CHANGE REPORT

cm.chemicals database – change report

Version 2.01, March 2024

carbonminds

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Version 2.01 2024, Carbon Minds

Content

1. Introduction

This document describes the cm.chemicals database changes when updating from V2.00 2023 to V2.01 2024. The document covers new features of the cm.chemicals database, database-wide changes, and updates of modeling of specific chemical processes. The cm.chemicals methodology document Version 2.01 2024 is the corresponding document to this change report.

All changes described in this document are adapted to the complete cm.chemicals database and the Carbon Minds datasets in ILCD and SimaPro.CSV data formats.

2. New features

This chapter describes database-wide new features of the updated cm.chemicals database. These include the extended third-party review and recertification by TÜV Rheinland Energy & Environment GmbH, including the review of additional compliance with the UEIL/ATIEL methodology for Product Carbon Footprint (PCF) calculations of lubricants and other specialities . Moreover, additional reporting features of the datasets have been introduced to comply with the recently published Together for Sustainability (TfS) data model requirements.

2.1 Extended third-party review and certification

The cm.chemicals database methodology is designed to provide data for ISO 14040/14044 compliant LCA studies, ISO 14067 compliant PCF studies, PCF calculations compliant with the Together for Sustainability guideline for PCF, as well as PCF calculations compliant with the Product Life Cycle Accounting and Reporting Standard of the Greenhouse Gas (GHG) Protocol. Moreover, from the V2.01 2024 update, the cm.chemicals database methodology is additionally compliant with the UEIL/ATIEL methodology for PCF calculation of lubricants and other specialities.

The compliance of the methodology to generate the cm.chemicals database with the ISO standards 14040, 14044 and 14067, as well as with the TfS guideline for product carbon footprints and the GHG product standard, is recertified by TÜV Rheinland Energy & Environment GmbH in an independent external review. Additionally, the review by TÜV Rheinland Energy & Environment GmbH certifies the compliance of the methodology with the UEIL/ATIEL methodology for PCF calculations of lubricants and other specialities. 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. In the Annex B of the cm.chemicals methodology document, a copy of the Review Report by TÜV Rheinland Energy & Environment GmbH on the 'Critical Review of the Methodology for the LCI Database "cm.chemicals" by Carbon Minds' is attached.

2.2 Additional reporting features of the cm.chemicals datasets

In compliance with the recently published TfS data model requirements, additional reporting features have been introduced into the datasets of the cm.chemicals database:

- The documentation of the corresponding cm.chemicals methodology version in each dataset, for example cm.chemicals methodology V2.01 2024.
- The documentation of the background data version used in the background of the cm.chemicals database. Currently, ecoinvent 3.10 is used in the background.
- The documentation of the compliant standards and sector specific guidelines in each dataset.
- The documentation in each dataset whether packaging emissions are included in the system boundaries of the dataset or not. Currently, all cm.chemicals datasets exclude packaging emissions from the system boundaries.
- The more detailed documentation of cut-off criteria in each dataset: Next to the cut-off rules, it is now also specified for each dataset, which percentage of emissions resulted to be excluded from the PCF in total. To determine this, all known and quantifiable flows are taken into account.
- The documentation of the corresponding IPCC Assessment Report (AR) version, from which the characterization factors for PCF calculations are obtained. Currently, the used global warming potential characterization factors are compliant with IPCC AR6, published in 2021.
- For PCF datasets: The provision of PCF values calculated according to the "Carbon Minds ISO 14067 (based on IPCC 2021)" LCIA method, as well as the additional provision of PCF values calculated according to the "IPCC 2021" LCIA method. The "Carbon Minds ISO 14067 (based on IPCC 2021)" LCIA method is compliant with the "PCF (incl. biogenic emissions and removals)" as described in the reporting requirements of the TfS guideline. In addition, TfS outlines the "PCF (excl. biogenic emissions and removals)" in its reporting requirements. The "PCF (excl. biogenic emissions and removals)" is characterized by assigning the characterization factor of 0 to the biogenic CO_2 emissions and biogenic CO_2 removals. Furthermore, other biogenic GHG emissions, such as biogenic methane, are considered in the "PCF (excl. biogenic emissions and removals)". Thus, the "PCF (excl. biogenic emissions and removals)" is not compliant with the ISO 14067 standard. Nevertheless, the "PCF (excl. biogenic emissions and removals)" is aligned with the current PEF guidelines. Carbon Minds provides PCF values calculated according to both LCIA methods, such that LCA practitioners can choose the LCIA method that is most suitable for their LCA or PCF study.

