CHANGE REPORT

cm.chemicals database – change report

Version 2.00, July 2023

Authors:

Laura Stellner, Aline Kalousdian, Dr. Raoul Meys

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carbonminds

www.carbon-minds.com

https://www.linkedin.com/company/carbon-minds

For more information, you can contact us.

info@carbon-minds.com

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Content

1. Introduction

This document describes the cm.chemicals database changes when updating from V1.01 2022 to V2.00 2023. 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 2.00 2023 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 GmbH, including the review of compliance with the Together for Sustainability (TfS) guideline for Product Carbon Footprint calculations. Moreover, additional reporting features of the datasets have been introduced to comply with the TfS guideline. Additionally, Carbon Minds developed an LCIA method compliant with ISO 14067 and the TfS guideline.

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 (TfS) guideline for product carbon footprints, as well as PCF calculations compliant with the Product Life Cycle Accounting and Reporting Standard of the Greenhouse Gas (GHG) Protocol. The compliance of the methodology to generate the cm.chemicals database with the ISO standards 14040, 14044 and 14067 is reviewed by TÜV Rheinland Energy GmbH in an independent external review. Additionally, the review by TÜV Rheinland Energy GmbH certifies the compliance of the methodology with the TfS guideline for product carbon footprints and the GHG product standard. 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 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 TfS guideline, additional reporting features have been introduced into the datasets of the cm.chemicals database:

- The cm.chemicals datasets now additionally report the data quality according to the TfS guideline's data quality indicators and levels while keeping the data quality indicators and levels defined by Carbon Minds (cf. Section 5.2 in the cm.chemicals methodology document). As a result, the database user has the option to choose between the TfS and Carbon Minds data quality indicators and levels, when performing their LCA/PCF calculation.

- The cm.chemicals datasets now report the data quality rating (DQR) calculated according to the TfS guideline (cf. Section 3.3.2 in the cm.chemicals methodology document).
- The cm.chemicals datasets now report the primary data share (PDS) calculated according to the TfS guideline (cf. Section 5.2.3 in the cm.chemicals methodology document).
- For technology-specific and plant-specific datasets (cf. Section 2.3 in the cm.chemicals methodology document), the applied allocation method for the technology used is defined in more detail.
- In addition to the biogenic carbon content, the cm.chemicals datasets now report the total carbon content of the respective reference flow.

2.3 Implementation of IPCC 2021 characterization factors for carbon footprints

When LCA practitioners use the cm.chemicals database to calculate product carbon footprints according to ISO 14067 or according to the TfS guideline, additional LCIA methods requirements must be considered. Due to the required additional specifications, we have implemented the latest IPCC 2021 characterization factors in compliance with ISO 14067 and the TfS guideline in the new LCIA method "Carbon Minds ISO 14067 (based on IPCC 2021)". The LCIA method follows the following principles:

- The 100-year GWP characterization factors (GWP 100a) are used in kg CO_2-eq per kg emission.
- The GWP 100a characterization factors are derived from the latest values reported by the Intergovernmental Panel on Climate Change (IPCC).
- The latest values available are based on IPCC's Sixth Assessment Report (AR6). Annex A of the cm.chemicals methodology document provides a detailed list of the characterization factors according to IPCC's AR 6.
- The developed LCIA method excludes the assessment of short-living climate forces.
- To accurately assess biogenic carbon, the removals of CO_2 into biomass are characterized as -1 kg CO_2-eq per kg CO_2. The emissions of biogenic CO_2 are characterized as +1 kg CO_2-eq per kg CO_2.
- The developed LCIA method can separately account for fossil GHG emissions, biogenic GHG emissions, biogenic GHG removals, as well as emissions and removals resulting from land use change in order to support the separate documentation of specific GHG emissions (cf. Table 1).

The additional reporting of GHG emissions due to aircraft transportation, as required in ISO 14067, is neglected in this methodology since aircraft transportation in the chemical value chain is neglectable.

Table 1: Implemented LCIA method for product carbon footprint calculations according to ISO 14067.

