CHANGE REPORT

cm.chemicals database – change report

Version 1.01, September 2022

carbonminds

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Content

1. Introduction

This document describes the cm.chemicals database changes when updating from V1.00 2021 to V1.01 2022. The document covers the introduction of new features of the cm.chemicals database, database-wide changes, changes in specific supply chains, and updates of modeling of specific chemical processes.

All changes described in this document are adapted to the complete cm.chemicals database, as well as to the Carbon Minds datasets in ILCD and SimaPro.CSV data formats. However, some changes have been adapted for particular datasets. These changes are described for each dataset.

2. New features

Chapter 2 describes database-wide new features of the updated cm.chemicals database. These include the introduction of biogenic carbon content calculations for every chemical and biogenic carbon emissions for every process. Moreover, the compliance of the methodology to generate the cm.chemicals database with the ISO standards 14040 and 14044 is reviewed by TÜV Rheinland Energy GmbH in an independent external review. Additionally, the CAS numbers of all chemicals included in the cm.chemicals database are updated using the official CAS Registry Numbers.

2.1 Biogenic carbon content and biogenic emissions

Biogenic emissions are greenhouse emissions that are based on a biological source. As an example, castor beans have a biogenic carbon content whereas fossil crude oil has a non-biogenic carbon content. This biogenic carbon content is based on the CO_2 emission (a biogenic emission) uptake during plant growth.

Due to the increased occurrence of biobased processes in the cm.chemicals database, a methodology has been developed to calculate the biogenic carbon content and biogenic carbon emissions of processes that are modeled in the core layer, extension layer, or simplified extension layer (cf. cm.chemicals database – methodology document). In our methodology, we subdivide the carbon dioxide, carbon monoxide, and methane emissions into biogenic carbon emissions and fossil carbon emissions, by tracking the carbon resources throughout the complete supply chain.

The methodology developed to calculate biogenic carbon contents and emissions includes five major steps:

1. For all chemicals, it is checked whether some of the raw materials are biobased. The biogenic carbon share is directly set to zero for all chemicals that are fully based on fossil raw materials and is set to one for all chemicals that are fully based on biogenic raw materials.

Example 1: The biogenic carbon share of carbon disulfide is directly set to 0 as it is produced from the raw materials natural gas and sulfur, which both have a completely fossil-based supply chain in our database.

Example 2: The biogenic carbon share of ethylamine is directly set to 1 as it is produced from the raw materials ethanol and ammonia. Ethanol, which has a completely bio-based supply chain in our database, supplies all carbon atoms for the ethylamine.

2. For all chemicals, which are partly based on biogenic raw materials, each chemical process is reviewed manually to quantify the percentage of carbon content originating from which raw material. This currently applies to around 5% of the chemicals in the cm.chemicals database, as the other 95% of the chemicals are either fully fossil-based or fully bio-based and thus do not need to be analyzed further.Example 1: Ethyl isothiocyanate is produced from ethylamine and carbon disulfide, thus it is partly based on fossil and partly based on biobased materials. Throughout a manual review, we find that 1/3 of the carbon is sourced from carbon disulfide, whereas 2/3 of the carbon is sourced from ethylamine (see table below).

Example 2: N,n-diethylthiourea is produced from ethyl isothiocyanate and ethylamine. Throughout a manual review, we find that 2/5 of the carbon is sourced from ethylamine, whereas 3/5 of the carbon is sourced from ethyl isothiocyanate (see table below).

				ethyl isothiocyanate process	n,n-diethylthiourea process
carbon disulfide	1	kg	CS2	-1/3	
ethylamine	1	kg	C2H7N	-2/3	-2/5
ethyl isothiocyanate	1	kg	C3H5NS	1	-3/5
n,n-diethylthiourea	1	kg	C5H12NS2		1

3. In the next step, a mathematical carbon supply chain model is built for the cm.chemicals database according to the mathematical calculation framework described in Section 4.5 of the cm.chemicals database methodology document.