3. Database-wide changes

This chapter describes database-wide changes. Database-wide changes occur from different database versions or input data used to update the reference year to 2022. Moreover, database-wide changes can occur from systematical changes in the methodology, e.g., different allocation approaches or changes in the modeling of raw materials at the beginning of the supply chain such that it affects the results of most other chemicals and plastics included in the database.

Database-wide changes occurred in the update from V2.00 2023 to V2.01 2024 regarding methodological changes and input data used. They are described in the following sections.

3.1 Background data

The ecoinvent database used in the background has been changed from ecoinvent Version 3.9.1 to 3.10. This adds more consistency between our modeling approach and ecoinvent's.

Due to the update from ecoinvent Version 3.9.1 to 3.10, our modeling and ecoinvent's modeling are more aligned regarding time representativeness. Especially for the electricity markets, ecoinvent updates the reference year to 2020 or 2021 for most countries, which is more in line with cm.chemicals' current reference year of 2022.

Furthermore, the background data for natural gas and crude oil, which incorporates the latest scientific findings regarding gas flaring, venting, and fugitive emissions, is maintained up-to-date through the use of data from ecoinvent 3.10 and Energie-Stoffe-Umwelt (ESU).

3.1.1 Natural gas supply

The modeling of natural gas as a background dataset provided by the ecoinvent 3.10 cut-off model is based on the same modeling approach as in version 3.9.1 but has been updated regarding time and geographical representativeness[1]. Ecoinvent's modeling is based on the life cycle inventories of crude oil and natural gas extraction, published by Energie-Stoffe-Umwelt (ESU)[2]. As a result, the geographical coverage of natural gas production and supply has expanded by additional thirteen (13) regions, resulting in a total of fifty-nine (59) available countries and regions for the ecoinvent process "market for natural gas, high pressure". Moreover, these datasets are updated regarding time representativeness, now reflecting international trade statistics for the average of the years 2019 to 2021.

3.1.2 Ethane, propane, n-butane, isobutane, and n-pentane supply

Ethane, propane, n-butane, isobutane, and n-pentane have been modeled in the background of the cm.chemicals database, ensuring that the chemical feedstock is

[1] Documentation of changes implemented in the ecoinvent database v3.10 (2023.11.28)

[2] Christoph Meili; Niels Jungbluth; Maresa Bussa (2023). Life cycle inventories of crude oil and natural gas extraction. ESU-services Ltd. Commissioned by ecoinvent & Carbon Minds, Schaffhausen, Switzerland. The detailed report is available upon request (info@carbon-minds.com)

modeled based on the latest scientific findings. Note that these datasets are not sold but modeled as background data to ensure high quality of the chemical datasets.

Compared to V2.00 2023, the modeling has improved by using a higher regionalized supply of the raw material natural gas to produce ethane, propane, n-butane, isobutane, and n-pentane (see section 3.1.1 for further details on natural gas).

3.2 Technology data

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

Updates were included for some technology data points compared to Version V2.00 2023. Thus, the reference year of this data is 2020 to 2022.

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.

The market data has been updated to the reference year 2022.

3.4 Trade data

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

The trade data has been updated to the reference year 2022.

3.5 Systematic methodological changes

As the cm.chemicals methodology remains compliant with the ISO standards 14040, 14044, and 14067, as well as with the TfS guideline, no systematic methodological changes have been introduced in the V2.01 2024 update.

