvent*, data are approximated to be representative for around 60% of the methanol production during an adequate period (Edelen et al., 2016). This is because the studied process for the production of methanol is steam reforming from natural gas. Therefore, representativity concerning energy is considered as good but low when it comes to average emissions. Therefore, the completeness category is assigned a score of 2 because the included sites do not represent the whole methanol production in the studied area. Finally, the dataset is representative for the process design and conditions of the low-pressure steam reforming process, with a modern process being considered as average and data from combined reforming and autothermal reforming also being considered but no data on the scale and materials is provided. The category for technology differences is therefore scored as 4. The fact that that this process only represents 60% of the total production, with the IEA report also including other processes, is already considered in the completeness category.

1.1.2.2 Ethylene and propylene

Further information on the date supplied for both chemicals is the same since they both come from the steam cracking of naphtha. Consequently, the assigned scores are equal. A score of 2 is assigned to the reliability category, since review was carried out for the data, which was collected from literature and company surveys (i.e., no estimates are reported), but data on some specific fluxes are omitted. As for the completeness indicator, a score of 3 is assigned to ethylene according to the calculations explained in Table 9-4 from the main report since the steam cracking of naphtha is the studied process and the total number of ethylene production sites could be found. For propylene, the cited sites do not represent a high enough percentage compared to the total production sites for the chemical, so a 3 is given as seen in Table 9-4 from the main report. For both cases, no information is provided neither on what technologies are considered, nor on the materials or the scale of the processes included. Applying the most pessimistic score, a 5 is assigned to the technology differences category.

1.1.2.3 Cumene

The cumene dataset does not provide much detail on the information used, therefore the score for completeness is 5 and the score for reliability is 4. Information is based on literature but also estimates and approximations, so even though it is reviewed a higher score cannot be assigned to reliability. As for the completeness indicator, even though all relevant technologies are studied, thus covering the total cumene production, no information is given on how many sites were included. For the technology category, the score is 4 since the activities from the IEA report (IEA, 2013) and *ecoinvent* match exactly (cumene from propylene and benzene) but no further information is supplied.

1.1.2.4 Ethylene glycol

The ethylene glycol dataset is based on literature, which is in turn based on measurements and subject to extensive review by more than one reviewer. However, the score assigned to the reliability category is 2 since default values are used for the impacts of the infrastructure of the process. The completeness category is assigned a score of 5 since the studied process is representative of the whole production and the time span is adequate. yet no specific number of sites is provided. The technological differences category can also be assgined a score of 2 since all technologies are well described and match with those in the IEA report (IEA, 2013).

1.1.2.5 Styrene

Since information comes from industry reports and is verified, a score of 2 was assigned to the reliability category. The details provided indicate that some approximations were done, which is in concordance with this category's description of verified data partly based on assumptions (Weidema & Wesnaes, 1996). For the completeness indicator, a score of 5 is assigned. Finally, a score of 4 is given to the technology category, since not all routes under study are included. Although the process studied (dehydrogenation of ethylbenzene) is the main route for the production of styrene (James et al., 2011), it is important to acknowledge that styrene from pyrolysis gasoline and styrene peroxidation of propylene and ethylbenzene also produce respectively the same amount of GHG emissions and around four times as much energy consumption (IEA, 2013).

1.1.2.6 Purified terephthalic acid

The terephthalic acid dataset was assigned a score of 2 for the reliability category and a score of 5 for completeness, since company data based on measurements were collected from several production sites within the studied area during an adequate period of time, but the exact number of sites is not reported so it is not possible to evaluate whether it is representative enough. The database acknowledges that missing parameters were estimated. Regarding technology, not much information is provided on the design of the processes, the materials, the scale or the conditions, so a score of 5 was assgined.

1.1.2.7 Propylene oxide

Ecoinvent indicates that the propylene oxide dataset was based on few literature sources due to a lack of data on process emissions. Therefore, estimations had to be made to calculate the energy demand, plant infrastructure and process emissions. Consequently, the reliability indicator was set to a score of 4 (since even if estimates were used, they were reviewed and qualified). As with the cumene case, a score of 5 was assigned to the completeness indicator since no data on what sites were considered is provided. As for the technology indicator, the dataset covers the production via the chlorohydrin process, but other technologies relevant for their environmental impact are missing, such as the hydroperoxidation route (IEA, 2013). Therefore, a score of 4 is assigned to this category.

1.1.2.8 Vinyl chloride

The vinyl chloride dataset collected data from literature values based on company surveys. Regardless, the score for reliability is 2 since waste data were obtained from an older report because the most recent one omitted such information. The report carefully describes the number of sites studied within the range area and includes the major part of the vinyl chloride production during an adequate period of time, so a score of 2 is given to the completeness indicator (Table 9-4 in the main report). The considered process matches with the IEA study, therefore a score of 2 is set to the technology category. The process starts with the chlorination of chlorine and ethylene to produce ethylene dichloride, which later goes through a process of oxychlorination to obtain vinyl chloride (European Patent No. EP0883588B1, 1996).

*1.1.2.9 Acryl*onitrile

Regarding the reliability category, the score is 2 because data are reviewed but partly based on estimations. For the completeness category, a score of 5 is assigned for the same reasons as in the ethylene glycol and styrene cases. As for the technology category, a score of 2 can be safely established since the dataset matches with the IEA report exactly, and the target route to produce acrylonitrile (the Sohio process) is accurately described.

*1.1.2.10 A*mmoni*a*

The two main processes for the production of ammonia currently operating in Europe are steam reforming and partial oxidation (EFMA, 2000). In this study, the two activities were separated (i.e., a different dataset was used for each) and analysed individually. In addition, and despite representing a market share lower than 0.1%, the cocamide DEA production process was also included since *ecoinvent* grouped it together with the two previously mentioned routes to create the dataset labelled *market for ammonia* in Europe. The uncertainty characterization is specific for each of these processes.

3.1.1.1.1 Ammonia production, partial oxidation & steam reforming

A score of 1 is given to the reliability category for both datasets since all literature sources are cited, extensive and reviewed. As for the completeness and technology indicators, the score assigned is 3 because the datasets do represent the production through both active processes correctly and take into account the different existent catalysts and variations, but no information on how many sites were studied is provided.

3.1.1.1.2 Ammonia production, cocamide diethanolamine production

Reliability is scored with a 2 in this case since data are collected from literature but also use stochiometric calculations partially based on a generic model. As for the completeness indicator, a score of 5 is assigned since only the average composition of DEA is considered, but its market share is unknown. Regarding the technology, the dataset is scored with a 2 since the process is very specific.

1.1.2.11 High Density Polyethylene; HDPE

For HDPE production, used mainly in packaging, two different datasets were included, one for the strict production of new granulate HDPE and a second one for the recycled fraction of HDPE. HDPE is often subject of poor handling after its use, which makes it difficult to correctly segregate the waste plastic for posterior recycling (Hahladakis & Iacovidou, 2018). However, it has been proved that it can be reprocessed and still offer similar mechanical properties to those of non-recycled HDPE (Vilaplana & Karlsson, 2008). Acknowledging that closed loop recycling only represents a low % of the market (Wernet et al., 2016), this input has been included in the study owing to the widespread use and high production volume of HDPE.

3.1.1.1.3 Polyethylene production, high density, granulate

For the principal PE dataset, a 2 is assigned to the reliability category since data are verified and claimed to proceed from company surveys. Even though no estimations were made, some data on specific fluxes were not included (see specifications, same case as other chemicals). However, for the completeness category, a score of 3 is set since the number of sources from where data were collected is cited, and the time period is also adequate. Regarding technological differences, the dataset represents the production of HDPE from the polymerization out of ethylene under normal pressure and temperature, which would encompass all three low-pressure routes to produce PE that the IEA report cites. Those would be the solution process, the Slurry process, and the gas phase process. They all present their own characteristics and contribute differently to the GHG emissions and energy use of the HDPE production. No further information is provided so it is unknown which of the possible catalysts and co-monomers, all required for the three low pressure polymerization techniques, were included in the study (Naguib & Marwan, 2013), were included in the study. Therefore, a score of 4 is assigned to the technology category to ensure the worst-case scenario policy is being respected.

3.1.1.1.4 Recycled to generic market for high density PE granulate

No specific information is supplied for this dataset since its use is to link recycled HDPE to the global market, even though its contribution to it is low. In this study, it is that of 0.08%. Since data for all categories is unknown, they are all scored with a 5.

1.1.2.12 Low density Polyetheylene; LDPE

Similar to the HDPE production dataset, the LDPE one has been scored with a 1 in the completeness category, since it used data from a reported number of sites distributed within the studied area during enough time. For reliability, the data set is missing the same inputs as the HDPE one, therefore a score of 3 is also assigned. Regarding technology, *ecoinvent* reports the study is for LDPE from the polymerization out of ethylene at high pressure and high temperature. Two processes should be included under such label, the autoclave process and the tubular process (IEA, 2013; Platzer, 1983). However, it is not specified which technologies were considered, so a score 4 is set.

1.1.2.13 Linear Low Density Polyethylene; LLDPE

A smaller number of sites was considered in this case, so a score of 3 is assigned to completeness, while a score of 2 is assigned to reliability because data was obtained from company surveys and are reviewed. As for technology, the dataset is representative of the LLDPE produced out of the polymerization of ethylene, but no further details are provided on which specific technologies are included. These should be the autoclave, gas phase, Slurry, solution, and tubular processes (IEA, 2013). As for the other types of PE, a score of 4 is assigned.

1.1.2.14 Polypropylene

All scores are the same as in the LDPE dataset since the same number of sites were considered and information was also from company surveys. As for technology, PP from propylene is included, but no information on whether all processes for its production were included, so the assigned score is 4. The gas phase, the bulk and the Slurry processes all have similar impacts on both GHG and energy consumption (IEA, 2013). The IEA report that produced the list of most environmentally damaging materials also includes an “others” category. This may comprise, for example, hybrid processes (Intratec, 2020).

1.1.2.15 Benzene

Two datasets were considered for the production of benzene, the catalytic reforming process, which is the most important within Europe, and a secondary one for coking benzene in Germany. The necessity to include this second process in the analysis despite its low market share stems from its environmental performance, as this process is highly unsustainable (Liao et al., 2015). The coking dataset has been allocated adequately to benzene out of all of coking’s byproducts.

3.1.1.1.5 Benzene production

For benzene, a 2 was given to the reliability category since data are based in measurements and reviewed, but estimations were also made. As for completeness, the dataset considers a smaller number of production sites and the time period is adequate as in the whole *ecoinvent* database, so a score of 3 is assigned. The technology differences category was scored with a score of 5 since it neglects processes which emit a considerable amount of greenhouse gases and are responsible for an important part of the energy consumption associated with benzene production (IEA, 2013).

3.1.1.1.6 Benzene, coking

A considerable number of assumptions was made for this dataset, therefore a score of 2 is assigned to the reliability category. Meanwhile, for the completeness category, a score of 2 is set since 70% of Germany production is covered with the dataset. As for technology, the dataset is already specific for the coking process of coal, lignite, or peat, so the score assigned is 2.

1.1.2.16 Xylene

All three isomers of xylene were grouped since the *ecoinvent* database information is supplied for mixed xylenes, even though p-xylene is the most used one and, thus, appears as a standalone chemical in the IEA report. For the reliability category, this dataset is assigned a score of 2 since data are collected from company surveys with some assumptions, but for completeness, no information is given so automatically the score is set to 5. Finally, for technology, a score of 5 is also assigned since the dataset only includes the catalytic reforming out of naphtha, while missing many other processes with important environmental impact.

1.1.2.17 Toluene

The toluene dataset receives a score of 2 for both the reliability (reviewed data from measurements) and the completeness categories, since only 11 plants were studied. For the technology indicator, a 5 is assigned as the worst-case scenario because relevant processes were omitted and no further information on the conditions is provided.

1.1.2.18 Ethylene oxide

Data were collected from literature, but estimations were made, so a 2 is assfined to the reliability category. As for the completeness category, a score of 3 is assigned since few sites were studied even if the principal manufacturers were cited in the dataset and the time span is adequate. A score of 2 is given to the technology category because the dataset does not omit any process described in the IEA list of products, and the oxidation from ethylene process is carefully described.

4 Results

The values of the average contributions represented in the bar plots in the main document can be consulted in Table 4-1 and Table 4-2.

Table 4-1 shows the total contributions to each PB (sum of the impacts of all chemicals), while Table 4-2 shows the breakdown of contributions where the fraction corresponding to each process can be seen. Note that in the first table, the values correspond to the fraction of occupied SoSOS, while in the second table, the impacts expressed in the units of every PB are shown.

Table 4-1:Occupied fraction of the assigned So, SOS for every allocation principle. Shaded cells indicate transgression of the corresponding PB.

EUSoSOS	**Share of SoS (EU): $SoSOS_{EUSoSOS}$ = $aSPB_{EUSoSOS*SoS,PB}$**	**Upper bound SoSoS**	**Remaining SOS**	**$occSoSOS_{PB,EUSoSOS}$**
Climate change (energy imalance at top of atmosphere)	$6.7\cdot10^{-2}$	$10.07\cdot10^{-2}$	$2.26\cdot10^{-2}$	$66.29\cdot10^{-2}$
Climate change (atmospheric CO2 concentration)	$483.43\cdot10^{-2}$	$1490.56\cdot10^{-2}$	$148.86\cdot10^{-2}$	$69.21\cdot10^{-2}$
Stratospheric ozone depletion	$97.35\cdot10^{-2}$	$194.71\cdot10^{-2}$	$97.33\cdot10^{-2}$	$0.029\cdot10^{-2}$
Ocean acidification	$4.62\cdot10^{-2}$	$6.93\cdot10^{-2}$	$3.59\cdot10^{-2}$	$22.13\cdot10^{-2}$
Biogeochemical flows (Nitrogen)	$416.28\cdot10^{-2}$	$550.57\cdot10^{-2}$	$414.63\cdot10^{-2}$	$0.39\cdot10^{-2}$
Biogeochemical flows (Phosphorus)	$66.47\cdot10^{-2}$	$664.04\cdot10^{-2}$	$66.43\cdot10^{-2}$	$0.062\cdot10^{-2}$
Land-system change	$167.85\cdot10^{-2}$	$308.85\cdot10^{-2}$	$167.85\cdot10^{-2}$	$0.00083\cdot10^{-2}$
Freshwater use	$26857.07\cdot10^{-2}$	$40285.61\cdot10^{-2}$	$26843.92\cdot10^{-2}$	$0.049\cdot10^{-2}$
Aerosol loading	$0.74\cdot10^{-2}$	$2.42\cdot10^{-2}$	$0.65\cdot10^{-2}$	$11.53\cdot10^{-2}$

