

# Supplier Carbon Footprints Methodology

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I·C·I·S

Supplier Carbon  
Footprints

In Partnership with

  
carbonminds

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## 1. About this document

This document summarizes the methodology used to calculate Supplier Carbon Footprints. The calculation is based on ISO 14040 and 14044 for Life Cycle Assessment, as well as on ISO 14067 for Product Carbon Footprint (PCF) calculations. Moreover, the methodology is compliant with the Together for Sustainability (TfS) guideline for PCF calculations.

## 2. Goal and Scope definition

### 2.1 Goal

The goal of Supplier Carbon Footprints data is to provide a representative, consistent, quality-assured, and transparent source of carbon footprint data representing the production of chemicals and plastics. Following the ISO standards, the goal can be defined as follows:

- **Intended application.** Supplier Carbon Footprints data aims to reflect the carbon footprints of the production of chemicals and plastics from different plants and suppliers as precisely as possible. The data can be used, for example, for the calculation of product or company carbon footprints.
- **Reasons.** Gathering environmental impact data is frequently seen as the major obstacle when performing environmental assessments for chemical products.<sup>1</sup> Providing representative, consistent, quality-assured, and transparent data is therefore key to conducting more representative and reliable assessments to support environmental decisions.
- **Intended audience.** Supplier Carbon Footprint data can be used for climate impact assessments in different fields, including industry, consulting, political decision support, and academia.
- **Comparative assertions.** The climate impact assessments carried out based on Supplier Carbon Footprints data can support various goals, including comparative assessments to be disclosed to the public. Nevertheless, Supplier Carbon Footprints data alone does not intend or support any comparative assertions to be disclosed to the public in the sense of ISO 14040/14044.

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<sup>1</sup> Maranghi, S. and Brondi, C., 2020. Life Cycle Assessment in the Chemical Product Chain. Springer International Publishing.

## 2.2 Scope

This section describes the scope of the Life Cycle Inventory (LCI) model used to calculate Supplier Carbon Footprints.

### 2.2.1 Function, functional unit and declared unit

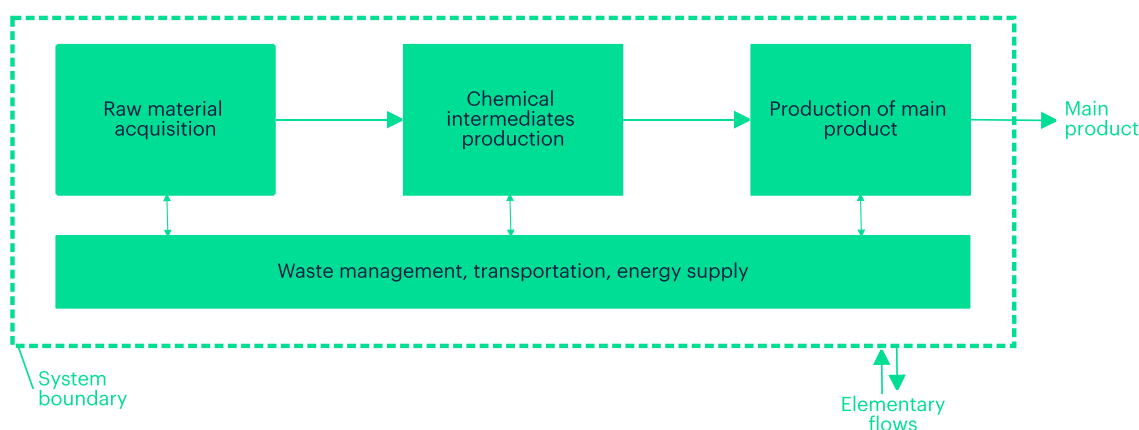
Life Cycle Assessments quantify the environmental impacts of a product system relative to its function, e.g. global warming impact per production of 1 kg of product. The so-called functional unit specifies and quantifies the function of the product system. Partial product systems, according to ISO 14067, are quantified by the declared unit instead of the functional unit. The declared unit specifies and quantifies the amount of a partial product system. The definition of a functional unit or declared unit serves as a basis for comparing the environmental impacts of different products or services.

The functional units or declared units of all Supplier Carbon Footprints are defined in relation to the reference products, i.e. the chemicals for which Supplier Carbon Footprints are compiled. Therefore, the functional unit or declared unit is defined as "Production of 1 kg of the reference product".

### 2.2.2 System boundaries

The system boundaries define which processes, material flows, and energy flows belong to the product system represented by a carbon footprint.