To additionally comply with the UEIL/ATIEL methodology for PCF calculations of lubricants and other specialities, no systematic methodological changes needed to be introduced, as the methodologies are already compliant. In particular, the allocation procedure of the cm.chemicals methodology, described in Section 4.3 of the cm.chemicals methodology document, aligns with the allocation hierarchy described in the UEIL/ATIEL methodology for PCF calculations of lubricants and other specialities. In the lubricant industry, the ratio between the economic values of products and co-products of blending processes is characterized by a value lower than 5. Consequently, these products and co-products are not allocated by price, but by mass. Note that due to this characteristic, the allocation of the production of lube base stock (type I) process has been changed to mass allocation in the cm.chemicals database V2.01 2024 (for further details, please refer to Section 4.1).

3.6 Carbon Minds LCIA method update

The "Carbon Minds ISO 14067 (based on IPCC 2021)" LCIA method, which has been implemented in V2.00 2023, has been updated in V2.01 2024.

The elementary flow nomenclature has been adapted to the general elementary flow nomenclature update, which is line with the ecoinvent elementary flow nomenclature of ecoinvent 3.10. Moreover, three elementary flows have been additionally characterized for the "Carbon Minds ISO 14067 (based on IPCC 2021)" LCIA method:

- Chloro-fluoromethane
- Difluoromethane
- Perfluoropentane

For more details on the LCIA method, see Section 3.2.4 of the cm.chemicals methodology document.

4. Updates and changes in datasets

This section describes the updates and changes for specific datasets. Additionally, Annex A. List of changed chemicals and process names lists all chemical and process names that were changed from Version 2.00 2023 to 2.01 2024.

4.1 Geographical update of datasets

Datasets formerly reflecting the region of "Serbia and Montenegro" have been updated to individually reflect the countries "Serbia" and "Montenegro".

4.2 Update of core layer datasets

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

- **Base oil (type I):** The allocation procedure for the process "*production of lube base stock type I*" was changed from price allocation to mass allocation. As base oils are used to manufacture lubricating oils, greases, and other specialities, and are not relevant in the chemical industry, they should be allocated according to the allocation procedure described in the UEIL/ATIEL methodology for PCF calculations of lubricants and other specialities. According to the UEIL/ATIEL methodology, allocation based on mass shall be applied. See Section 4.3 of the cm.chemicals methodology document for more details on allocation.
- **Acetic acid:** The allocation procedure for the process "*carbonylation of methanol with coal-based CO (average process of 8% Cativa, 31% Celanese, and 61% Monsanto)*" was changed from price allocation to energy content allocation, due to the existing hydrogen co-product (see Section 4.3 of the cm.chemicals methodology document for more details on allocation).
- **Acetic acid:** The allocation procedure for the process "*carbonylation of methanol with coal-based CO (Cativa)*" was changed from price allocation to energy content allocation, due to the existing hydrogen co-product (see Section 4.3 of the cm.chemicals methodology document for more details on allocation).
- **Acetic acid:** The allocation procedure for the process "*carbonylation of methanol with coal-based CO (Celanese)*" was changed from price allocation to energy content allocation, due to the existing hydrogen co-product (see Section 4.3 of the cm.chemicals methodology document for more details on allocation).

4.3 Update of extension layer datasets

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

- **White oil (technical grade):** The supply chain of the dataset for the production of white oil (technical grade) has been changed to reflect a more industry representative supply chain. According to industry experts, white oil (technical grade) is mainly produced on the basis of base oil (type I). Thus, the old dataset "*catalytic hydrotreating of vacuum gas oil*" is now exchanged with the new dataset "*catalytic hydrotreating of base oil (type I)*".

- **Stripped oil:** Stripped oil is a co-product of white oil production. The supply chain of the dataset for the production of white oil (technical grade) has been changed to reflect a more industry representative supply chain. Therefore, the supply chain of stripped oil has also been changed. Thus, the old dataset "*catalytic hydrotreating of vacuum gas oil*" is now exchanged with the new dataset "*catalytic hydrotreating of base oil (type I)*".
- **Paraffin wax:** Paraffin wax is a co-product of base oil (type I) production. The allocation procedure for the process "*production of lube base stock type I*" was changed from price allocation to mass allocation (see Section 4.2 for more details).
- **Isobutylene, high purity:** The emissions due to direct emissions, energy recovery, and waste treatment were corrected for the process "*high purity isobutylene from MTBE cracking*".