EUCISoSOS	**Share of SoS (EU & Chemical Industry): $SoSOS_{EUCISoSOS}$ = $aSPB_{EUCISoSOS*SoS,PB}$**	**Upper bound SoSoS**	**Remaining SOS**	**$occSoSOS_{PB,EUCISoSOS}$**
Climate change (energy imalance at top of atmosphere)	$0.32\cdot10^{-2}$	$0.048\cdot10^{-2}$	$-4.13\cdot10^{-2}$	13.8346
Climate change (atmospheric CO2 concentration)	$23.16\cdot10^{-2}$	$41.43\cdot10^{-2}$	$-311.40\cdot10^{-2}$	14.4425
Stratospheric ozone depletion	$4.66\cdot10^{-2}$	$9.33\cdot10^{-2}$	$4.63\cdot10^{-2}$	0.0062
Ocean acidification	$0.22\cdot10^{-2}$	$0.33\cdot10^{-2}$	$-0.80\cdot10^{-2}$	4.6185
Biogeochemical flows (Nitrogen)	$19.94\cdot10^{-2}$	$26.38\cdot10^{-2}$	$18.29\cdot10^{-2}$	0.0828
Biogeochemical flows (Phosphorus)	$3.28\cdot10^{-2}$	$31.82\cdot10^{-2}$	$3.14\cdot10^{-2}$	0.0129
Land-system change	$8.04\cdot10^{-2}$	$14.80\cdot10^{-2}$	$8.04\cdot10^{-2}$	0.0002
Freshwater use	$1286.96\cdot10^{-2}$	$1930.45\cdot10^{-2}$	$1273.81\cdot10^{-2}$	0.0102
Aerosol loading	$0.035\cdot10^{-2}$	$0.11\cdot10^{-2}$	$-0.049\cdot10^{-2}$	2.4068

FSoSOS	**Share of SoS (EU, chemical industry & selected chemicals): $SoSOSPB_{FSoSOS}$ = $aSPB_{FSoSOS*SoS,PB}$**	**Upper bound SoSoS**	**Remaining SOS**	**$occSoSOS_{PB,FSoSOS}$**
Climate change (energy imalance at top of atmosphere)	$4.14\cdot10^{-4}$	$6.19\cdot10^{-4}$	$-440.98\cdot10^{-4}$	107.755
Climate change (atmospheric CO2 concentration)	$297.41\cdot10^{-4}$	$917.04\cdot10^{-4}$	$-33159.17\cdot10^{-4}$	112.490
Stratospheric ozone depletion	$59.89\cdot10^{-4}$	$119.79\cdot10^{-4}$	$57.00\cdot10^{-4}$	0.048
Ocean acidification	$2.84\cdot10^{-4}$	$4.26\cdot10^{-4}$	$-99.39\cdot10^{-4}$	35.973
Biogeochemical flows (Nitrogen)	$256.11\cdot10^{-4}$	$338.72\cdot10^{-4}$	$90.84\cdot10^{-4}$	0.645
Biogeochemical flows (Phosphorus)	$40.89\cdot10^{-4}$	$408.53\cdot10^{-4}$	$36.77\cdot10^{-4}$	0.101
Land-system change	$103.27\cdot10^{-4}$	$190.01\cdot10^{-4}$	$103.13\cdot10^{-4}$	0.001
Freshwater use	$16523.25\cdot10^{-4}$	$24784.87\cdot10^{-4}$	$15207.93\cdot10^{-4}$	0.080
Aerosol loading	$0.45\cdot10^{-4}$	$1.49\cdot10^{-4}$	$-8.06\cdot10^{-4}$	18.746

SQSoSOS	**Share of SoS (Status quo): $SoSOS_{PB,SQ}$ = $aSPB_{SQ*SoS,PB}$**	**Upper bound SoSOS**	**Remaining SOS**	**$occSoSOS_{PB, SQ}$**
Climate change (energy imalance at top of atmosphere)	$193.53\cdot10^{-4}$	$290.29\cdot10^{-4}$	$-251.58\cdot10^{-4}$	2.30
Climate change (atmospheric CO2 concentration)	$19990.66\cdot10^{-4}$	$61637.87\cdot10^{-4}$	$-123465.93\cdot10^{-4}$	1.67
Stratospheric ozone depletion	$0.47\cdot10^{-4}$	$0.93\cdot10^{-4}$	$-2.43\cdot10^{-4}$	6.21
Ocean acidification	$127.79\cdot10^{-4}$	$191.68\cdot10^{-4}$	$25.56\cdot10^{-4}$	0.80
Biogeochemical flows (Nitrogen)	$68.31\cdot10^{-4}$	$90.34\cdot10^{-4}$	$-96.95\cdot10^{-4}$	2.42
Biogeochemical flows (Phosphorus)	$1.95\cdot10^{-4}$	$19.51\cdot10^{-4}$	$-2.17\cdot10^{-4}$	2.11
Land-system change	$0.092\cdot10^{-4}$	$0.17\cdot10^{-4}$	$-0.045\cdot10^{-4}$	1.52
Freshwater use	$2023.55\cdot10^{-4}$	$3035.33\cdot10^{-4}$	$708.24\cdot10^{-4}$	0.65
Aerosol loading	$5.87\cdot10^{-4}$	$19.16\cdot10^{-4}$	$-2.66\cdot10^{-4}$	1.45

Table 4-2: Impact values per chemical and PB (for chemicals which include more than one production process, a weighted calculation based on market shares has been carried out).

Chemical list	Energy imbalance at top of atmosphere (W m^{-2})	Atmospheric CO_2 concentration (ppm CO_2)	Stratospheric ozone depletion (DU)	Ocean acidification (Ω_{arag})	Biogeochemical flows, N (Tg N yr^{-1})
Methanol	$2.58 \cdot 10^{-4}$	$1.91 \cdot 10^{-2}$	$458.43 \cdot 10^{-8}$	$5.83 \cdot 10^{-5}$	$1.69 \cdot 10^{-5}$
Ethylene	$7.94 \cdot 10^{-4}$	$5.96 \cdot 10^{-2}$	$5.57 \cdot 10^{-8}$	$18.23 \cdot 10^{-5}$	$4.11 \cdot 10^{-5}$
Propylene	0	0	0	0	0
Cumene	$13.93 \cdot 10^{-4}$	$10.43 \cdot 10^{-2}$	$652.90 \cdot 10^{-8}$	$31.87 \cdot 10^{-5}$	$19.44 \cdot 10^{-5}$
Ethylene glycol	$7.65 \cdot 10^{-4}$	$5.67 \cdot 10^{-2}$	$637.17 \cdot 10^{-8}$	$17.33 \cdot 10^{-5}$	$16.18 \cdot 10^{-5}$
Styrene	$42.16 \cdot 10^{-4}$	$31.48 \cdot 10^{-2}$	$2690.25 \cdot 10^{-8}$	$96.20 \cdot 10^{-5}$	$60.09 \cdot 10^{-5}$
Terephthalic acid	$12.54 \cdot 10^{-4}$	$9.36 \cdot 10^{-2}$	$749.61 \cdot 10^{-8}$	$28.61 \cdot 10^{-5}$	$23.05 \cdot 10^{-5}$
Propylene oxide	$34.30 \cdot 10^{-4}$	$25.23 \cdot 10^{-2}$	$7429.59 \cdot 10^{-8}$	$77.10 \cdot 10^{-5}$	$590.68 \cdot 10^{-5}$
Vinyl chloride	$25.41 \cdot 10^{-4}$	$19.23 \cdot 10^{-2}$	$2781.89 \cdot 10^{-8}$	$58.76 \cdot 10^{-5}$	$21.62 \cdot 10^{-5}$
Acrylonitrile	$6.52 \cdot 10^{-4}$	$4.91 \cdot 10^{-2}$	$324.54 \cdot 10^{-8}$	$15.00 \cdot 10^{-5}$	$7.56 \cdot 10^{-5}$
Ammonia	$110.95 \cdot 10^{-4}$	$83.98 \cdot 10^{-2}$	$12558.50 \cdot 10^{-8}$	$256.65 \cdot 10^{-5}$	$104.06 \cdot 10^{-5}$
Polyethylene/HD	$35.53 \cdot 10^{-4}$	$26.83 \cdot 10^{-2}$	$43.25 \cdot 10^{-8}$	$81.98 \cdot 10^{-5}$	$17.73 \cdot 10^{-5}$
Polyethylene/LD/linear	$11.96 \cdot 10^{-4}$	$8.98 \cdot 10^{-2}$	$12.35 \cdot 10^{-8}$	$27.44 \cdot 10^{-5}$	$8.12 \cdot 10^{-5}$
Polyethylene/LD	$26.11 \cdot 10^{-4}$	$19.60 \cdot 10^{-2}$	$23.07 \cdot 10^{-8}$	$59.89 \cdot 10^{-5}$	$11.32 \cdot 10^{-5}$
Polypropylene	$66.25 \cdot 10^{-4}$	$50.02 \cdot 10^{-2}$	$58.92 \cdot 10^{-8}$	$152.86 \cdot 10^{-5}$	$728.85 \cdot 10^{-5}$
Benzene	$26.67 \cdot 10^{-4}$	$20.04 \cdot 10^{-2}$	$82.67 \cdot 10^{-8}$	$61.23 \cdot 10^{-5}$	$19.05 \cdot 10^{-5}$
Toluene	$5.17 \cdot 10^{-4}$	$3.88 \cdot 10^{-2}$	$2.82 \cdot 10^{-8}$	$11.85 \cdot 10^{-5}$	$4.11 \cdot 10^{-5}$
Mixed xylene	$1.55 \cdot 10^{-4}$	$1.16 \cdot 10^{-2}$	$0.87 \cdot 10^{-8}$	$3.55 \cdot 10^{-5}$	$1.04 \cdot 10^{-5}$
Ethylene oxide	$7.86 \cdot 10^{-4}$	$5.85 \cdot 10^{-2}$	$446.77 \cdot 10^{-8}$	$17.88 \cdot 10^{-5}$	$13.96 \cdot 10^{-5}$
Phenol	$21.21 \cdot 10^{-4}$	$15.84 \cdot 10^{-2}$	$1393.45 \cdot 10^{-8}$	$48.42 \cdot 10^{-5}$	$35.26 \cdot 10^{-5}$

Chemical list	Biogeochemical flows, P (Tg P yr^{-1})	Land-system change (%)	Freshwater use (m^3 yr^{-1})	Aerosol loading (AOD)
Methanol	$2.59 \cdot 10^{-8}$	$51.76 \cdot 10^{-8}$	$26.04 \cdot 10^{-4}$	$4.26 \cdot 10^{-6}$
Ethylene	$9.84 \cdot 10^{-8}$	$-0.094 \cdot 10^{-8}$	$7.81 \cdot 10^{-4}$	$9.57 \cdot 10^{-6}$
Propylene	0	0	0	0
Cumene	$23.97 \cdot 10^{-8}$	$9.57 \cdot 10^{-8}$	$61.57 \cdot 10^{-4}$	$44.75 \cdot 10^{-6}$
Ethylene glycol	$16.82 \cdot 10^{-8}$	$13.73 \cdot 10^{-8}$	$31.37 \cdot 10^{-4}$	$24.03 \cdot 10^{-6}$
Styrene	$71.92 \cdot 10^{-8}$	$44.34 \cdot 10^{-8}$	$393.73 \cdot 10^{-4}$	$134.80 \cdot 10^{-6}$
Terephthalic acid	$25.86 \cdot 10^{-8}$	$30.65 \cdot 10^{-8}$	$54.17 \cdot 10^{-4}$	$22.87 \cdot 10^{-6}$
Propylene oxide	$336.34 \cdot 10^{-8}$	$81.54 \cdot 10^{-8}$	$221.15 \cdot 10^{-4}$	$113.21 \cdot 10^{-6}$
Vinyl chloride	$1029.07 \cdot 10^{-8}$	$-1.11 \cdot 10^{-8}$	$71.77 \cdot 10^{-4}$	$27.06 \cdot 10^{-6}$
Acrylonitrile	$10.32 \cdot 10^{-8}$	$21.95 \cdot 10^{-8}$	$41.29 \cdot 10^{-4}$	$9.12 \cdot 10^{-6}$
Ammonia	$163.38 \cdot 10^{-8}$	$1142.84 \cdot 10^{-8}$	$138.94 \cdot 10^{-4}$	$196.02 \cdot 10^{-6}$
Polyethylene/HD	$93.52 \cdot 10^{-8}$	$-0.78 \cdot 10^{-8}$	$66.77 \cdot 10^{-4}$	$54.35 \cdot 10^{-6}$
Polyethylene/LD/linear	$11.66 \cdot 10^{-8}$	$-0.13 \cdot 10^{-8}$	$5.65 \cdot 10^{-4}$	$19.44 \cdot 10^{-6}$
Polyethylene/LD	$82.25 \cdot 10^{-8}$	$-0.87 \cdot 10^{-8}$	$39.26 \cdot 10^{-4}$	$43.90 \cdot 10^{-6}$
Polypropylene	$39311.30 \cdot 10^{-8}$	$-1.27 \cdot 10^{-8}$	$104.81 \cdot 10^{-4}$	$87.83 \cdot 10^{-6}$
Benzene	$28.18 \cdot 10^{-8}$	$0.78 \cdot 10^{-8}$	$13.81 \cdot 10^{-4}$	$40.34 \cdot 10^{-6}$
Toluene	$5.82 \cdot 10^{-8}$	$-0.059 \cdot 10^{-8}$	$2.49 \cdot 10^{-4}$	$5.75 \cdot 10^{-6}$
Mixed xylene	$1.53 \cdot 10^{-8}$	$-0.023 \cdot 10^{-8}$	$0.80 \cdot 10^{-4}$	$1.83 \cdot 10^{-6}$
Ethylene oxide	$16.83 \cdot 10^{-8}$	$5.47 \cdot 10^{-8}$	$33.81 \cdot 10^{-4}$	$12.27 \cdot 10^{-6}$
Phenol	$40.27 \cdot 10^{-8}$	$28.53 \cdot 10^{-8}$	$141.31 \cdot 10^{-4}$	$64.83 \cdot 10^{-6}$

5 Discussion of results

5.1 Insight into the environmental burdens

LCIs that contribute to the transgression of the climate change boundaries include all types of GHGs. Despite 45 GHGs being considered, the selected activities have been found to predominantly emit 3 kinds of CO_2. Fig. 5-1 and Fig. 5-2 show the total GHG emissions for the considered chemicals (for chemicals for which more than one process is considered, a weighted value has been calculated using market shares). It can be appreciated that the three principal GHGs emitted by the industry are fossil emissions of CO_2 directed to non-urban air or from high stacks (in orange), and to urban air or close to ground (in yellow), or unspecified but also fossil CO_2 emissions (in grey).

Fig. 5-3 and Fig. 5-4 present the breakdown of the emissions contributing to the ocean acidification boundary, to which fossil CO_2 and CH_4 have the highest impact again (as in the climate change boundaries).

Regarding the aerosol loading boundary, the breakdown of the emitted compounds by each process can be seen in Fig. 5-5 and Fig. 5-6, which note that the most relevant aerosols are NMVOCs (emitted to urban air or close to ground), sulfur dioxide (emitted to non-urban and urban air to both high and low heights) and nitrogen oxides to urban air or close to ground.

Fig. 5-7 and Fig. 5-8 give insight in the ODS emissions per process and show how dinitrogen monoxide is the principal emission caused by the industry that poses a threat to the ozone layer. The rest of included substances are regulated by the European Council Regulation (EC) No. 1005/2009 (2009), and thus their use is limited. Five different emission subcompartments are considered for N_2O, but as with CO_2, emissions to urban and rural air (atmosphere) and low heights and unspecified emissions eclipse emissions to higher layers (troposphere and stratosphere).

Both the land-system change, and the freshwater use boundaries have double figures, since not only the resource uptakes are evaluated but also the returns to the environment. For land-system change, the areas of deforested land are classified according to the type of land transformation in Fig. 5-9 and Fig.

5-10(which show how transformation is mainly intensive), while the areas of reforested land are illustrated in Fig. 5-11 and Fig. 5-12 (which confirm reforestation is also generally intensive, even at a greater level than deforestation). Regarding freshwater use, water uptakes are classified according to the type of source they originate from in Fig. 5-13 and Fig. 5-14 (which reveal most withdrawn water comes from rivers or underground reservoirs). After adequate treatment, a fraction of the collected water is returned to water bodies. Fig. 5-15 and Fig. 5-16show how most water is returned to surface water bodies rather than to ground.