Item	Method	Impact	Indicator	Comment
1	Carbon Minds ISO 14067 (based on IPCC 2021)	climate change	GWP 100a	Including all GHG emissions. Sum of Items 2, 3, 4, and 5.
2	Carbon Minds ISO 14067 (based on IPCC 2021)	climate change: fossil	GWP 100a	Including only fossil GHG emissions.
3	Carbon Minds ISO 14067 (based on IPCC 2021)	climate change: biogenic emissions	GWP 100a	Including only biogenic GHG emissions.
4	Carbon Minds ISO 14067 (based on IPCC 2021)	climate change: biogenic removal	GWP 100a	Including only biogenic GHG removals.
5	Carbon Minds ISO 14067 (based on IPCC 2021)	climate change: land use	GWP 100a	Including only emissions and removals resulting from land use change.

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 2021. 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.

Major database-wide changes occurred in the update from V1.01 2022 to V2.00 2023 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 3.8 to 3.9.1. This adds more consistency between our modeling approach and ecoinvent's.

Due to the update from ecoinvent Version 3.8 to 3.9.1, our modeling and ecoinvent's modeling are more aligned regarding time representativeness. Especially for the electricity markets, ecoinvent updates the reference year to 2019 or 2020 for most countries, which is more in line with cm.chemicals' current reference year of 2021.

Moreover, to maintain the cm.chemicals database at the highest scientific standards, we have implemented the latest scientific findings regarding gas flaring, venting, and fugitive emissions by incorporating the updated background datasets of ecoinvent 3.9.1 and ESU-services Ltd. This is described in more detail in the following sections.

3.1.1 Natural gas supply

The modeling of natural gas as a background dataset provided by the ecoinvent 3.9.1 cut-off model has been updated regarding technical and geographical representativeness[1]. The technical representativeness includes incorporating the latest scientific findings regarding gas flaring, venting, and fugitive emissions. The geographical representativeness has been extended to cover nineteen (19) additional regions for the ecoinvent process "market for natural gas, high pressure", resulting in a total of forty-six (46) regions. By this means, the background data for natural gas can be even more regionalized, in line with the cm.chemicals database methodology. These datasets are calculated based on national data and international trade statistics for 2019.

3.1.2 Crude oil supply

The geographical representativeness of crude oil supply is essential, in particular, when modeling the chemical value chain. Therefore, Energie-Stoffe-Umwelt (ESU) was com-

[1] Documentation of changes implemented in the ecoinvent database v3.9 (2022.10.13)

missioned by ecoinvent and Carbon Minds to expand the geographical representativeness of crude oil supply[2]. As a result, a total of thirty-five (35) country and regional-specific "market for petroleum" processes have been generated. By this means, the background data for crude oil can be even more regionalized, in line with the cm.chemicals database methodology. These datasets are calculated based on international trade statistics for 2021.

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

The modeling is improved by using more regionalized raw materials (e.g., natural gas and crude oil) and energy market supply to produce ethane, propane, n-butane, isobutane, and n-pentane.

3.1.4 Naphtha and LPG supply

The modeling is improved by using more regionalized raw materials (e.g., natural gas and crude oil) and energy market supply to naphtha and liquefied petroleum gas (LPG).

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 V1.01 2022. 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 2021.

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 2021.

[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)

3.5 Systematic methodological changes

This update introduces systematic changes in the cm.chemicals methodology to achieve methodological compliance with ISO 14067 and the TfS guideline. The major methodological changes include a more detailed modeling of precious metal catalysts and a more precise definition of the system boundaries in the cm.chemicals methodology document. Moreover, our allocation approach to solving multifunctionality complies with the TfS guideline and ISO 14067.

3.5.1 System boundaries and cut-offs

The system boundaries have been defined more clearly in the cm.chemicals methodology document (cf. Section 3.2.2) to be more transparent about the included and excluded parts of the chemical's cradle-to-gate life cycle compliant with the TfS guideline.