4.4 Update of simplified extension layer datasets

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

- **Methyl formate:** The allocation procedure for the process "*carbonylation of methanol*" was changed from price allocation to energy content allocation, due to the existing hydrogen co-product (see Section 4.3 of the cm.chemicals methodology document for more details on allocation).
- **Amyl ethyl ketone:** The allocation procedure for the process "*reaction of 2-butanol*" was changed from price allocation to energy content allocation, due to the existing hydrogen co-product (see Section 4.3 of the cm.chemicals methodology document for more details on allocation).
- **Methyl ethyl ketone (butanol-based):** The allocation procedure for the process "*reaction of 2-butanol*" was changed from price allocation to energy content allocation, due to the existing hydrogen co-product (see Section 4.3 of the cm.chemicals methodology document for more details on allocation).
- **Alpha-methyl styrene:** The allocation procedure for the process "*dehydrogenation of cumene*" was changed from price allocation to energy content allocation, due to the existing hydrogen co-product (see Section 4.3 of the cm.chemicals methodology document for more details on allocation).
- **N-(2,3-Dichloro-phenyl)acetamide:** The production process has been corrected and remodeled by substituting acetic acid with acetic anhydride as the raw material. The process name has changed accordingly from "*reaction of 2,3-dichloroaniline and acetic acid*" to "*reaction of 2,3-dichloroaniline and acetic anhydride*".
- **N-(4-fluorophenyl)acetamide:** The production process has been corrected and remodeled by substituting acetic acid with acetic anhydride as the raw material. The process name has changed accordingly from "*reaction of p-fluoroaniline and acetic acid*" to "*reaction of p-fluoroaniline and acetic anhydride*".
- **Hexamethylene diisocyanate homopolymer (30 hexamethylene diisocyanate units):** The "*reaction of hexamethylene diisocyanate*" process has been remodeled from 100 to 30 hexamethylene diisocyanate units. The product name has

changed accordingly from "*hexamethylene diisocyanate homopolymer (100 hexamethylene diisocyanate units)*" to "*hexamethylene diisocyanate homopolymer (30 hexamethylene diisocyanate units*".

- **Methyl hydrogen sulfate:** The "*hydrolysis of dimethyl sulfate*" process has been corrected by adding the co-product methanol to the process. As a consequence, the "*hydrolysis of dimethyl sulfate*" is now a multifunctional process, leading to the decision of price allocation (see Section 4.3 of the cm.chemicals methodology document for more details on allocation).
- **Sulfur dichloride:** The "reaction of sulfur and chlorine" process was corrected since the chlorine demand was previously overestimated.

Annexes

Annex A. List of changed chemicals and process names

This annex lists all chemical and process names that were changed from Version 2.00 2023 to 2.01 2024.

old product name	old process name	new product name	new process name
Changes in the extension layer			
white oil (technical grade)	catalytic hydrotreating of vacuum gas oil	white oil (technical grade)	catalytic hydrotreating of base oil (type I)
stripped oil	catalytic hydrotreating of vacuum gas oil	stripped oil	catalytic hydrotreating of base oil (type I)
phosphoric acid (as P2O5)	themal oxidation reaction of phosphorus	phosphoric acid (as P2O5)	thermal oxidation reaction of phosphorus
hydrogen peroxide	anthraquinone process	hydrogen peroxide	anthraquinone process (production of 70% hydrogen peroxide)
Changes in the simplified extension layer			
hexamethylene diisocyanate homopolymer (100 hexamethylene diisocyanate units)	reaction of hexamethylene diisocyanate	hexamethylene diisocyanate homopolymer (30 hexamethylene diisocyanate units)	reaction of hexamethylene diisocyanate
N-(4-fluorophenyl)acetamide	reaction of p-fluoroaniline and acetic acid	N-(4-fluorophenyl)acetamide	reaction of p-fluoroaniline and acetic anhydride
N-(2,3-Dichlorophenyl)acetamide	reaction of 2,3-dichloroaniline and acetic acid	N-(2,3-Dichlorophenyl)acetamide	reaction of 2,3-dichloroaniline and acetic anhydride