No graphs are presented for the biogeochemical flows boundaries since there is only one flux which contributed to each of them, in accordance with the PBs framework and the study's specifications (see the section that details the application of the PB-LCIA damage assessment model in the project's main report). For the N cycle, only the runoff of nitrates to surface waters is considered, while for the P cycle, phosphorus also to surface waters is the studied flux.

In Fig. 5-17 and Fig. 5-18, the labels for all fluxes which have low or negligible contributions to the total have not been included for visual simplicity. These illustrate the final emissions or resource uptakes caused by the considered activities taking into account their total production volumes (including chemicals destined to exports). These are not equal to the final contributions to the PBs, since they have not been related to any characterization factors. Final pressures put on every Earth cycle are presented in the main document (Table 10-3).

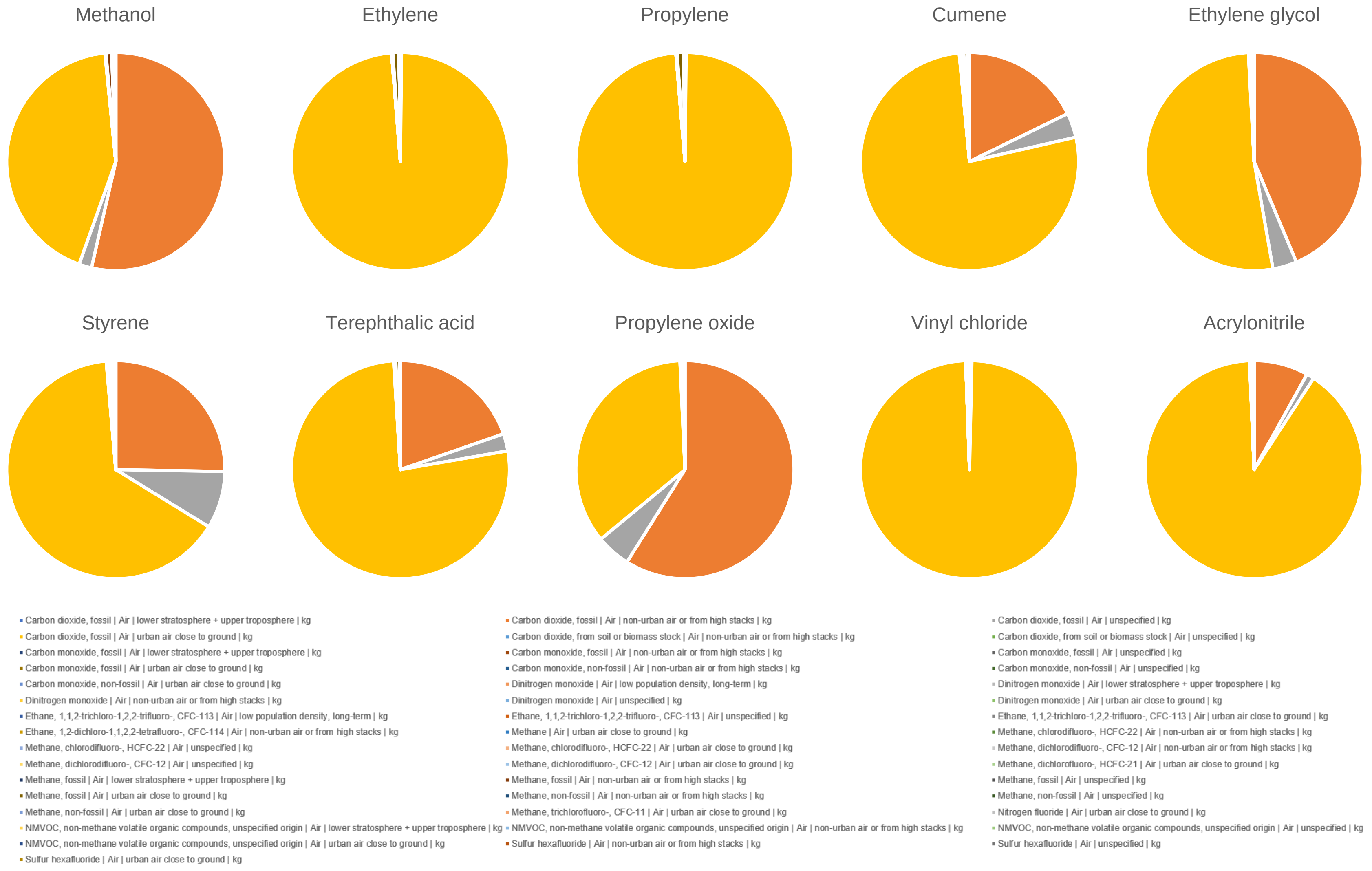


Fig. 5-1: GHG emissions (in kg) per kg of chemical classified by compound emitted and type of emission (1).

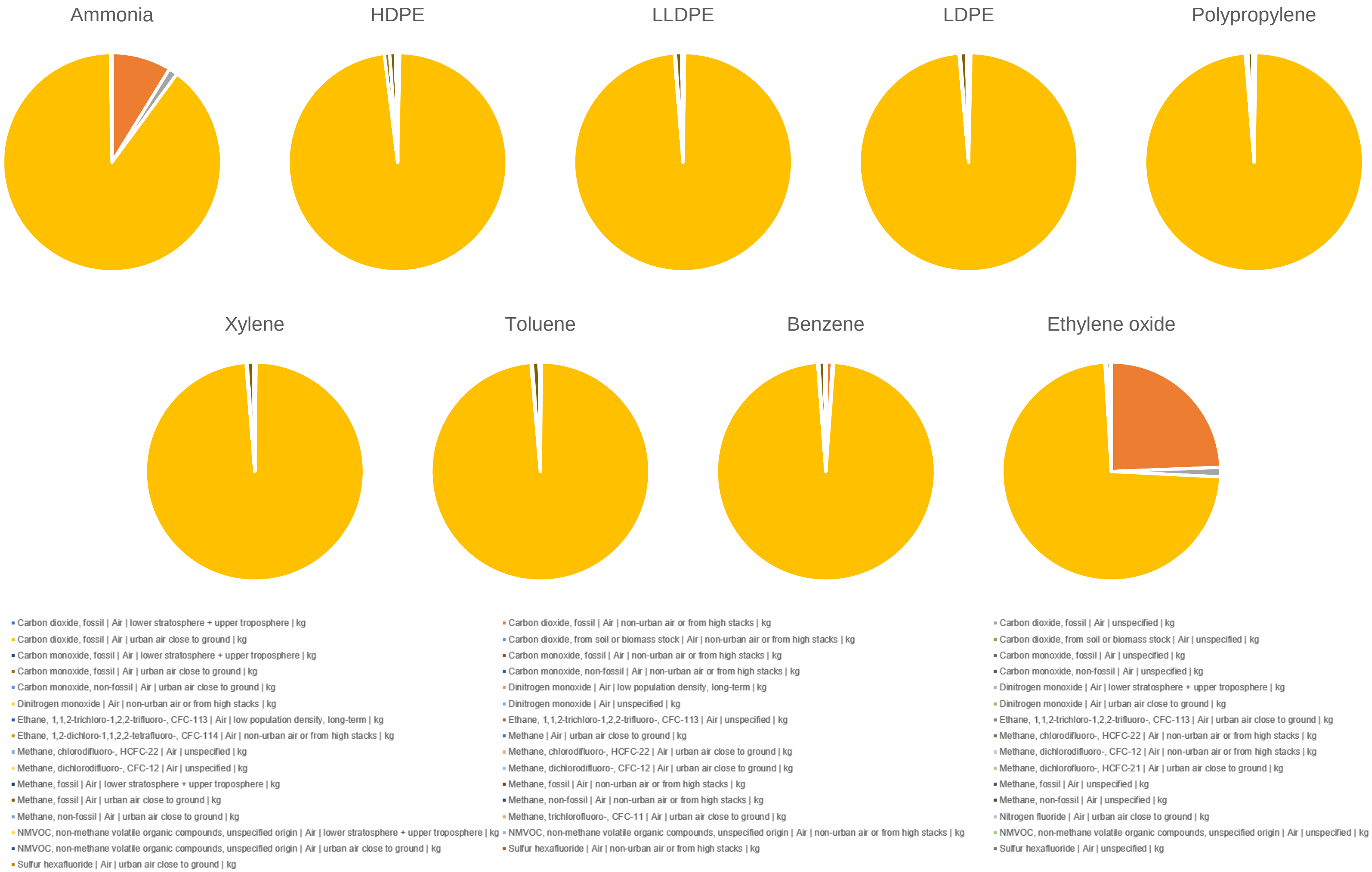


Fig. 5-2: GHG emissions (in kg) per kg of chemical classified by compound emitted and type of emission (2).

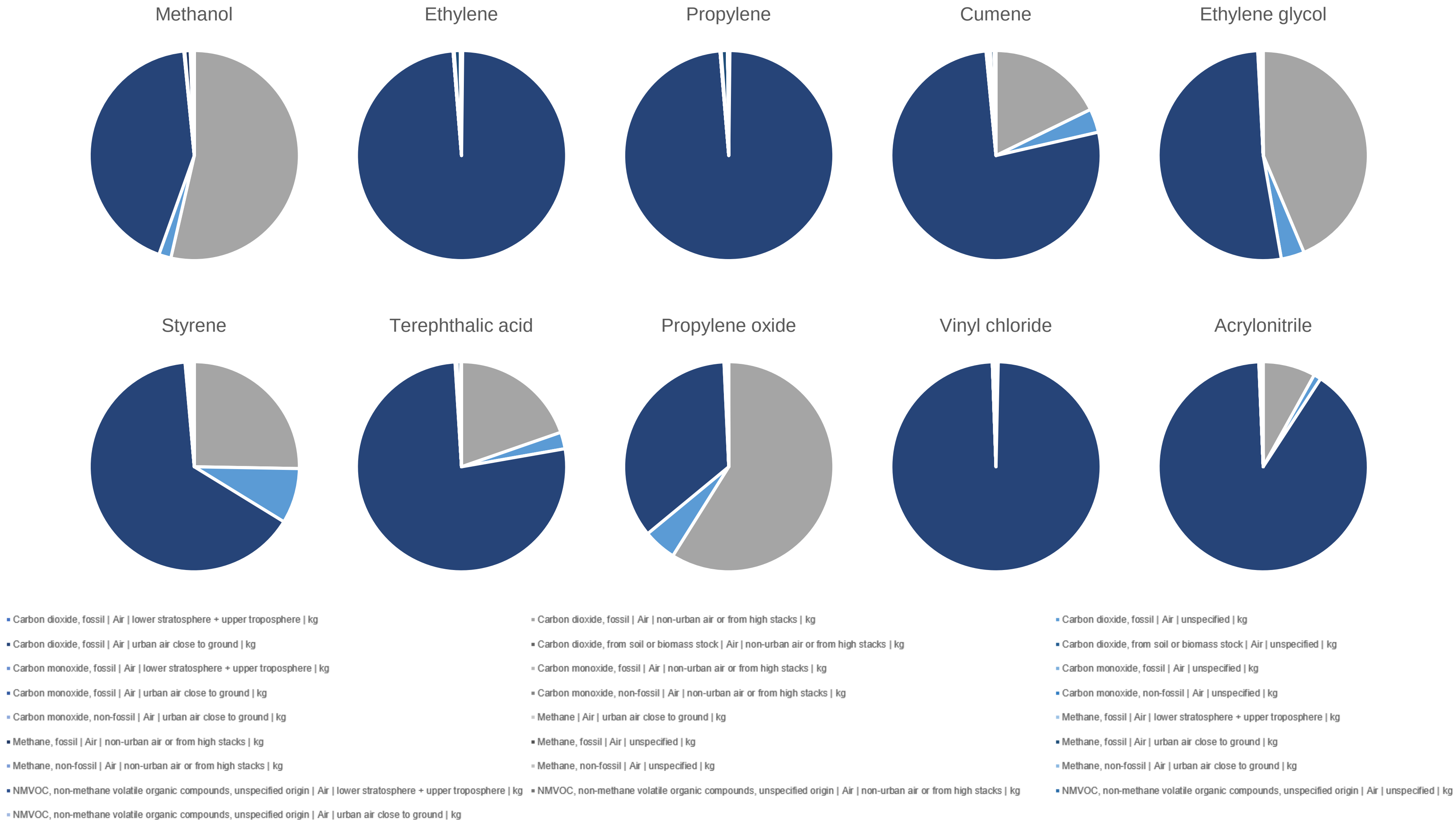


Fig. 5-3: Environmental burdens (kg) contributing to the acidification of ocean water per kg of chemical (1).

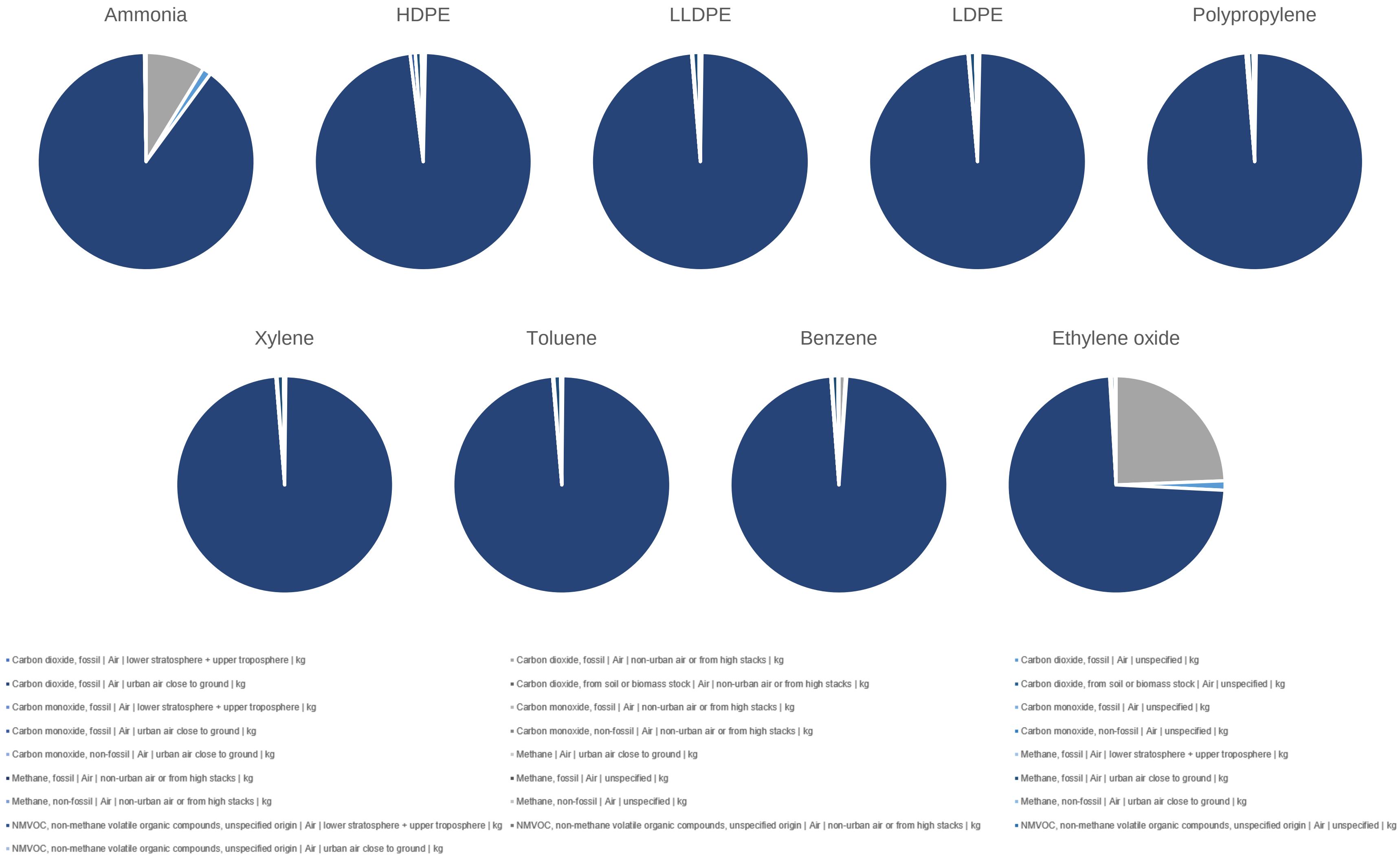


Fig. 5-4: Environmental burdens (kg) contributing to the acidification of ocean water per kg of chemical (2).