Specifically, the inclusion and exclusion of transportation activities is discussed in more detail in the methodology document. For chemical products in the core layer, the system boundary includes upstream transportation services related to international trade. For chemical products in the extension layer, upstream transportation is only considered for those core layer chemical products which are part of the value chain of extension layer chemical product. Additionally, for consumption mix datasets, downstream transportation is included since the location of the supply of the chemical product is known. For other datasets in the cm.chemicals database, downstream transportation is excluded and might need to be added by the user of the dataset depending on their specific application.

Moreover, consumed precious metal catalysts are now included in the system boundaries of the cm.chemicals datasets (cf. Section 3.2.2. in the cm.chemicals methodology document). Furthermore, the cut-off criteria are not applied to consumed precious metal catalysts with high environmental impacts, as their contribution to the total environmental impacts of the respective process is usually not neglectable. To ensure the correct calculation of environmental impacts of the respective process, the loss of precious metal catalysts with an environmental impact equal to the environmental impact of the respective virgin catalyst is considered (cf. Section 3.2.3 in the cm.chemicals methodology document).

Precious metal catalysts have been added to modeling the following processes as shown in the table below.

Process name	Main product name
Changes in the core layer	
acetoxylation of butadiene	1,4-butanediol
propylene oxide isomerization and hydroformulation	1,4-butanediol
carbonylation of methanol with coal-based CO (average process of 8% Cativa, 31% Celanese, and 61% Monsanto)	acetic acid
carbonylation of methanol with coal-based CO (Monsanto)	acetic acid
carbonylation of methanol with natural gas-based CO (average process of 8% Cativa, 31% Celanese, and 61% Monsanto)	acetic acid
carbonylation of methanol with natural gas-based CO (Monsanto)	acetic acid
oxidation of ethanol via acetaldehyde	acetic acid
oxidation of ethylene via acetaldehyde	acetic acid
oxidation and esterification of isobutylene	methyl methacrylate
oxidation of p-xylene (Amoco)	terephthalic acid
oxidation of p-xylene (average process of 36% Invista, 4% Mitsubishi, 5% BP, 2% Eastman, and 13% Amoco)	terephthalic acid
oxidation of p-xylene (Invista)	terephthalic acid
oxidation of p-xylene (Mitsubishi)	terephthalic acid
TDI production from toluene (CO from coal)	toluene diisocyanate
TDI production from toluene (CO from natural gas)	toluene diisocyanate
acetoxylation of ethylene with acetic acid and oxygen	vinyl acetate
Changes in the extension layer	
hydrogenation of dimethyl terephthalate (DMT)	1,4-cyclohexanedimethanol
chlorination of acetic acid	chloroacetic acid
cataltic reduction of ammonia, oxygen, hydrogen and sulfuric acid	hydroxylammonium sulfate
catalytic air oxidation of m-xylene	isophthalic acid
hydrogenation and hydroformation of propylene	n-butyraldehyde
hydroformylation of C4 olefins	n-valeraldehyde
hydrogenation of o-nitrochlorobenzene	o-phenylenediamine
TDI production from toluene (CO from natural gas)	o-toluenediamine

3.5.2 Solving multifunctionality (allocation procedure)

The ISO standard 14044 has defined a hierarchy among the methodological approaches to guide the selection of methodological approaches. In this version and previous versions of the cm.chemicals database, we apply this hierarchy to all multifunctionality problems.

However, in case multifunctionality problems are solved according to other allocation criteria – which is the last step of the allocation hierarchy – we have updated our approach to be compliant with the TfS guideline (cf. Section 4.3 in the cm.chemicals methodology document). If allocation according to other criteria is applied, we allocate the environmental exchanges of the process and its supply chain in proportion to the mass or price of the products. The decision criteria on whether to use allocation based on mass or price are defined according to the proposition of the World Business

Council for Sustainable Development (WBCSD)[3]. If the ratio of the economic values of the products and co-products is greater than 5, allocation based on price shall be used. Otherwise, allocation based on mass content shall be used. An update process for the chemical prices is yet to be established. If a co-product comprises less than 1% (by mass or volume), it can be excluded from allocation method decisions.