Example: A small example of a matrix-based carbon supply chain model is shown in the table below. The carbon disulfide process and ethylamine process are aggregated because the biogenic carbon share was directly set in step 1.

	carbon disulfide process	ethylamine process	ethyl isothiocyanate process	n,n-diethylthiourea process
carbon disulfide	1		-1/3	
ethylamine		1	-2/3	-2/5
ethyl isothiocyanate			1	-3/5
n,n-diethylthiourea				1

4. After calculating the scaling vectors of the processes in the carbon supply chain model, as described in Section 4.5 of the cm.chemicals database methodology document, the biogenic and fossil carbon shares can be calculated by tracking the carbon atoms across the complete carbon supply chain. Moreover, the biogenic carbon content can be calculated by multiplying the carbon content with the previously calculated biogenic carbon share.

Example 1: For ethyl isothiocyanate, the scaling vectors of the carbon supply chain model are calculated (see table below). Afterwards the biogenic carbon share of ethyl isothiocyanate is calculated as follows: $\frac{1}{3} \cdot 0 + \frac{2}{3} \cdot 1 = 0.67$.

Example 2: For n,n-diethylthiourea, the scaling vectors of the carbon supply chain model are calculated (see table below). Afterwards the biogenic carbon share of n,n-diethylthiourea is calculated as follows: $\frac{1}{5} \cdot 0 + \frac{4}{5} \cdot 1 = 0.8$.

	ethyl isothiocyanate	n,n-diethylthiourea
carbon disulfide process	1/3	1/5
ethylamine process	2/3	4/5
ethyl isothiocyanate process	1	3/5
n,n-diethylthiourea process	0	1

5. Finally, based on the shares of biogenic and fossil carbon contents previously calculated in step 4, the carbon monoxide, carbon dioxide, and methane emissions to air are recalculated. Accordingly, emissions that were previously attributed to fossil emissions are now partly or fully attributed to biogenic emissions.

Due to the differentiation between biogenic and fossil carbon emissions in the cm.chemicals database, biogenic and fossil-based environmental impacts can be calculated. However, not all LCIA methods have characterization factors defined for biogenic emissions. Therefore, depending on the LCIA method, biogenic emissions can be taken into account or can be neglected. Thus, an LCIA method should be selected carefully in order to properly cover the desired scope of an LCA study. However, the definition of LCIA methods depends on the detailed scope of an LCA study and is out of the scope of the cm.chemicals database (cf. cm.chemicals database – methodology document).

LCIA methods commonly used to calculate carbon footprints, more specifically the global warming potential for 100 years, are listed in the table below. The table shows that the LCIA methods EF v2.0 2018, EF v3.0, and EF v3.0 EN15804 provide a distinction between fossil-based and biogenic carbon footprints which is necessary to meet the requirements of ISO 14067 for carbon footprint calculations. Moreover, the table lists other LCIA methods that can only be used for a total carbon footprint calculation and without any distinction between fossil-based and biogenic emissions.

LCIA method	**total CF**	**fossil-based CF**	**biogenic CF**
EF v2.0 2018	yes	yes	yes
EF v3.0	yes	yes	yes
EF v3.0 EN15804	yes	yes	yes
IPCC 2013	yes	no	no
ReCiPe Midpoint (H)	yes	no	no
ReCiPe Midpoint (H) V1.13	yes	no	no
CML v4.8 2016	yes	no	no
EDIP2003	yes	no	no
TRACI	yes	no	no

2.2TÜV review

To assure data quality, the compliance of the methodology to generate the cm.chemicals database with the ISO standards 14040 and 14044 is reviewed and certified by TÜV Rheinland Energy GmbH in an independent external review.

The review covers the check of methodological approaches, a selected sample of primary and secondary input data, the documentation, the qualification of our employees, the calculation model, and the check of a selected number of output datasets.