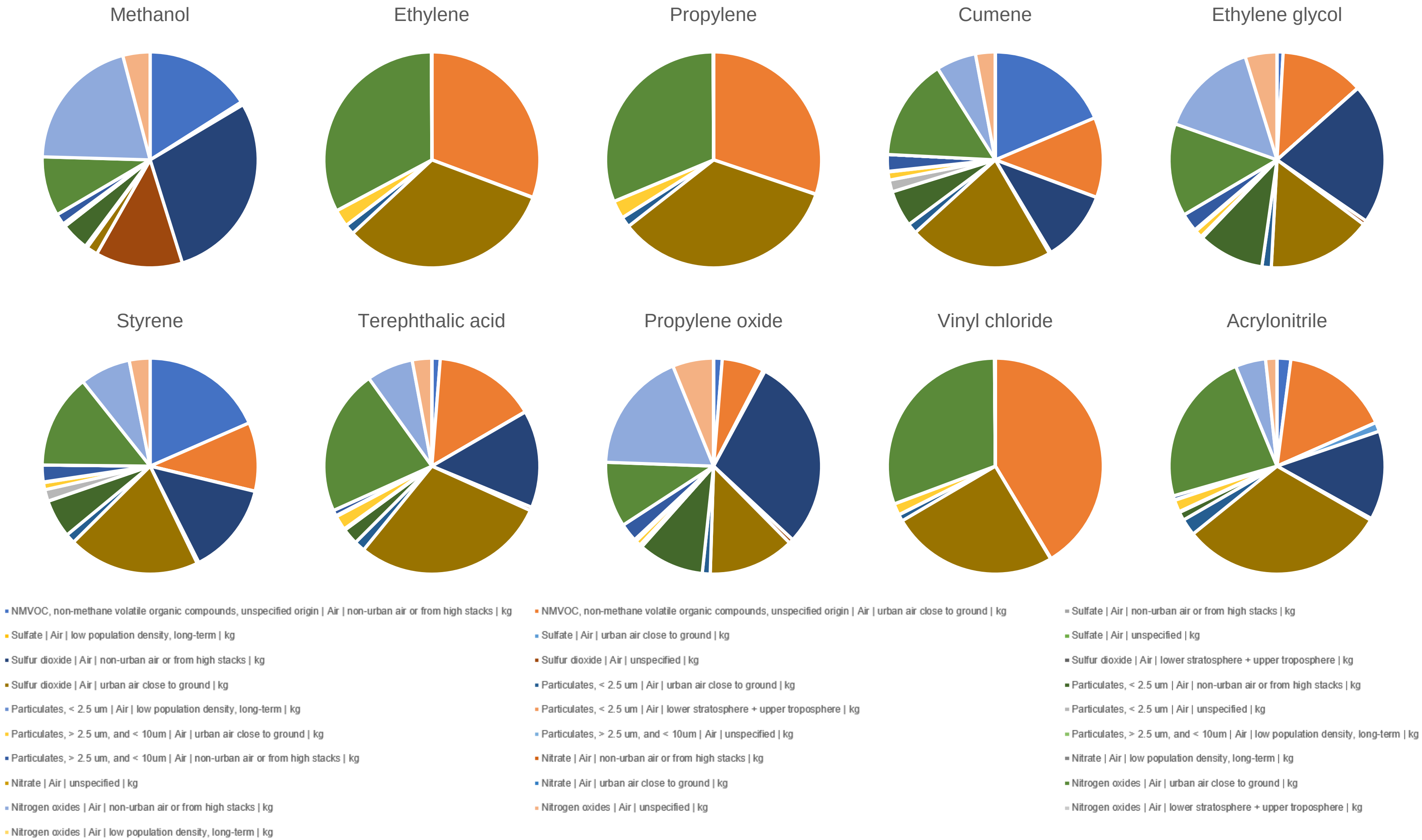


Fig. 5-5: Environmental burdens (kg) contributing to the aerosol loading boundary per kg of chemical (1).

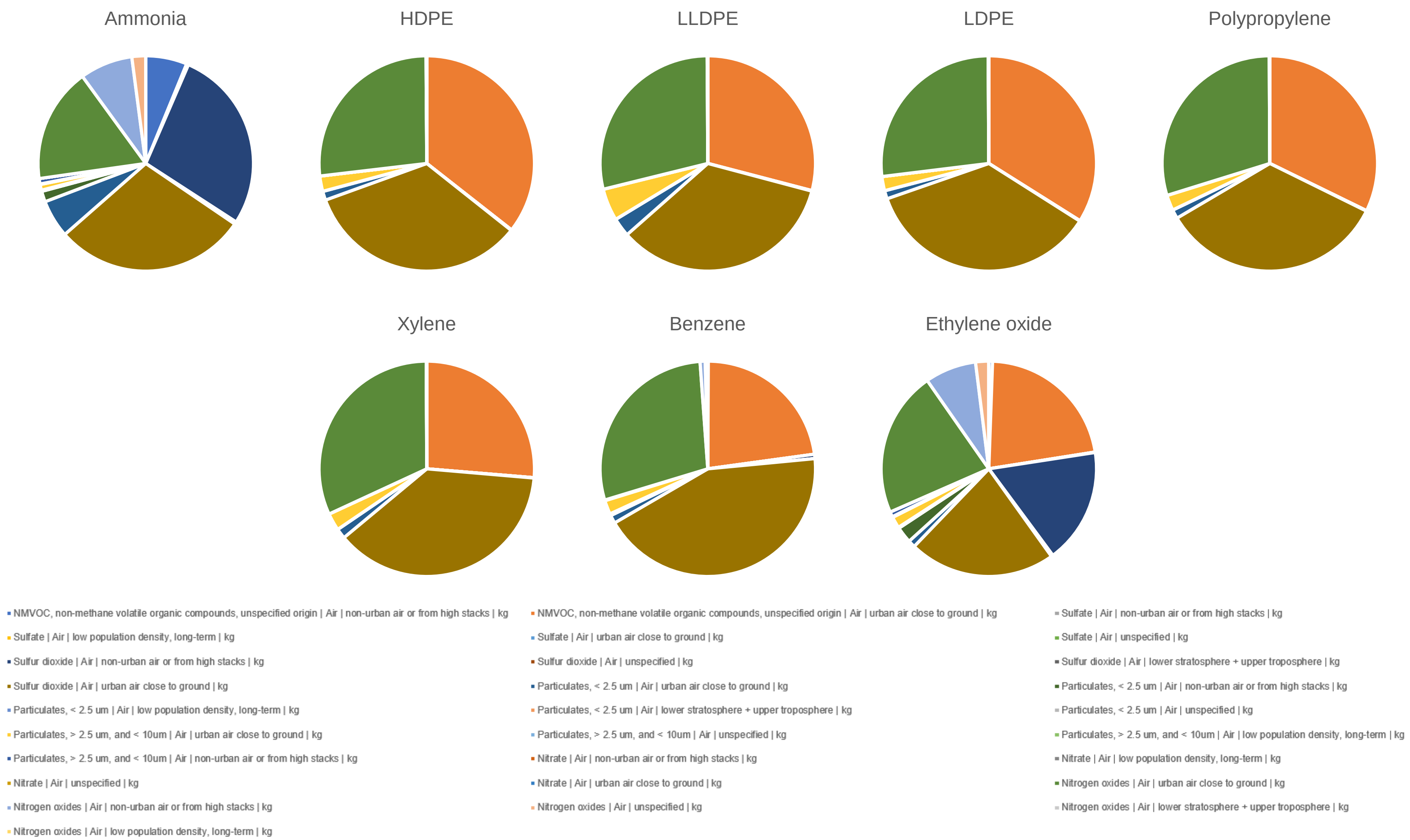


Fig. 5-6: Environmental burdens (kg) contributing to the aerosol loading boundary per kg of chemical (2).

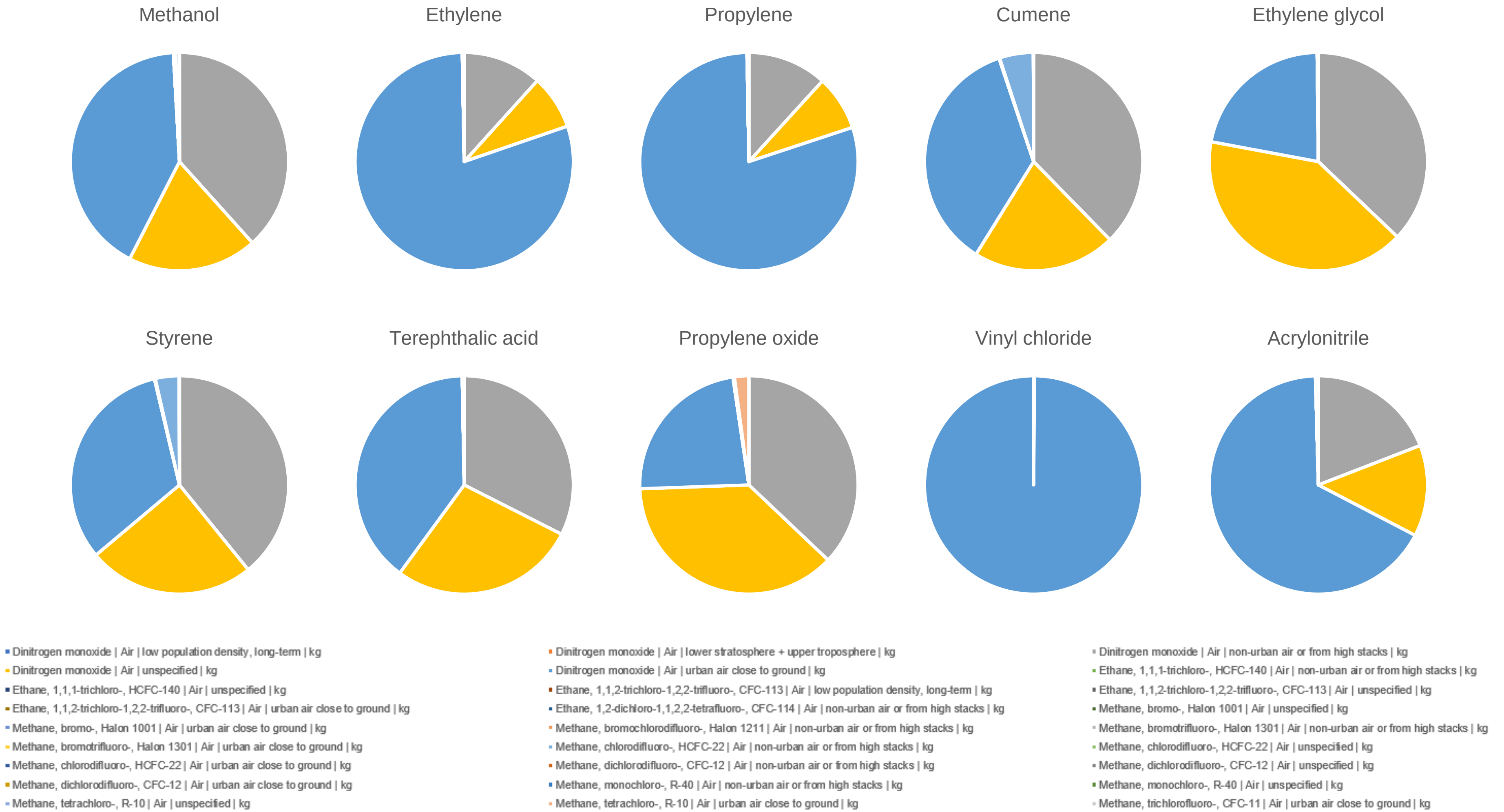


Fig. 5-7: Environmental burdens (kg) contributing to the depletion of stratospheric ozone per kg of chemical (1).

Fig. 5-8: Environmental burdens (kg) contributing to the depletion of stratospheric ozone per kg of chemical (2).

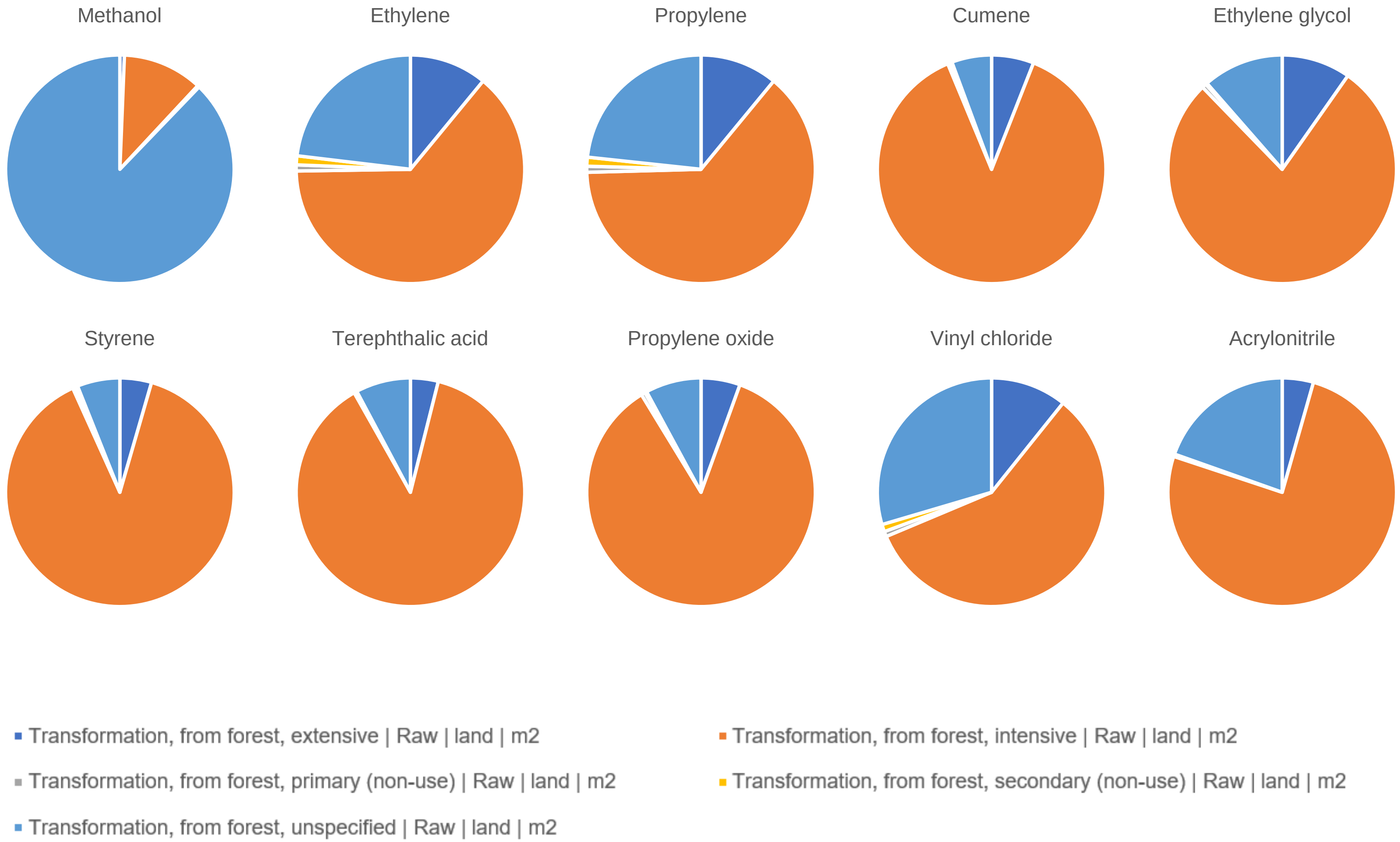


Fig. 5-9: Areas of deforested land (m^2) contributing to the land-system change PB per kg of chemical (1).