Moreover, specific allocation procedures have been introduced according to the TfS guideline (cf. Section 4.3 in the cm.chemicals methodology document). Specific allocation procedures to solve multifunctionality are:

- For processes that co-produce hydrogen, allocation based on energy content shall be applied unless one or more products have an energy content of zero. In that case, allocation according to other criteria (mass or price) is applied.

- For processes that co-produce CO_2, the system expansion via avoided burden approach is applied. An avoided operation of the Direct Air Capture process is assumed for the avoided burden. To model the Direct Air Capture, the following assumptions are made[4]:
    - 2.52 MJ electricity is consumed per kg captured CO_2.
    - 4.74 MJ electricity is consumed for the provision of low temperature heat.
    - 0.02 kg CO_2-eq per kg captured CO_2 are emitted to account for the CO_2 losses during Direct Air Capture.
    - In the Direct Air Capture process, the modeled CO_2 uptake from the atmosphere is considered by the elementary flow "carbon dioxide, in air" in the compartment "resource, in air". However, this elementary flow is typically used to model CO_2 uptakes due to biomass growth, which is why this elementary flow is taken into account in the biogenic part of product carbon footprint calculations. This leads to a negative biogenic carbon footprint for the DAC-process. For instance, this leads to a positive biogenic carbon footprint for the ammonia pro-cesses with CO_2-capture, as the avoided burden approach (avoided operation of the Direct Air Capture process) is applied.

- For the following processes, allocation according to the official Product Category Rule (PCR), *Plastics Europe's recommendation on Steam Cracker allocation*[5], is applied:
    - Steam cracking of naphtha
    - Steam cracking of LPG
    - Steam cracking of ethane
    - Steam cracking of atmospheric gas oil
    - Steam cracking of vacuum gas oil

[3] WBCSD, 2014. Lifecycle Metrics for Chemical Products. A guideline by the chemical sector to assess and report on the environmental footprint of products, based on life cycle assessment.
[4] The Assumptions are based on: Deutz, S. and Bardow, A., 2021. Life-cycle assessment of an industrial direct air capture process based on temperature–vacuum swing adsorption. Nat Energy 6.
[5] Life Cycle and Sustainability working group of PlasticsEurope, 2017. PlasticsEurope recommendation on Steam Cracker allocation.

- For the following processes, allocation according to the official Product Category Rule (PCR), *The Chlor-Alkali Process by Euro Chlor*[6], is applied:
    - Electrolysis of NaCl in mercury cells
    - Electrolysis of NaCl in diaphragm cells
    - Electrolysis of NaCl in membrane cells

- For the following processes, allocation according to the official Product Category Rule (PCR), *Toluene Diisocyanate (TDI) & Methylenediphenyl Diisocyanate (MDI), Eco-profiles and Environmental Product Declaration of the European Plastic Manufacturers by ISOPA*[7], is applied:
    - production of MDI by phosgenation
    - TDI production from toluene
    - hydrogenation of methylenedianiline

- In the TfS guideline, allocation according to the official Product Category Rules (PCR) from the *Surfactant Life Cycle and Ecofootprinting Project by ERASM*[8] shall be applied for C12-14 fatty alcohols (oleo), methyl esters, as well as refined and crude oils from palm oil and coconut oil. As these products are currently not covered in the cm.chemicals database, the PCRs by ERASM are not implemented in this methodology.

Potential deviations from this approach are illustrated in the metadata of the respective dataset.

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[6] Euro Chlor, 2022. Chlorine (The Chlor-Alkali Process). An Eco-profile and Environmental Product Declaration of the European Chlor-Alkali Industry. Final report.
[7] ISOPA, 2012. Toluene Diisocyanate (TDI) & Methylenediphenyl Diisocyanate (MDI). Eco-profiles and Environmental Product Declaration of the European Plastic Manufacturers.
[8] ERASM, 2014. Surfactant Life Cycle and Ecofootprinting Project. Updating the life cycle inventories for commercial surfactant production. Final Report for ERASM.

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 1.01 2022 to 2.00 2023. Furthermore, Annex B. List of replaced chemicals lists all chemicals that were deleted and replaced by already existing other datasets.