For more information on the review, you can also check the Annex of the cm.chemicals database methodology document. Alternatively, you can check the certificate database Certipedia of TÜV Rheinland by using the review ID 0000081021 (https://www.certipedia.com/quality_marks/0000081021?locale=en).

2.3 Updated CAS numbers

The CAS Registry Numbers have been updated for all chemicals and plastics included in the cm.chemicals database. This was done by using the official CAS Registry Numbers website (www.cas.org). This adds more value and usability to the database for customers, as they can easier find chemicals they are looking for using the most updated versions of CAS numbers.

3. Database-wide changes

This chapter describes database-wide changes. Database-wide changes occur from different database versions or databases used in the background of the modeling. Moreover, database-wide changes can occur from systematical changes in the methodology or changes in the modeling of raw materials at the beginning of the supply chain so that it affects the results of most other chemicals and plastics included in the database.

In the update from V1 2021 to V1 2022, only minor database-wide changes occurred. They are described in the following sections:

3.1 Background data

The ecoinvent database used in the background is changed from ecoinvent Version 3.7.1 to 3.8. Additionally, we also changed from the ecoinvent APOS system model to the ecoinvent cut-off model. This adds more consistency between our own modeling approach and ecoinvent's modeling approach.

Based on the update from ecoinvent Version 3.7.1 to 3.8, our own modeling and ecoinvent's modeling is more aligned in terms of time representativeness. Especially for the electricity markets, ecoinvent updates the reference year from 2017 to 2018 for most countries. In the case of US and Canada in Ecoinvent, the reference year is updated from 2018 to 2019 when updating from ecoinvent Version 3.7.1 to 3.8. Thus, this is more consistent with Carbon Minds current reference year 2019.

Moreover, due to the switch from the ecoinvent APOS system model to the ecoinvent cut-off model, our own modeling and ecoinvent's modeling is more aligned in terms of the allocation procedure. For both ecoinvent system models, APOS and cut-off, the way by-products are handled is the same and in accordance with the ISO 14040 and ISO 14044 standards. However, the allocation approach for waste differs between the APOS and the cut-off model. In the APOS model, the burdens associated to the treatment of the waste will be shared between all valuable products generated in the

value chain. Thus, the burdens of treating a waste will be shared between the producer of the waste and eventually other processes using products obtained from treating the waste. On the other hand, in the cut-off model, the burdens of treating a waste are associated to the producer of the waste only. As an exception, recyclable materials are treated as burden free. Thus, the ecoinvent cut-off approach is more consistent with Carbon Minds modeling approach and allocation procedure. However, the change of the ecoinvent system model is primarily relevant for end-of-life activities and therefore has only small impacts on the cradle-to-gate processes in the cm.chemicals database.

Furthermore, the modeling of natural gas as a background dataset provided by the ecoinvent 3.8 cut-off model has been extended: In addition to the ecoinvent process "market for natural gas, high pressure", the use of the ecoinvent process "market group for natural gas, high pressure" for modeling natural gas supply in the background of the cm.chemicals database is now also allowed. By also allowing the "market group for natural gas, high pressure" process, the cm.chemicals database has the option to choose three additional regional background datasets for natural gas: for Canada, Global, and Europe without Switzerland. By this means, the background data for natural gas can be even more regionalized, in line with the cm.chemicals database methodology.

3.2 Technology data

This data depicts the full mass and energy balances for each production technology. For instance, this data includes information about the raw material consumption, utilities (e.g., energy use), resource extractions, emissions, co-products, and waste consumption of the steam cracking of naphtha.

No updates were included compared to Version V1 2021 due to the Covid crisis in 2020. Thus, we still use the reference year 2019.

3.3 Market data

This data includes, for instance, how much ethylene is produced in Ludwigshafen via the steam cracking of naphtha. Furthermore, this data includes meta-information, like the company operating the plant (e.g., the BASF in Ludwigshafen) or the first year of operation.

No updates were included compared to Version V1 2021 due to the Covid crisis. Thus, we still use the reference year 2019.