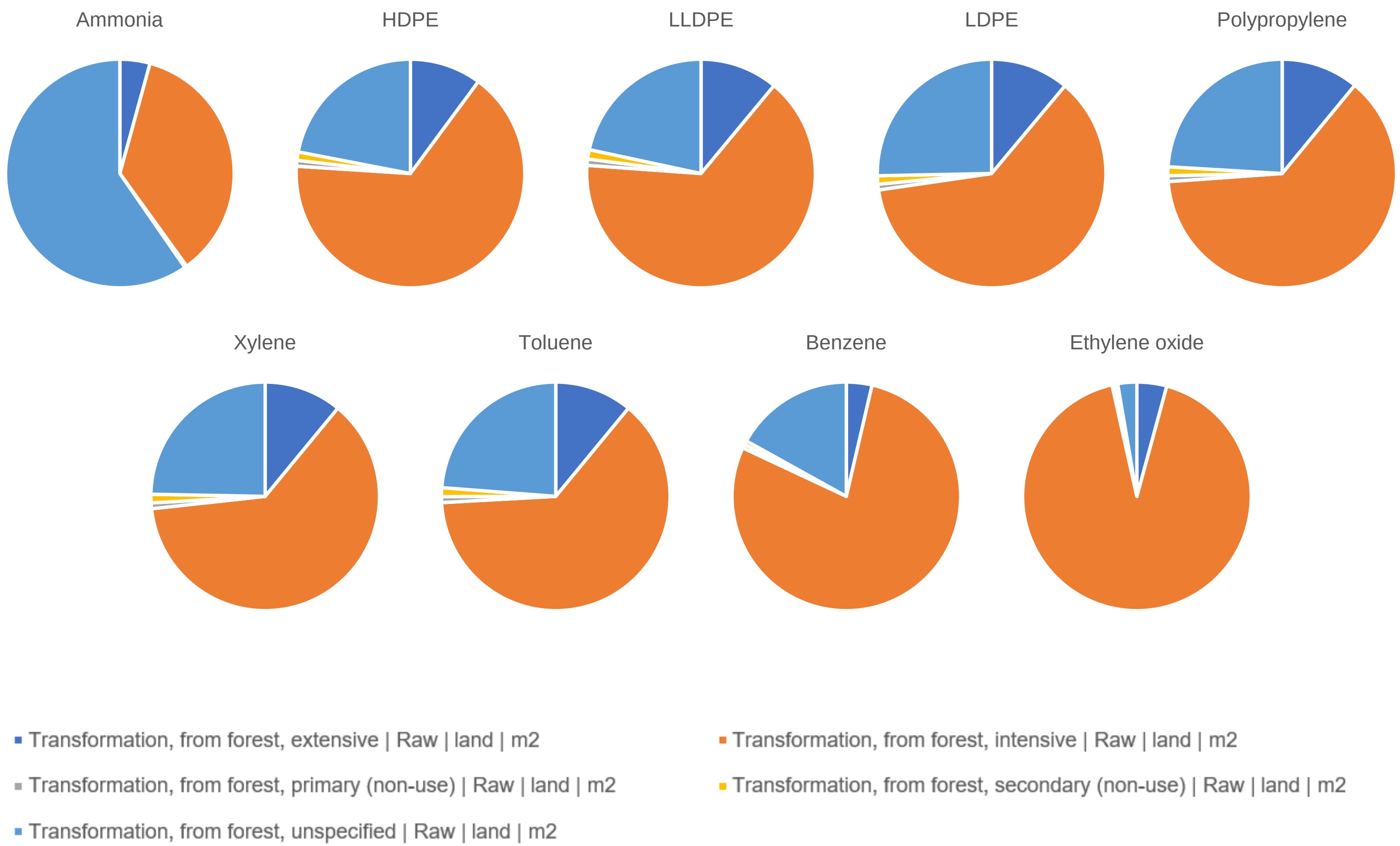


Fig. 5-10: Areas of deforested land (m^2) contributing to the land-system change PB per kg of chemical (2).

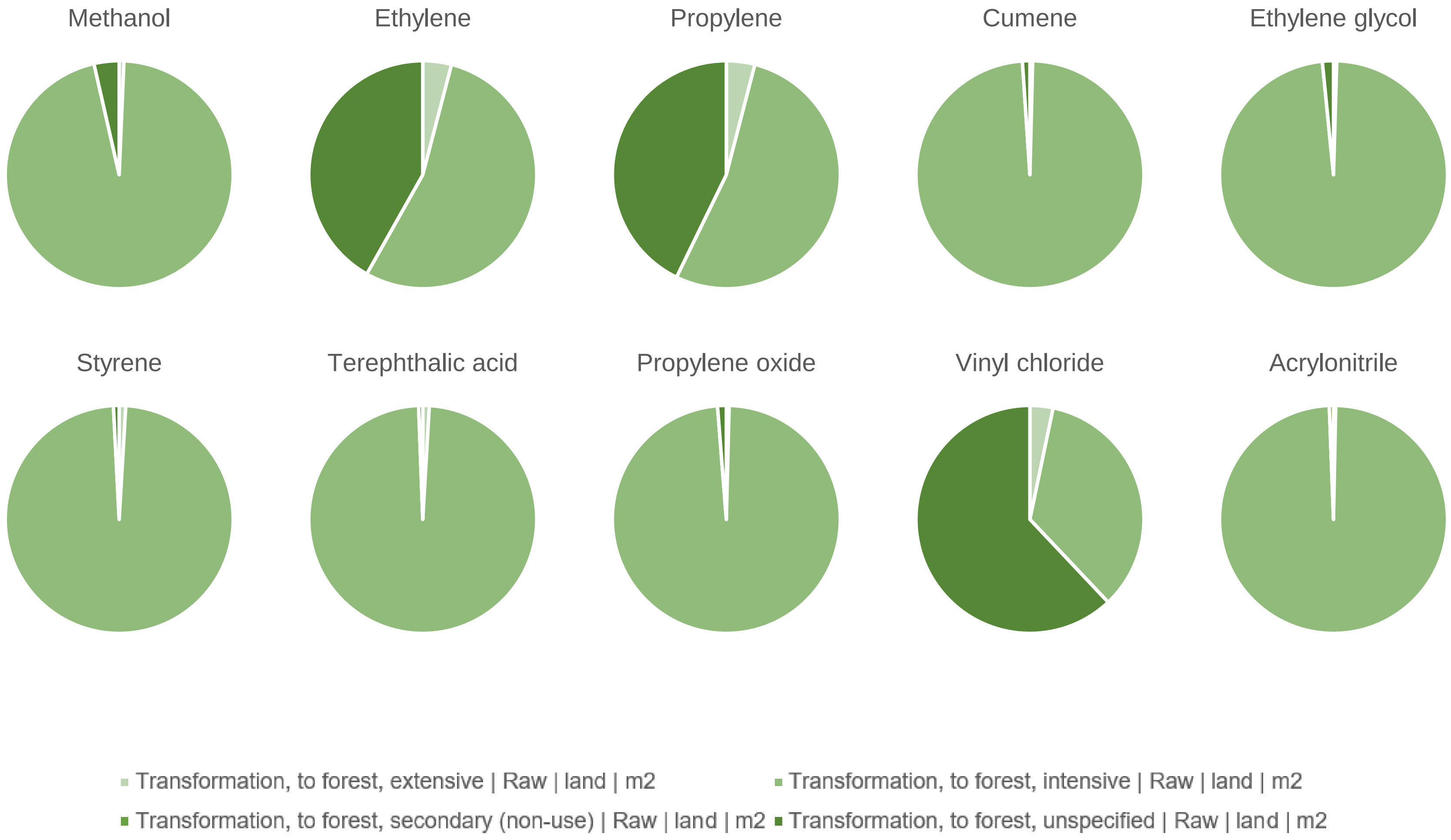


Fig. 5-11: Areas of reforested land (m^2) per kg of chemical (1).

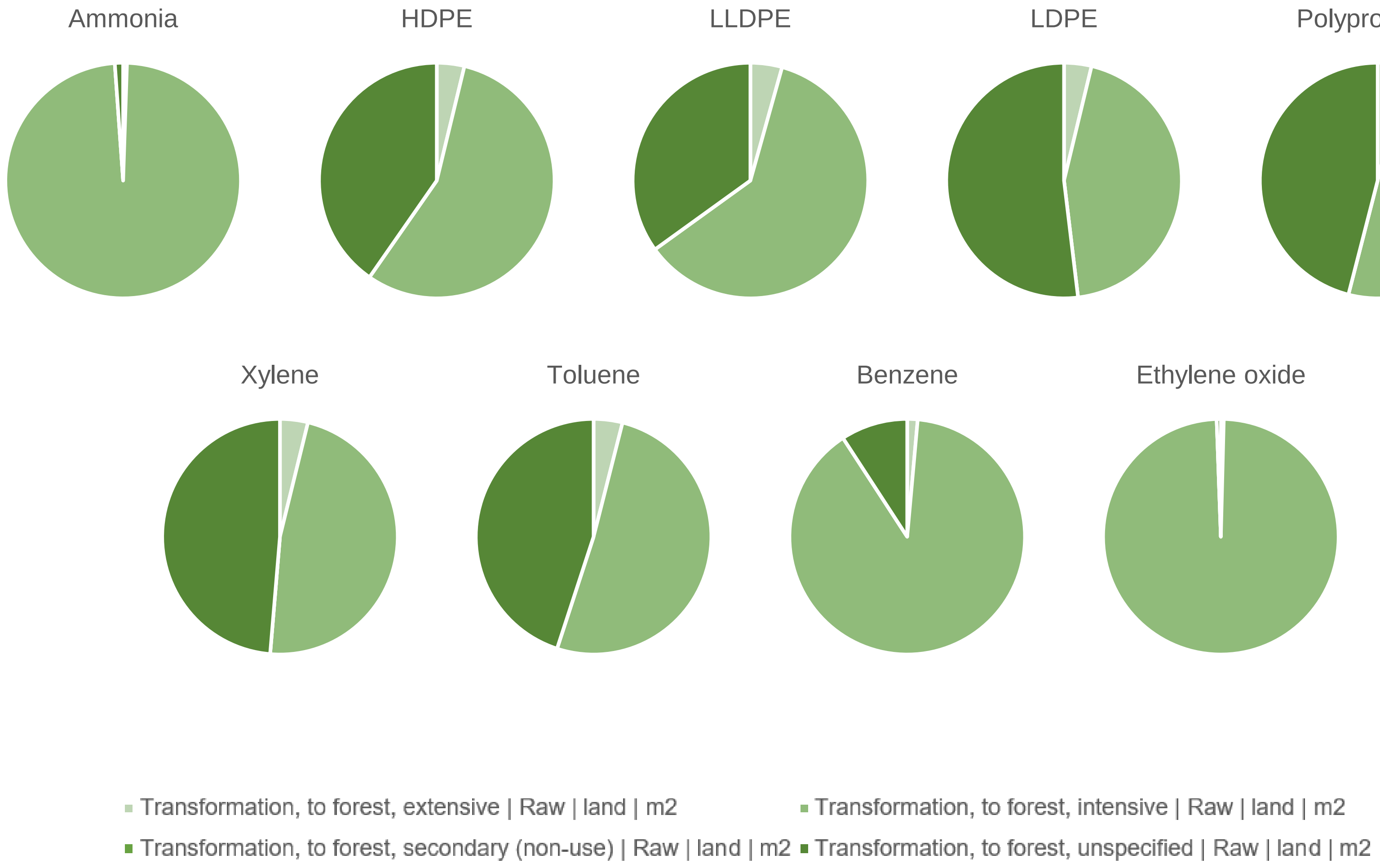


Fig. 5-12: Areas of reforested land (m^2) per kg of chemical (2).

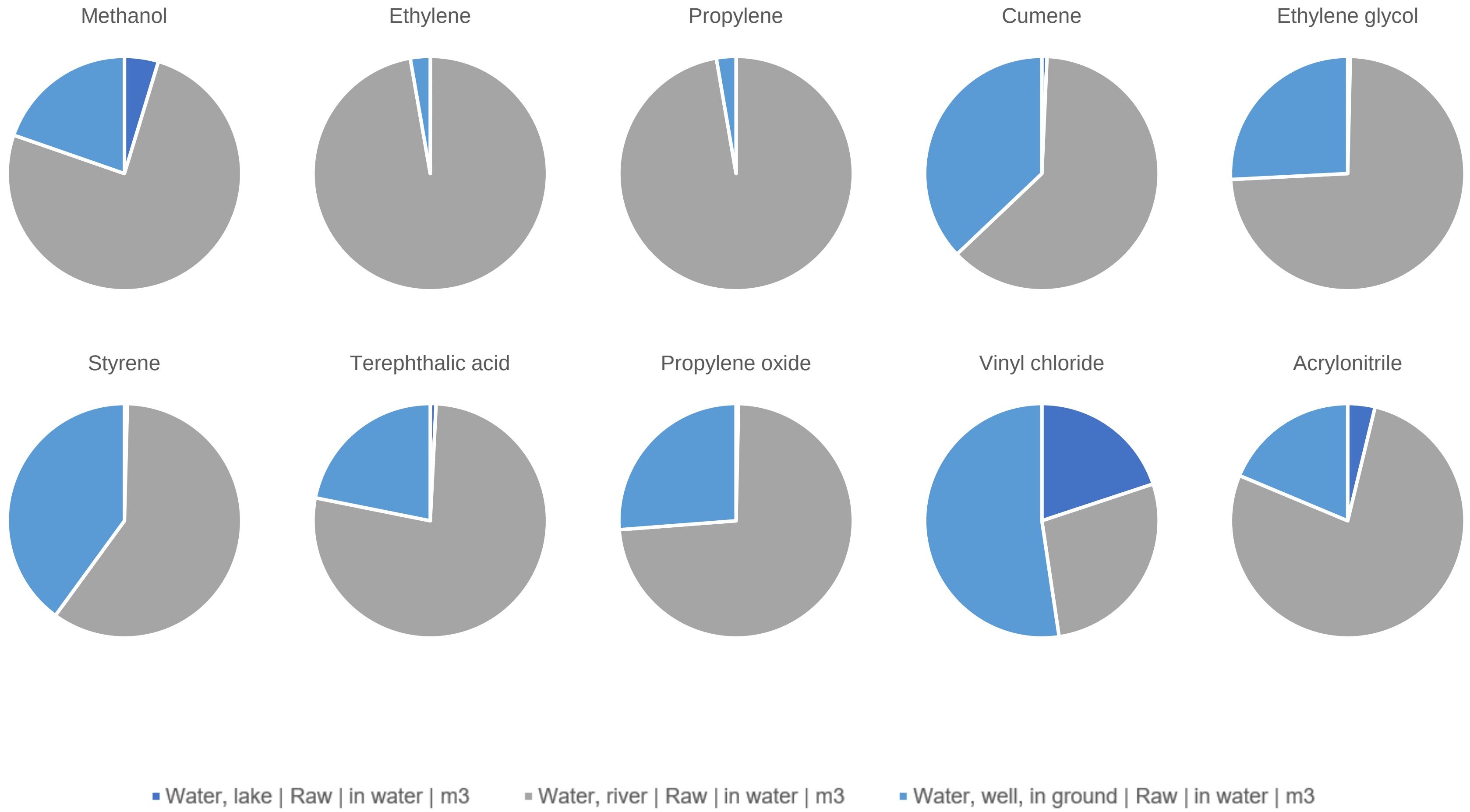


Fig. 5-13: Water consumption (m^3) per kg of chemical (1).