4.1 Core layer

No changes have been made for chemicals and processes in the core layer, except for the methodological changes described in Section 3.5.

4.2 Extension layer

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

- Carbon disulfide: The process "reaction of sulfur and natural gas" process was corrected since we previously overestimated the natural gas demand.
- Naphthalene: The carbon dioxide emissions due to direct emissions, energy recovery, and waste treatment, were corrected for the process "coal tar hydro-refining".
- Pitch: The carbon dioxide emissions due to direct emissions, energy recovery, and waste treatment, were corrected for the process "coal tar fractionation".

Annexes

Annex A. List of changed chemicals and process names

This annex lists all chemical and process names that were changed from Version 1.01 2022 to 2.00 2023.

old product name	old process name	new product name	new process name
Changes in the core layer			
polyethylene (LLD)	slurry loop process (ChevronPhillips Martech)	polyethylene (LLD)	slurry loop process (Chevron Phillips Martech)
polyethylene (HD)	slurry loop process (Chevronphillips Martech)	polyethylene (HD)	slurry loop process (Chevron Phillips Martech)
Changes in the extension layer			
ABS resin	emulsion polymerization	acrylonitrile butadiene styrene (ABS) resin	emulsion polymerization
CFC-11	reaction of anhydrous hydrogen fluoride and carbon tetrachloride	trichlorofluoromethane (CFC-11)	reaction of anhydrous hydrogen fluoride and carbon tetrachloride
CFC-12	reaction of anhydrous hydrogen fluoride and carbon tetrachloride	dichlorodifluoromethane (CFC-12)	reaction of anhydrous hydrogen fluoride and carbon tetrachloride
DGEBPA	o-alkylation of bisphenol A with epichlorohydrin	bisphenol A diglycidyl ether (DGEBPA)	o-alkylation of bisphenol A with epichlorohydrin
DGEBPA & BPA epoxy resin	reaction of DGEBPA and bisphenol A	bisphenol A diglycidyl ether (DGEBPA) & bisphenol A (BPA) epoxy resin	reaction of bisphenol A diglycidyl ether (DGEBPA) and bisphenol A
DGEBPA epoxy resin	reaction and dehydrochlorination of bisphenol A and epichlorhydrin	bisphenol A diglycidyl ether (DGEBPA) epoxy resin	reaction and dehydrochlorination of bisphenol A and epichlorhydrin
DMPCT	reaction of phosphorus pentasulfide, methanol and chlorine	dimethyl chlorothiophosphate	reaction of phosphorus pentasulfide, methanol and chlorine
ECN epoxy resin	condensation and subsequent epoxidation of o-cresol and formaldehyde	epoxycresol novolak (ECN) resin	condensation and subsequent epoxidation of o-cresol and formaldehyde
EPN epoxy resin	condensation and subsequent epoxidation of phenol and formaldehyde	epoxyphenol novolak (EPN) resin	condensation and subsequent epoxidation of phenol and formaldehyde
ethylene/va copolymer	autoclave reactor	ethylene/vinyl acetate (EVA) copolymer	autoclave reactor