3.4 Trade data

This data depicts, for instance, the imports of ethylene from the Netherlands to Germany. Including this data offers the possibility of understanding which chemical is traded between countries.

No updates were included compared to Version V1 2021 due to the Covid crisis in 2020. Thus, we still use the reference year 2019.

4. Updates and changes in datasets

4.1 Core layer

Some plant-specific datasets, supplier-specific datasets, and technology-specific datasets were excluded and partly moved to the extension layer to be methodologically consistent with regard to bio-based modeling (cf. Section 2.1). We expect to reverse these changes in future versions.

The changes in the core layer are listed in the table below. The percentage in the *plants* column represents the amount of plants that have been omitted or remodeled.

product	country	route	plants	comments
acetaldehyde	Colombia	Ethanol	7.7%	omitted
acetaldehyde	Indonesia	Ethanol	7.7%	omitted
acetaldehyde	Iran	Ethanol	7.7%	omitted
acetaldehyde	Sweden	Ethanol	7.7%	omitted
acetaldehyde	Taiwan, Province of China	Ethylene	7.7%	omitted
acetic acid	Colombia	Acetaldehyde	2.3%	omitted
acetic acid	Indonesia	Acetaldehyde	2.3%	omitted
acetic acid	Sweden	Acetaldehyde	2.3%	omitted
acetic acid	Switzerland	Acetaldehyde	2.3%	omitted
diethylene glycol	India	Ethylene Oxide	0.9%	omitted
epichlorohydrin	China	Glycerin	28.6%	remodeled in extension layer
epichlorohydrin	Czechia	Glycerin	2.9%	remodeled in extension layer
epichlorohydrin	France	Glycerin	2.9%	remodeled in extension layer
epichlorohydrin	Thailand	Glycerin	2.9%	remodeled in extension layer
ethyl acrylate	China	Ethyl Acrylate	30.0%	remodeled in extension layer
ethyl acrylate	Czechia	Ethyl Acrylate	5.0%	remodeled in extension layer
ethyl acrylate	France	Ethyl Acrylate	5.0%	remodeled in extension layer
ethyl acrylate	Germany	Ethyl Acrylate	5.0%	remodeled in extension layer
ethyl acrylate	India	Ethyl Acrylate	5.0%	remodeled in extension layer
ethyl acrylate	Indonesia	Ethyl Acrylate	5.0%	remodeled in extension layer
ethyl acrylate	Japan	Ethyl Acrylate	5.0%	remodeled in extension layer
ethyl acrylate	Republic of Korea	Ethyl Acrylate	5.0%	remodeled in extension layer
ethyl acrylate	Singapore	Ethyl Acrylate	5.0%	remodeled in extension layer
ethyl acrylate	Taiwan, Province of China	Ethyl Acrylate	10.0%	remodeled in extension layer
ethyl acrylate	United States	Ethyl Acrylate	20.0%	remodeled in extension layer
ethylene	Brazil	Ethanol	0.4%	omitted
ethylene	China	Ethanol	0.5%	omitted
ethylene	India	Ethanol	0.4%	omitted
ethylene	Taiwan, Province of China	Ethanol	0.2%	omitted
ethylene	United States	Ethanol	0.2%	omitted
ethylene dichloride	India	Ethylene/HCl	0.5%	omitted
ethylene glycol	India	Ethylene Oxide	0.7%	omitted
ethylene oxide	China	Ethylene	2.0%	omitted
ethylene oxide	India	Ethylene	0.7%	omitted
ethylene oxide	United States	Ethylene	0.7%	omitted
isobutanol	Colombia	Butyraldehyde	1.4%	omitted

n-butanol	Colombia	Butyraldehyde	2.0%	omitted
polyethylene (HD)	Taiwan, Province of China	Virgin Resin	0.4%	omitted
polyethylene (LD)	Taiwan, Province of China	Virgin Resin	0.6%	omitted
polyethylene (LLD)	Taiwan, Province of China	Virgin Resin	0.6%	omitted
polyvinyl chloride	India	Emulsion	0.3%	omitted
polyvinyl chloride	India	Suspension	0.3%	omitted
propylene glycol	Belgium	Glycerin	1.9%	omitted
propylene glycol	Poland	Glycerin	1.9%	omitted
propylene glycol	United States	Glycerin	1.9%	omitted
vinyl chloride	India	Edc	0.4%	omitted