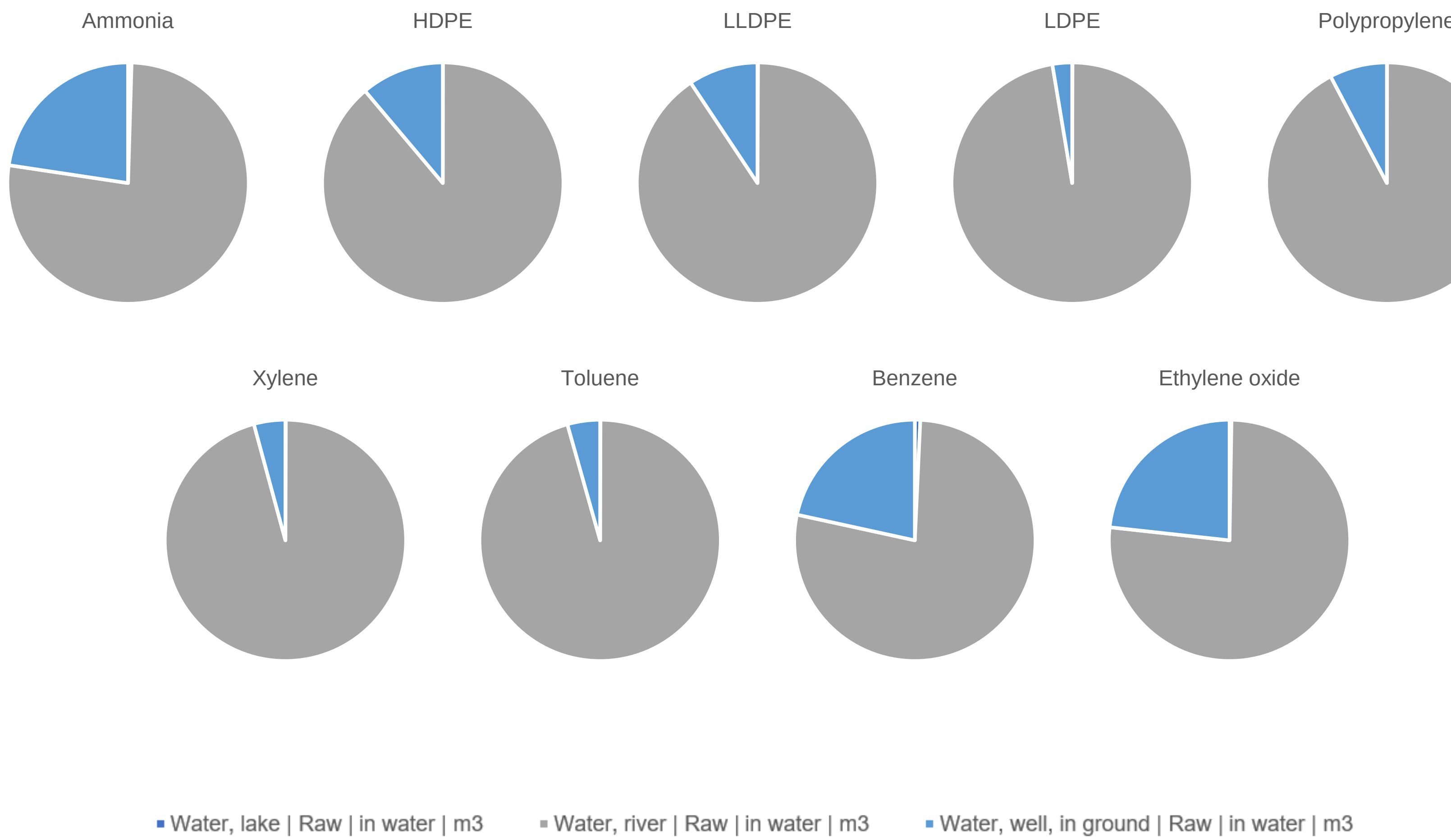


Fig. 5-14: Water consumption (m³) per kg of chemical (2).

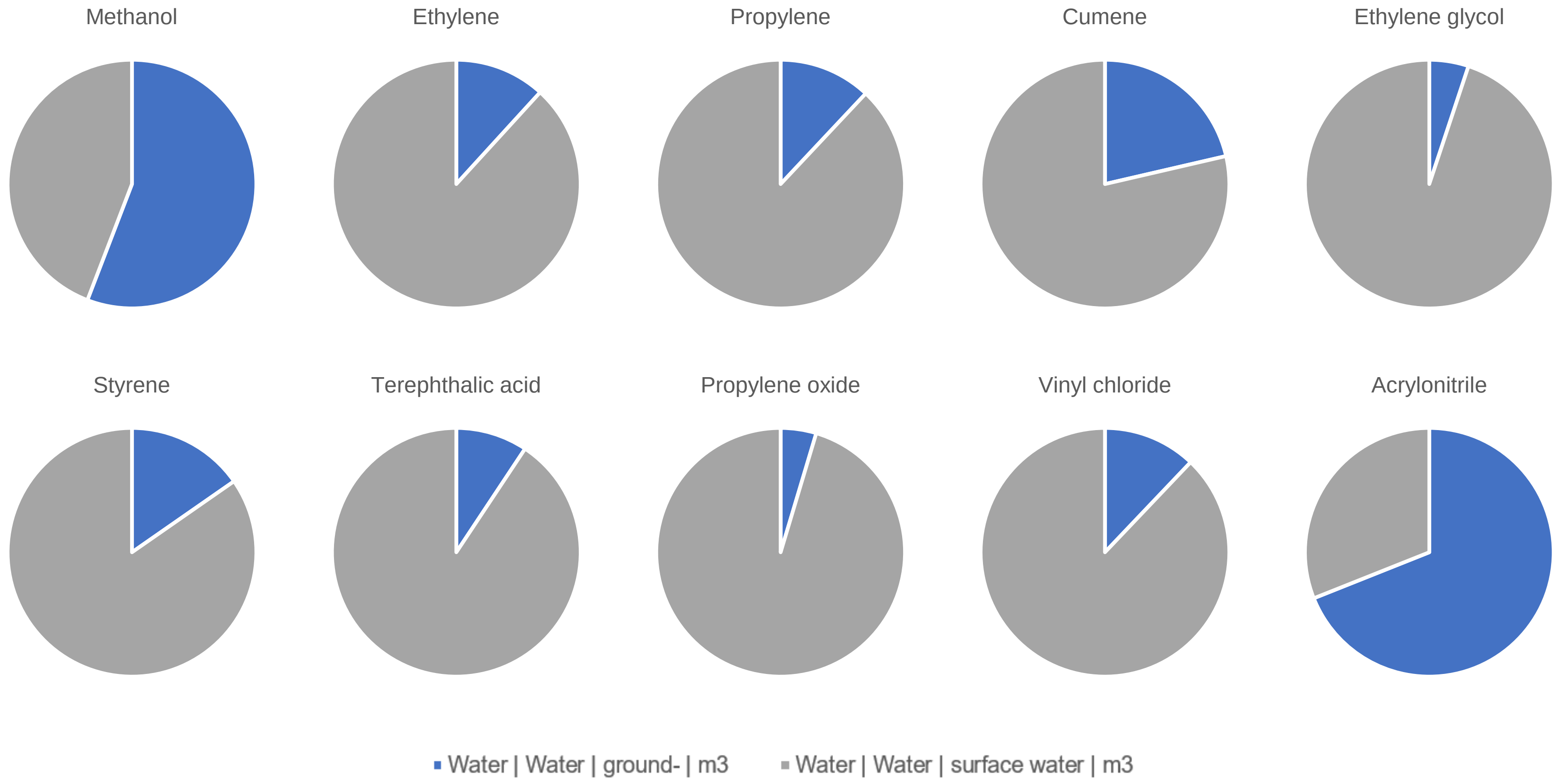


Fig. 5-15: Water return (m³) per kg of chemical (1).

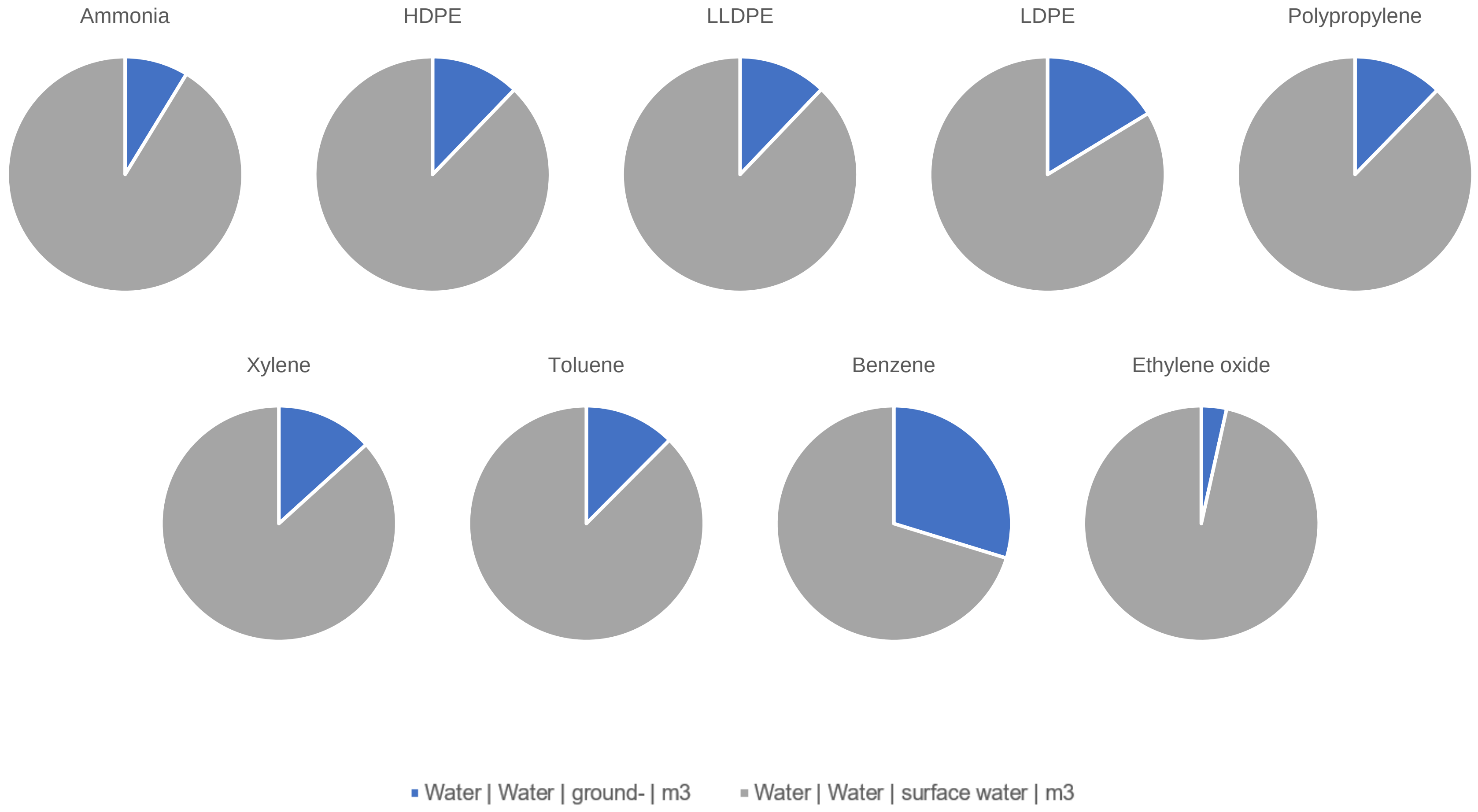


Fig. 5-16: Water return (m^3) per kg of chemical (2).

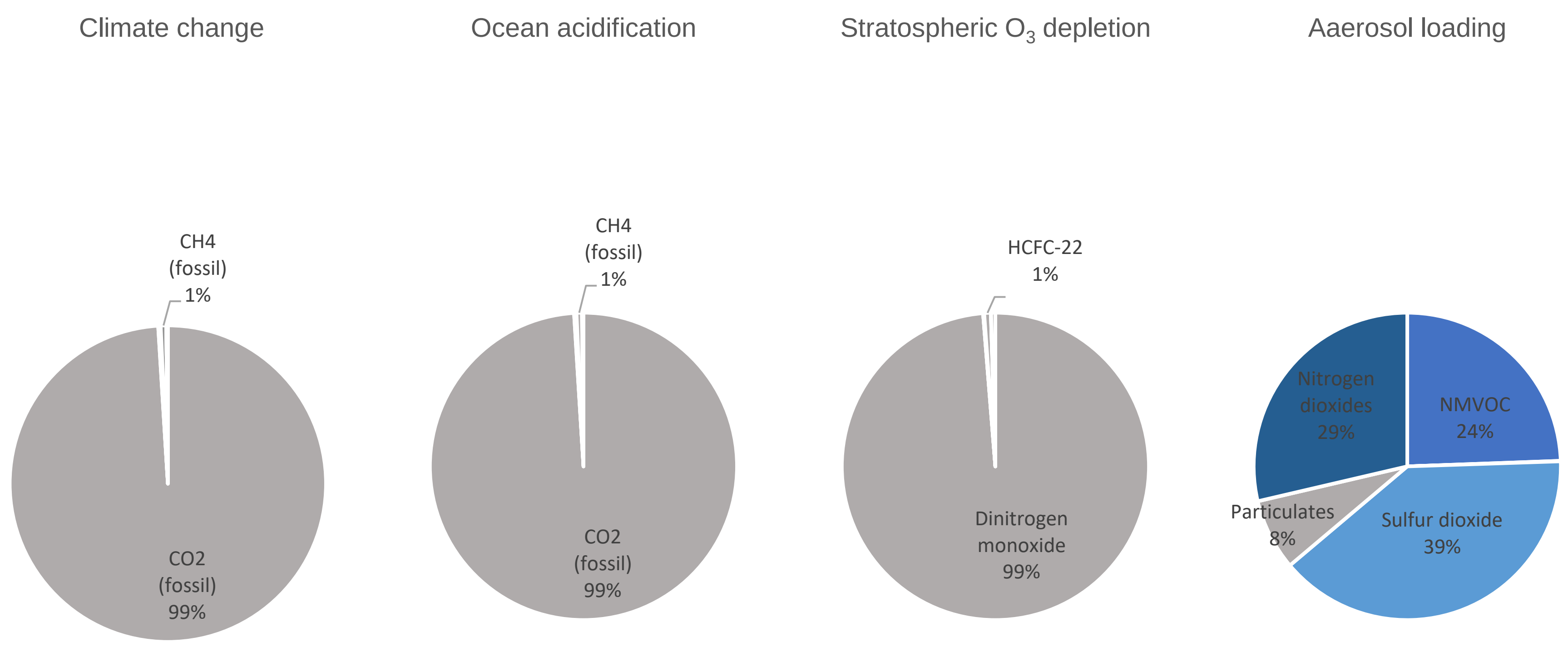


Fig. 5-17: Total emitted substances (kg) for the transgressed PBs (climate change, ocean acidification, stratospheric ozone depletion and aerosol loading).