ethylene-nor-bornene copolymer	polymerization of ethylene and nobronene	ethylene-nor-bornene copolymer	polymerization of ethylene and nor-bornene
FEP resin	polymerization of hexafluoropropylene and tetrafluoroeth-ylene	hexafluoropropylene tetrafluoroethylene copolymer (FEP resin)	polymerization of hexafluoropropylene and tetrafluoroeth-ylene
hydroxylammonium sulfate	catalic reduction of ammonia, oxygen, hydrogen and sulfu-ric acid	hydroxylammonium sulfate	catalytic reduction of ammonia, oxy-gen, hydrogen and sulfuric acid
methamidophos	reaction of DMPCT and ammonium hy-droxide	methamidophos	reaction of dimethyl chlorothiophosphate (DMPCT) and ammo-nium hydroxide
methyl chloride	reaction of methanol and HCl	methyl chloride	reaction of methanol and hydrochloric acid
norbornene	reaction of toluene, ethylene and DCPD	norbornene	reaction of toluene, ethylene and dicy-clopentadien (DCPD)
PBT pellets	polyesterification of DMT and butanediol	polybutylene tereph-thalate (PBT)	polyesterification of dimethyl tereph-thalate (DMT) and butanediol
PBT pellets (30% glass-filled)	blending of PBT pel-lets (IV=0.85) with glass fibers	polybutylene tereph-thalate (PBT) pellets (30% glass-filled)	blending of poly-butylene tereph-thalate (PBT) pellets (IV=0.85) with glass fi-bers
PBT pellets (IV=0.85)	polymerization of di-methyl terephthalate and 1,4-butanediol	polybutylene tereph-thalate (PBT) pellets (IV=0.85)	polymerization of di-methyl terephthalate and 1,4-butanediol
PBT pellets (IV>1.1)	polymerization of di-methyl terephthalate and 1,4-butanediol	polybutylene tereph-thalate (PBT) pellets (IV>1.1)	polymerization of di-methyl terephthalate and 1,4-butanediol
PCT pellets	polymerization of di-methyl terephthalate and 1,4-cyclohex-anedimethanol	poly cyclo-hexylenedi-methylene tereph-thalate (PCT) pellets	polymerization of di-methyl terephthalate and 1,4-cyclohex-anedimethanol
PCT pellets (glycol modified)	polymerization of di-methyl tereph-thalate, 1,4-cyclo-hexanedimethanol and ethylene glycol	poly cyclo-hexylenedi-methylene tereph-thalate (PCT) pellets (glycol modified)	polymerization of di-methyl tereph-thalate, 1,4-cyclo-hexanedimethanol and ethylene glycol
PET polymer melt	polymerization of ter-ephatalic acid and ethylene glycol	PET polymer melt	polymerization of ter-ephthalic acid and ethylene glycol
plastic film (coex-truded EVA/LLDPE/EVA)	coextrusion of eth-ylene vinyl acetat copolymer with poly-ethylene (LLDPE)	plastic film (coex-truded EVA/LLDPE/EVA)	coextrusion of eth-ylene vinyl acetate copolymer with poly-ethylene (LLDPE)
plastic film (coex-truded EVA/polyam-ide/EVA)	coextrusion of eth-ylene vinyl acetat copolymer with poly-amide	plastic film (coex-truded EVA/polyam-ide/EVA)	coextrusion of eth-ylene vinyl acetate copolymer with poly-amide

plastic film (coextruded HDPE/EVA)	coextrusion of ethylene vinyl acetat copolymer and polyethylene (HDPE)	plastic film (coextruded HDPE/EVA)	coextrusion of ethylene vinyl acetate copolymer and polyethylene (HDPE)
plastic film (unorientes PP)	chill-roll casting process	plastic film (unoriented PP)	chill-roll casting process
PMMPA	reaction of aniline and formaldehyde	polymethylene polyphenylene polyamine (PMPPA)	reaction of aniline and formaldehyde
polyacrylamide (mole wight=10millon)	solution polymeriation of acrylamide and ally chloride	polyacrylamide (mole weight=10million)	solution polymerization of acrylamide and allyl chloride
polyacrylamide (mole wight=20millon)	solution polymeriation of acrylamide and acrylic acid	polyacrylamide (mole weight=20million)	solution polymerization of acrylamide and acrylic acid
polyacrylamide (mole wight=7millon)	solution polymeriation of acrylamide and urea	polyacrylamide (mole weight=7million)	solution polymerization of acrylamide and urea
polyacrylate resin (superabsorbent)	suspension polymerization of acrlic acid	polyacrylate resin (superabsorbent)	suspension polymerization of acrylic acid
polyarylate (DPIP-DPTP-BPA)	melt polymerization of bisphenol A, diphenyl tere- and isophatalate	polyarylate (DPIP-DPTP-BPA)	melt polymerization of bisphenol A, diphenyl tere- and isophthalate
polyphenylene sulfide	polymerization of sodiumsulfide and dichlorobenzene	polyphenylene sulfide	polymerization of sodium sulfide and dichlorobenzene
polyphthalamide (glass-filled)	polymerization of terephatalic acid, isophthalic acid, and hexamethylenediamine with glass fibers	polyphthalamide (glass-filled)	polymerization of terephthalic acid, isophthalic acid, and hexamethylenediamine with glass fibers
polystyrene-methyl methacrylate	continious bulk process of methyl methacrylate, polybutadiene and styrene	polystyrene-methyl methacrylate	continuous bulk process of methyl methacrylate, polybutadiene and styrene
SAN resin	polymerization of styrene and acrylonitrile	styrene acrylonitrile (SAN) resin	polymerization of styrene and acrylonitrile
specialty film (PEN)	esterification, polymerisation, and film casting of polyethylene 2,6-naphthalate	specialty film (polyethylene naphthalate (PEN))	esterification, polymerisation, and film casting of polyethylene 2,6-naphthalate
stripped oil	catalytic hydrotreating of white oil (technical grade)	stripped oil	catalytic hydrotreating of vacuum gas oil
TGETPE epoxy resin	reaction of epichlorohydrin and phenol	tetraglycidyl ether of tetraphenylol ethane epoxy resin (TGETPE epoxy resin)	reaction of epichlorohydrin and phenol
TGMDA epoxy resin	reaction of MDA and epichlorhydrin	tetraglycidyl methylene dianiline epoxy resin (TGMDA epoxy resin)	reaction of methylene dianiline and epichlorhydrin
thermoplastic polyurethane (polyester-based)	reaction of polyester polyol, MDI and butanediol	thermoplastic polyurethane (polyester-based)	reaction of polyester polyol, methylene diphenyl diisocyanate