4.2 Extension layer

The following chemicals and processes were remodeled in the extension layer:

process	included chemicals
hydrochlorination of glycerin	epichlorohydrin (from biomass)
esterification of acrylic acid with ethanol	ethyl acrylate

5. Updates in chemicals and plastics modeling

In some cases, process modeling errors have been identified, or processes were wrongly assigned to the corresponding production plants in the core layer of the database. In the update to V1 2022, these processes have been remodeled or reassigned correctly.

Moreover, for some processes, the allocation procedure for multifunctional processes was changed from allocation by energy content to allocation by mass to be more consistent with our methodology.

5.1 Adipic acid

For some adipic acid production plants, the process was reassigned to the respective production plant:

product	country	company	site	route
adipic acid	France	Alsachimie	Chalampe	Cyclohexane

For this plant, the technology was changed from hydrogenation and oxidation of benzene with nitric acid (95.5% N2O abatement) to hydrogenation and oxidation of benzene with nitric acid (99.5% N2O abatement).

product	country	company	site	route
adipic acid	United States	Ascend Performance Material	Pensacola/Fl	Cyclohexane

For this plant, the technology was changed from hydrogenation and oxidation of benzene with nitric acid (90% N2O abatement) to hydrogenation and oxidation of phenol with nitric acid (99.3% N2O abatement).

In both cases, the abatement rates have been found to be higher[1].

5.2 Isopropanol

All production plants using the processes "indirect hydration of propylene to isopropanol" and "direct hydration of propylene to isopropanol" were accidentally exchanged and thus wrongly assigned to the corresponding production plants. In the V1 2022 update, the assignment was redone so that the correct process was assigned to each production plant.

5.3 Ammonium sulfate

For the following processes, the allocation procedure was changed from allocation by energy content to allocation by mass. Allocation by energy content could not be applied because some co-products do not have a heating value. Thus, this adds more consistency to our methodology.

product	process name
ammonium sulfate	hydrogenation and oximation of phenol with hydroxylamine
ammonium sulfate	hydrogenation, oxidation and oximation of benzene with hydroxylamine
ammonium sulfate	oxidation, hydrogenation, and decarboxylation of toluene

5.4 Caprolactam

For the following processes, the allocation procedure was changed from allocation by energy content to allocation by mass. Allocation by energy content could not be applied because some co-products do not have a heating value. Thus, this adds more consistency to our methodology.

product	process name
caprolactam	hydrogenation and oximation of phenol with hydroxylamine
caprolactam	hydrogenation, oxidation and oximation of benzene with hydroxylamine
caprolactam	oxidation, hydrogenation, and decarboxylation of toluene

5.5 Chlorobenzene

For the following processes, the allocation procedure was changed from allocation by energy content to allocation by mass. Allocation by energy content could not be applied because some co-products do not have a heating value. Thus, this adds more consistency to our methodology.

product	process name
chlorobenzene	chlorination of benzene

[1] Bart, Jan C. J.; Cavallaro, Stefano (2015): Transiting from Adipic Acid to Bioadipic Acid. 1, Petroleum-Based Processes. In *Ind. Eng. Chem. Res.* 54 (1), pp. 1–46. DOI: 10.1021/ie5020734.