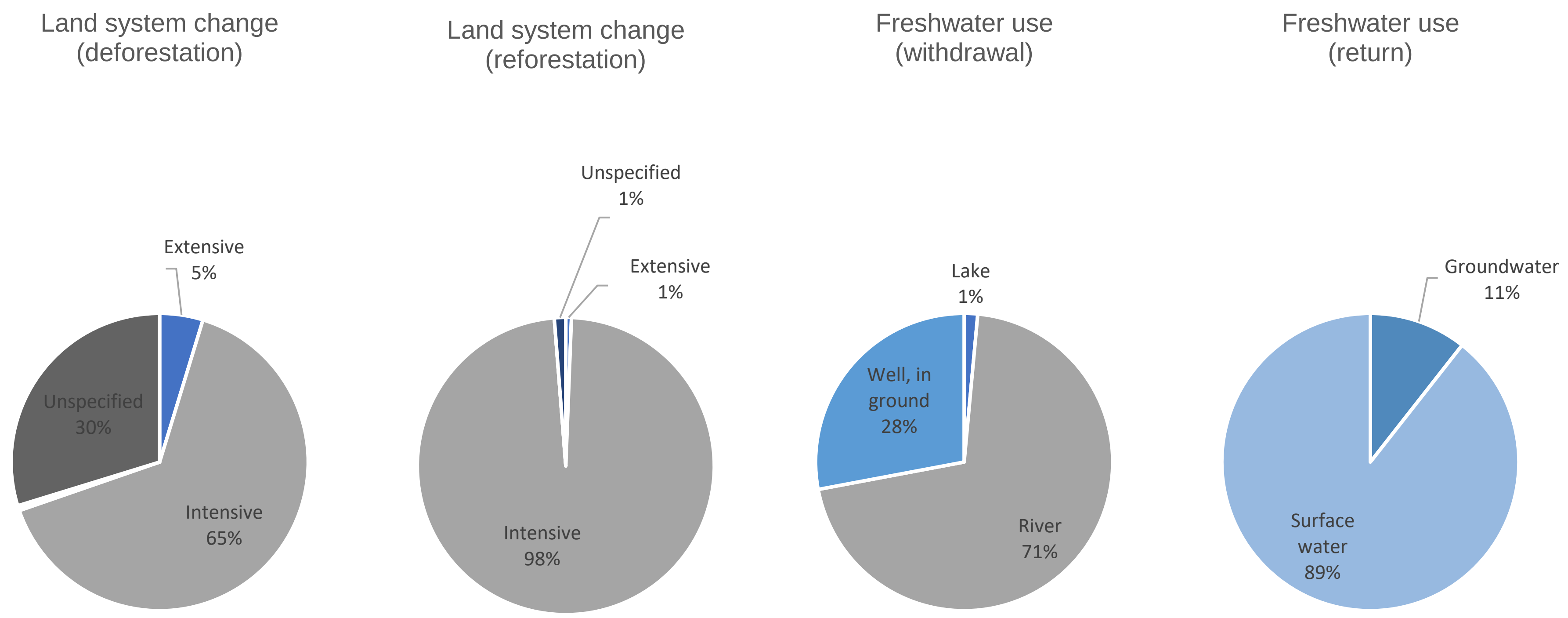


Fig. 5-18: Total transformed land area (m^2) and withdrawn or returned water (m^3) for the land-system change and freshwater use PBs.

5.2 Breakdown of impacts

5.2.1 Electricity demand

The electricity demand of the processes has been evaluated to understand GHG emissions. Fig. 5-19 shows the energy demand [kWh] per kg of produced chemical for the assessed activities.

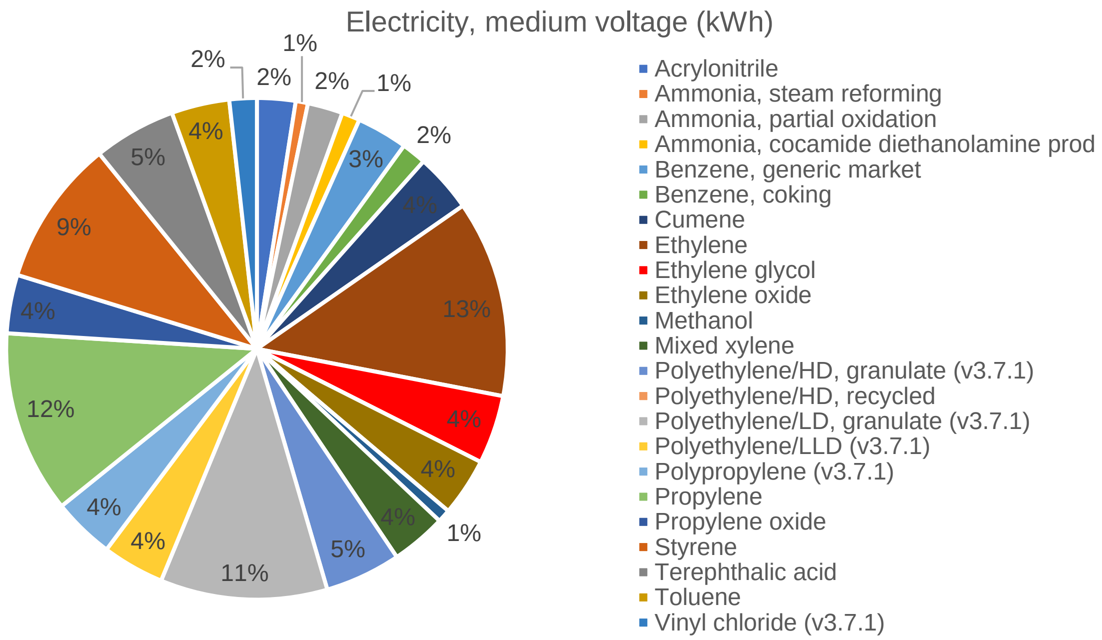


Fig. 5-19: Energy demand per process (for those processes for which ecoinvent did not provide infomatino on energy demand (i.e., benzene-generic market, xylene, ethylene, and propylene), LCIs have been collected from PlasticsEurope and Pozo et al., 2021).

5.2.2 GHG and nutrient emissions

Additionally, the production of propylene oxide through the chlorohydrin process has been individually studied to analyse the source of its CO_2 and N_2O emissions, as well as those of nitrates and phosphorus to surface waters (Fig. 5-20 and Fig. 5-21).

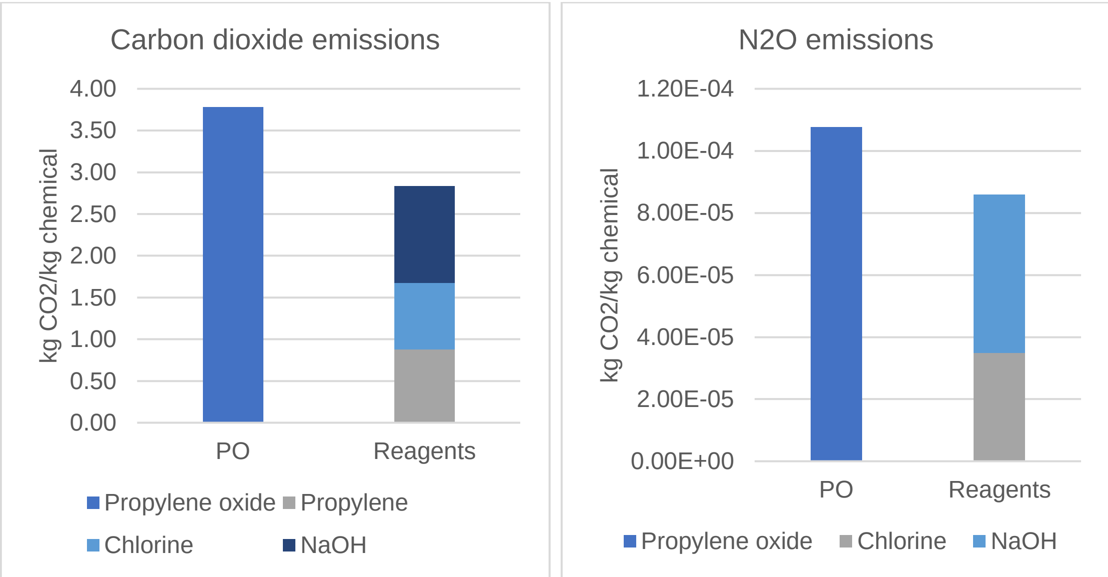


Fig. 5-20: Carbon dioxide and dinitrogen monoxide emissions per kg of chemical attributed to propylene oxide versus its baseline reagents (chlorine and sodium hydroxide in a 50% solution state).

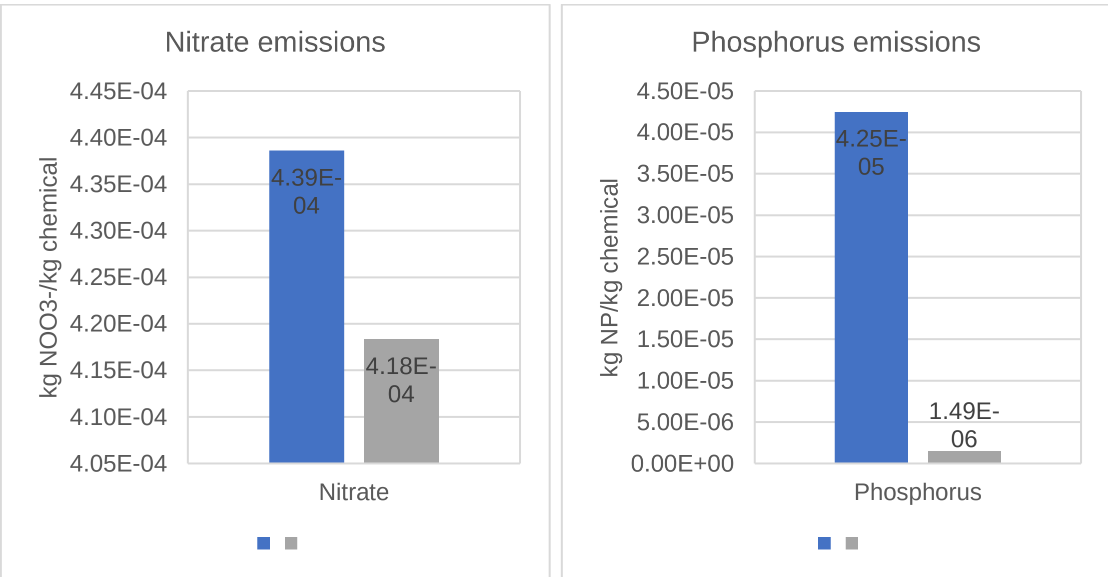


Fig. 5-21: Carbon dioxide and dinitrogen monoxide emissions per kg of chemical attributed to propylene oxide versus its baseline reagents (chlorine and sodium hydroxide in a 50% solution state).

5.2.3 Infrastructure

The necessity for a chemical plant is also considered as a possible origin for land use. Information for all chemicals for which data was available is presented in Fig. 5-22.

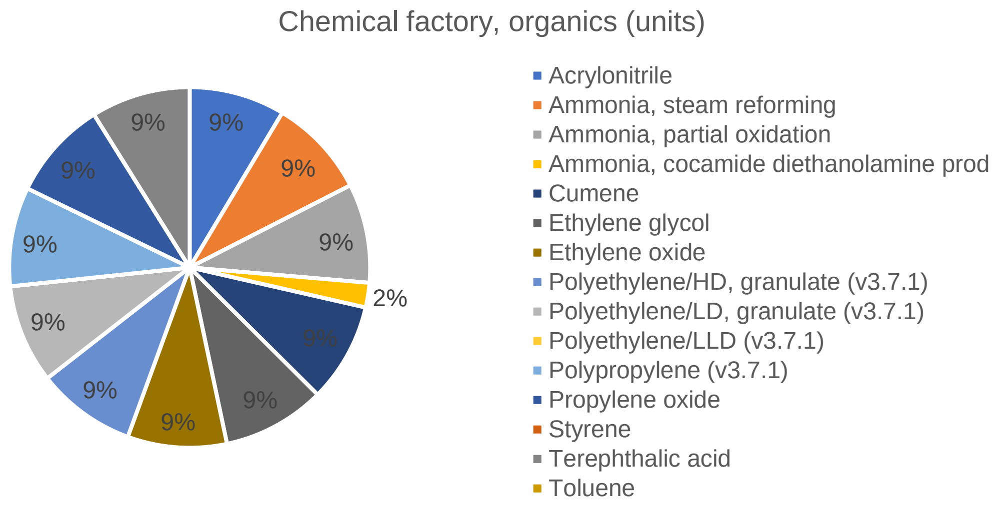


Fig. 5-22: Energy demand per process (some processes for which no information is available have been omitted: benzene, ethylene, toluene, recycled HDPE, methanol, propylene, and xylene).

5.2.4 Deforestation

The disturbed surface of forest was analysed for the reagents of the four chemicals which have the highest impact per kilogram of product (i.e., propylene oxide, terephthalic acid, acrylonitrile, and styrene) to determine the origin of the need for land use. Results are shown in Fig. 5-23.