			(MDI) and butanediol
thermoplastic polyurethane (polyether-based)	reaction of polyether polyol, MDI and butanediol	thermoplastic polyurethane (polyether-based)	reaction of polyether polyol, methylene diphenyl diisocyanate (MDI) and butanediol
urea (agricultural grade)	reaction of ammonin and carbon dioxide	urea (agricultural grade)	reaction of ammonia and carbon dioxide
vdc/vcm copolymer	suspension polymerization of vinylidene chloride and vinyl chloride	vinylidene chloride/vinyl chloride monomer (VDC/VCM) copolymer	suspension polymerization of vinylidene chloride and vinyl chloride
vinyl acetate/ethylene copolymer	emulsion polymerization of ethylene and vinyl acetate	vinyl acetate/ethylene (EVA) copolymer	emulsion polymerization of ethylene and vinyl acetate
vinyl ester resin	esterification of styrene, bisphenol A and DGEBA	vinyl ester resin	esterification of styrene, bisphenol A and bisphenol A diglycidyl ether (DGEBPA)
white oil (medical grade)	catalytic hydrotreating of vacuum gas oil	white oil (medical grade)	catalytic hydrotreating of white oil (technical grade)
white oil (technical grade)	catalytic hydrotreating of white oil (technical grade)	white oil (technical grade)	catalytic hydrotreating of vacuum gas oil
Changes in the simplified extension layer			
PAG (EO/PO, 1:1)	polymerization of propylene oxide and ethylene oxide	polyalkylene glycol (PAG) (ethylene oxide/propylene oxide, 1:1)	polymerization of propylene oxide and ethylene oxide

Annex B. List of replaced chemicals

This annex lists all chemicals that were deleted and replaced by already existing other datasets.

Deleted chemical	Replacement chemical
3-methylpyridine	beta-picoline
o-chloronitrobenzene	o-nitrochlorobenzene
stearyl alcohol	1-octadecanol
2-methoxyaniline	o-anisidine
2-methoxynitrobenzene	o-nitroanisole
4-aminodiphenylamine	n-phenyl-p-phenylenediamine
soda ash (sodium carbonate)	sodium carbonate (ammonia-based)
benzylchloride	benzyl chloride
tri n-butylamine	tri-n-butylamine
EPDM (ethylidenenorbornene, ethylene and 1-propene copolymer)	ethylene propylene diene monomer rubber (EPDM rubber)
1,2-propanediol	propylene glycol