5.6 Epichlorohydrin

For the following processes, the allocation procedure was changed from allocation by energy content to allocation by mass. Allocation by energy content could not be applied because some co-products do not have a heating value. Thus, this adds more consistency to our methodology.

product	process name
epichlorohydrin	hydrochlorination of allyl chloride from propylene

5.7 Hydrochloric acid

For the following processes, the allocation procedure was changed from allocation by energy content to allocation by mass. Allocation by energy content could not be applied because some co-products do not have a heating value. Thus, this adds more consistency to our methodology.

product	process name
hydrochloric acid	chlorination of benzene
hydrochloric acid	cracking of EDC
hydrochloric acid	hydrochlorination of allyl chloride from propylene
hydrochloric acid	production of MDI by phosgenation (CO from coal)
hydrochloric acid	production of MDI by phosgenation (CO from NG)
hydrochloric acid	TDI production from toluene (CO from coal)
hydrochloric acid	TDI production from toluene (CO from natural gas)

5.8 Hydrogen

For the following processes, the allocation procedure was changed from allocation by energy content to allocation by mass. Allocation by energy content could not be applied because some co-products do not have a heating value. Thus, this adds more consistency to our methodology.

product	process name
hydrogen	production of MDI by phosgenation (CO from coal)
hydrogen	production of MDI by phosgenation (CO from NG)

5.9 Methane

For the following processes, the allocation procedure was changed from allocation by energy content to allocation by mass. Allocation by energy content could not be applied because some co-products do not have a heating value. Thus, this adds more consistency to our methodology.

product	process name
methane	production of MDI by phosgenation (CO from coal)
methane	production of MDI by phosgenation (CO from NG)
methane	TDI production from toluene (CO from coal)
methane	TDI production from toluene (CO from natural gas)

5.10 Methylene diphenyl diisocyanate

For the following processes, the allocation procedure was changed from allocation by energy content to allocation by mass. Allocation by energy content could not be applied because some co-products do not have a heating value. Thus, this adds more consistency to our methodology.

product	process name
methylene diphenyl diisocyanate	production of MDI by phosgenation (CO from coal)
methylene diphenyl diisocyanate	production of MDI by phosgenation (CO from NG)

5.11 Dichlorobenzenes

For the following processes, the allocation procedure was changed from allocation by energy content to allocation by mass. Allocation by energy content could not be applied because some co-products do not have a heating value. Thus, this adds more consistency to our methodology.

product	process name
o-dichlorobenzene	chlorination of benzene
p-dichlorobenzene	chlorination of benzene

5.12 O-toluenediamine

For the following processes, the allocation procedure was changed from allocation by energy content to allocation by mass. Allocation by energy content could not be applied because some co-products do not have a heating value. Thus, this adds more consistency to our methodology.

product	process name
o-toluenediamine	TDI production from toluene (CO from coal)
o-toluenediamine	TDI production from toluene (CO from natural gas)

5.13 Propylene dichloride

For the following processes, the allocation procedure was changed from allocation by energy content to allocation by mass. Allocation by energy content could not be applied because some co-products do not have a heating value. Thus, this adds more consistency to our methodology.

product	process name
propylene dichloride	hydrochlorination of allyl chloride from propylene

5.14 Sulfur

For the following processes, the allocation procedure was changed from allocation by energy content to allocation by mass. Allocation by energy content could not be applied because some co-products do not have a heating value. Thus, this adds more consistency to our methodology.

product	process name
sulfur	production of MDI by phosgenation (CO from coal)

sulfur	TDI production from toluene (CO from coal)

5.15 Toluene diisocyanate

For the following processes, the allocation procedure was changed from allocation by energy content to allocation by mass. Allocation by energy content could not be applied because some co-products do not have a heating value. Thus, this adds more consistency to our methodology.

product	process name
toluene diisocyanate	TDI production from toluene (CO from coal)
toluene diisocyanate	TDI production from toluene (CO from natural gas)

5.16 Vinyl chloride

For the following processes, the allocation procedure was changed from allocation by energy content to allocation by mass. Allocation by energy content could not be applied because some co-products do not have a heating value. Thus, this adds more consistency to our methodology.

product	process name
vinyl chloride	cracking of EDC