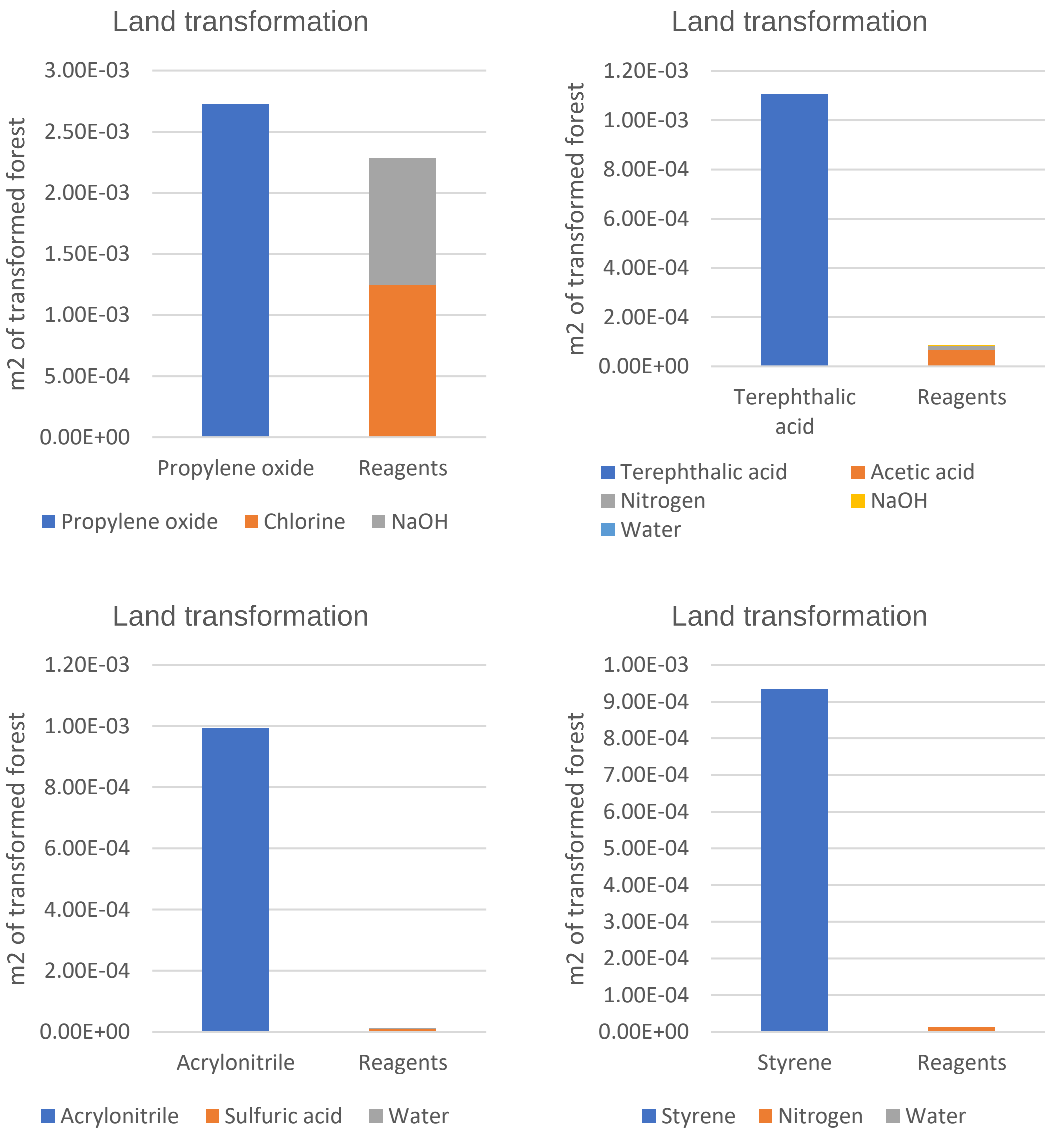


Fig. 5-23: Land transformation (m^2) per kg of chemical for the chemicals with the highest impact/kg product.

5.2.5 Aerosol emissions

For the aerosol loading boundary, the emissions for kg of chemical are highly homogeneous, and only propylene oxide and styrene present slightly higher pollution rates. The analysis of the fraction of these caused by the obtention of baseline reagents is analysed, with special importance given to the chlor-alkali process (Fig. 5-24).

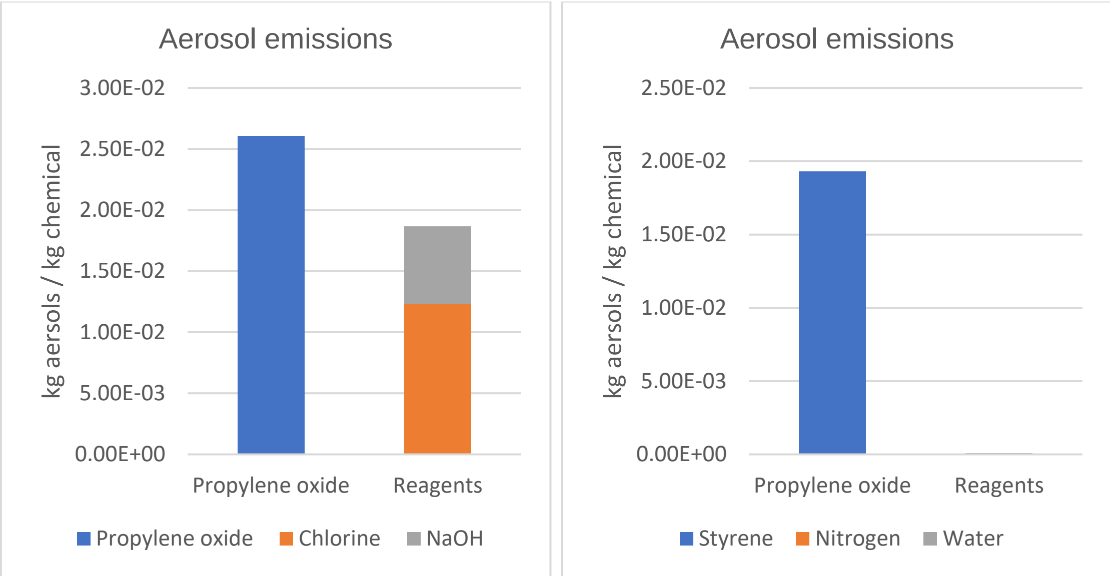


Fig. 5-24: Aerosol emissions (kg) per kg of chemical for propylene oxide and styrene (which show the highest emissions).

5.3 Scenarios

5.3.1 Energy mix

The technologies included as part of the renewable energy mix are presented in Table 5-1 along with the *ecoinvent* inventories used for their modelling.

Table 5-1: Activities conforming the renewable energy mix proposed in the scenarios section.

Technology	**Renewable mix (%)**	***Ecoinvent* activity name**
Coal	3.71	Electricity production, hard coal
Coal plant with CCS	2.57	Modelled individually
Natural gas	12.10	Electricity production, natural gas, combined cycle power plant
Natural gas plant with CCS	2.31	Modelled individually
Oil	0.51	Electricity production, oil
Nuclear	11.40	Electricity production, nuclear, pressure water reactor
Hydropower	18.00	Electricity production, hydro, reservoir, non-alpine region
Bioenergy	5.89	Heat and power co-generation, wood chips, 6667 kW, state-of- the-art 2014
Wind	21.50	Electricity production, wind, >3MW turbine, onshore
Solar photovoltaic	18.70	Electricity production, photovoltaic, 570kWp open ground installation, multi-Si
Geothermal	1.43	Electricity production, deep geothermal
Solar thermal	2.08	Electricity production, solar thermal parabolic trough, 50 MW

The plants involving CCS had to be modelled from basic inventory flows regulating the contribution of each of them in concordance with the inputs, outputs, and emissions of the plants, which were obtained from *Galán-Martín et al., 2021*. The adapted values to the production of 1 kWh in these plants are shown in Table 5-2 and Table 5-3 with the e*coinvent* datasets used in the study.

Table 5-2: Flux inventory for the production of 1 kWh in a coal plant with CCS.

	Amount (kg)	*Ecoinvent* activity name
Inputs		
Coal	6.72E-01	Market for hard coal
Natural gas	1.06E-03	Market for natural gas, liquid
Ammonia	1.48E-04	Market for ammonia, liquid
Limestone	5.56E-02	Market for limestone, crushed, washed
Sodium hydroxide	1.60E-04	Market for sodium hydroxide, without water, in 50% solution state
Solvent (MEA)	1.99E-04	Market for monoethanolamine
Fuel oil	8.03E-03	Market for light fuel oil
Outputs		
Hazardous waste	2.93E-03	Treatment of hazardous waste, underground deposit
Municipal waste	3.63E-03	Treatment of municipal solid waste, open dump, moist infiltration class (300mm)
Emissions		
Carbon dioxide	6.76E-02	
Sulfur dioxide	9.01E-05	
Nitrogen oxides	1.37E-03	
Ammonia	3.50E-04	
Particulates, <2.5	1.39E-04	
Monoethanolamine	1.10E-04	

In the cases where the datasets were available for the RER area, these have been selected. Otherwise, datasets labelled as GLO (global) or RoW (rest of world, when no or insufficient data is given for Europe, or when only data for non-European countries is provided) have been employed. The transport and storage of CO_2 in all scenarios involving carbon capture has been modelled using the fluxes described in Table 5-4.

Table 5-3: Flux inventory for the production of 1 kWh in a natural gas plant with CCS.

	Amount (kg)	***Ecoinvent* activity name**
Inputs		
Natural gas	1.48E-01	Market for natural gas, liquid
Water	3.28E-01	Market group for tap water
Rhodium catalyst	4.61E-08	Market for rhodium
Aluminium oxide catalyst	8.73E-07	Market for aluminium oxide
Solvent (MEA)	2.72E-03	Market for monoethanolamine
Outputs		
Catalysts	9.20E-07	Treatment of spent catalyst base from ethylene oxide production, residual material landfill
Wastewater	5.11E-04	Market for wastewater, average
Emissions		
Carbon dioxide	1.02E-01	

Table 5-4: Inventory of fluxes associated with the transport and storage of 1 kg of captured CO_2.

Inputs, CO_2 pipeline transportation	**Amount**	**Units**	***Ecoinvent* activity name**
Land occupation pipeline	4.22E-06	m^2yr	Occupation, construction
Land transformation pipeline	2.54E-06	m^2	Transformation, from forest, unspecified
Land transformation pipeline	2.54E-06	m^2	Transformation, to heterogeneous, agricultural
Water	2.37E-07	m^3	Water, unspecified natural origin
Diesel	4.20E-03	MJ	Diesel, burned in building machine, processing
Steel for pipelines	3.42E-04	kg	Market for steel, low-alloyed
Sand for filling	5.58E-03	kg	Market for sand
Assembly drawing of pipelines	3.42E-04	kg	Drawing of pipe, steel, processing

Table 5-4 (continued).

Stone wool	6.49E-06	kg	Stone wool production, packed
Monitoring by helicopter	3.30E-08	hr	Market for transport, helicopter
Monitoring by helicopter	1.32E-08	p	Market for transport, helicopter, LTO cycle
Transport materials	3.99E-04	tkm	Market for transport, freight, lorry 16-32 metric ton, euro6
Transport materials	6.99E-05	km	Market group for transport, freight train
Inputs, well double aquifer			
Land occupation well	2.29E-08	m^2yr	Occupation, industrial area
Land occupation well	2.06E-07	m^2yr	Occupation, industrial area, vegetation
Land occupation well	1.52E-08	m^2yr	Transformation, from grassland/pasture/meadow
Land occupation well	1-52E-9	m^2yr	Transformation, to an industrial area
Land occupation well	1.37E-08	m^2yr	Transformation, to an industrial area, vegetation
Well drilling	9.14E-08	m	Market for deep well, drilled, for geothermal power
Cement	3.20E-06	kg	Market for cement, unspecified
Gravel	3.35E-05	kg	Market for gravel, crushed
Transport of materials	7.34E-07	tkm	Market for transport, freight, lorry 16-32 metric ton, euro6
Transport of materials	3.20E-07	tkm	Market group for transport, freight train
Land occupation well	2.29E-08	m^2yr	Occupation, industrial area
Outputs, emissions to air			
Carbon dioxide	5.20E-05	kg	Carbon dioxide, fossil
Outputs, wastes			
Disposal land	5.58E-03	kg	Treatment of inert waste, inert material landfill
Dismantling and disposal pipelines	1.71E-04	kg	Treatment of, inert material landfill
Disposal rock wool	6.49E-06	kg	Treatment of waste mineral wool, inert material landfill

5.3.2 DACCS

The fluxes needed for the modelling of DAC are shown in Table 5-5. The transport and storage of CO_2 were included (Table 5-4).

Table 5-5: Flow inventory for the capture of 1 kg of CO_2 using DAC.

	Amount	**Units**	***Ecoinvent* activity name**
Inputs			
Carbon dioxide from air	7.69E-01	kg	Negative input
Natural gas	9.62E-02	kg	Market for natural gas, liquid
Electricity	2.82E-01	kWh	BAU and renewable mixes
Avoided electricity compression	1.02E-01	kWh	
Water	2.39E+00	kg	Market group for tap water
Calcium carbonate	1.53E-02	kg	Market for calcium carbonate, precipitated
Outputs			
Carbon dioxide	2.56E-02	kg	

5.3.3 BECCS

As for the capture of CO_2 through biomass, the inputs and outputs of the energy-production plant using CCS used for the modelling are found in Table 5-6. The transport of the captured CO_2 is included as well (Table 5-4). The data shown were already transformed to represent the capture of 1 kg of CO_2 and allocated to include the proportional fraction of impacts related to carbon capture.

Table 5-6: Flow inventory for the capture of 1 kg of CO_2 using BECCS.

	Amount	Units	*Ecoinvent* activity name
Inputs			
Electricity from wood chips	4.18E-01	kWh	Electricity, high voltage, heat and power co-generation, wood chips, 6667 kW
Carbon dioxide (biogenic) in wood chips	1.11E+00	kg	Negative input (fossil CO_2)
Outputs			
Metal working	1.81E-06	kg	Market for metal working, average for steel products
Concrete	1.38E-08	m3	Market for concrete, normal
Cooper	6.43E-08	kg	Market for cooper
Polyethylene	1.84E-07	kg	Market for polyethylene, low density, granulate
MEA solvent	2.28E-03	kg	Market for monoethanolamine
Concrete for compression unit	5.95E-10	m3	Market for concrete, normal
Metal for compression unit	5.95E-07	kg	Market for metal working, average for steel product manufacturing
Copper for compression unit	6.43E-08	kg	Market for copper
Polyethylene for compression unit	1.84E-07	kg	Market for polyethylene, low density, granulate
Diesel for MEA unit	1.82E-05	MJ	Market for diesel, burned in building machine
Electricity for MEA unit	5.61E-07	kWh	
Diesel for compression unit	1.82E-05	MJ	Market for diesel, burned in building machine

Table 5-6 (continued).

Electricity for compression unit	5.61E-07	kWh	Market for metal working, average for steel product manufacturing
Outputs, emissions to air			
Carbon dioxide biogenic	6.36E-02	kg	
Hydrogen sulfide	-6.87E-06	kg	
Hydrogen chloride	-6.29E-07	kg	
Ammonia	3.28E-05	kg	
Particulates, <2.5 um	9.76E-06	kg	
Nitrogen oxides	6.87E-06	kg	
Sulfur oxides	-3.22E-04	kg	
Methylamine	6.12E-09	kg	
Dimethylamine	4.49E-09	kg	
Ethylamine	4.49E-09	kg	
Diethylamine	2.17E-08	kg	
Monoethanolamine	3.03E-08	kg	
Diethanolamine	2.09E-09	kg	
Morpholine	8.68E-09	kg	
Formaldehyde	1.32E-07	kg	
Acetaldehyde	2.04E-06	kg	
Acetone	5.17E-07	kg	
Acetic acid	7.28E-08	kg	
Formamide	5.95E-08	kg	
Acetamide	8.44E-08	kg	
Carbon dioxide biogenic	1.66E-04	kg	

Table 5-6 (continued).

Outputs, wastes			
Solvent disposal	2.28E-03	kg	Treatment of hazardous waste, incineration (spent solvent mixture)

5.3.4 Green hydrogen

The production process of hydrogen from the electrolysis of water using wind energy is modelled according to the inventory presented in Table 5-7. The electricity required for the compression of H_2 to the feeding pressure in the synthesis processes is considered, as well as the energy consumption of the compression of H_2 for storage in tanks. Since wind energy is intermittent, the storage of a fraction of the produced hydrogen can ensure the functioning of the plant in continuous operation.

Table 5-7: Flow inventory for the production of 1 kg of green H_2.

	Amount	Units	*Ecoinvent* activity name
Inputs			
Water	11	kg	Market for water, deionised, from tap water, at user
Electricity	52.26	kWh	Market for electricity, high voltage, wind, >3MW turbine, onshore (GB)
Electricity for the preparation of H_2 (compression to 30 bars)	0.68	kWh	Market for electricity, high voltage, wind, >3MW turbine, onshore (GB)
Electricity for the storage of H_2 (compression to 200 bars for wind energy)	1.77	kWh	Market for electricity, high voltage, wind, >3MW turbine, onshore (GB)

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