**All Supplier Carbon Footprints have cradle-to-gate system boundaries.** These cradle-to-gate system boundaries include all relevant processes needed for the production of a respective chemical ([Figure 1](#)): from the extraction of raw materials ("cradle") through the production of all energy and material flows required to the factory gate of the of the plant in which the chemical is produced.



**Figure 1.** Overview of life cycle stages considered in the cradle-to-gate analysis of chemicals.

To ensure accurate and comparable Supplier Carbon Footprints, the system boundaries need to be defined clearly and the included and excluded parts of the chemical's cradle-to-gate life cycle need to be specified [Table 1](#) outlines these components, providing clarity on any exclusions or simplifications made.

**Table 1. Included and excluded parts of the chemical's cradle-to-gate life cycle.**

Included	Excluded
Direct emissions from manufacturing and related on-site utilities production/generation	Services such as engineering of infrastructure services, R&D activities
Production related raw materials (including precious metal catalysts and ancillary materials that are consumed)	Production of investment goods
Energy consumption	Business travel and employee commuting
Utilities consumption	Upstream packaging
Treatment or disposal of process wastes and wastewater treatment	Downstream packaging
Upstream transportation	Site-to-site transportation
	Downstream transportation

The Supplier Carbon Footprints generally exclude activities, as described in [Table 1](#). The reasons for the exclusion of activities are described in the following:

- The following activities are excluded from the system boundary of Supplier Carbon Footprints because these activities are not directly linked to the production activities of the respective chemical products: Services such as engineering of infrastructure services and R&D activities, as well as the production of investment goods, business travel and employee commuting.
- The upstream and downstream packaging is not considered, as there are no standardized package sizes used in every individual supply chain. Depending on the scope of the respective PCF calculation, the user of the Supplier Carbon Footprints needs to add information on packaging for their specific supply chain in their LCA calculations. However, we expect the environmental impacts of upstream and downstream packaging to be small.
- National site-to-site transportation is not included as it is considered to be neglectable in comparison to the total multiregional transportation and falls under the cut-off rules of the total environmental impact of a chemical.
- For Supplier Carbon Footprints, downstream transportation is excluded from the system boundaries since downstream transportation distances depend on the individual consumers' location. From a perspective of a chemical producing materials needs to be added.

### 2.2.3 Cut-offs

We have neglected flows that are used in small quantities in a respective process and are not relevant for any other process in the LCI model. The sum of all cut-offs in a respective process is lower than 1% of the mass of all input flows, excluding cooling water.

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.

### 2.2.4 Solving multifunctionality (allocation procedure)

Processes in the chemical industry often have more than one function (e.g. the joint production of more than one product) and are therefore multifunctional. To calculate product-specific LCIs (and resulting carbon footprints) for products from multifunctional processes, technical flows and environmental exchanges of these processes need to be allocated between the processes' functions. The problem of how to allocate environmental exchanges between products is called a multifunctionality problem.

For the calculation of Supplier Carbon Footprints, all multifunctionality problems are solved according to the allocation hierarchy provided in ISO 14044, as well as according to the further provisions from the Together for Sustainability Guideline for PCF calculations. The hierarchy is applied as follows.

**Step 1: Subdivision.** Whenever possible, we solve the multifunctionality problem through subdivision. Subdivision is a methodological approach to address multifunctionality problems due to data aggregation. It can be applied when the data from different single-functional sub-processes are aggregated to one aggregated process. The aggregated (black-box) process then seems to be multifunctional only due to the level of aggregation. Subdivision solves this multifunctionality problem by collecting additional process data for all relevant underlying single functional processes and including only the relevant processes into the model.

**Step 2: System expansion.** If subdivision cannot solve the multifunctionality problem, we use system expansion via avoided burden in the next step. In this approach, a credit is given for the joint provision of all functions not included in the functional unit. This credit represents the avoided environmental burden associated with the conventional way to provide these functions that would be used in the absence of the product system under study.

We use the method of system expansion via avoided burden for all fuels and steam outputs that are co-produced in chemical processes and not used internally in the process. We assume that all fuels are used for heat production and avoid the conventional production of heat based on natural gas. In the case of steam, we assume that conventional steam production based on natural gas is avoided. Consequently, the avoided burden represents the environmental burden associated with producing the same amount of heat from natural gas.

**Step 3: Allocation.** Finally, whenever system expansion via avoided burden cannot solve the multifunctionality problem, we apply allocation. Allocation divides the multifunctional process into processes with exactly one function. Then the environmental exchanges of the multifunctional process and its production chain are distributed to the functions reflecting either an underlying physical relationship or an underlying other relationship.

According to ISO 14044, an underlying physical relationship must be applied whenever possible by quantifying how inputs and outputs physically relate to the system's function. A way to determine physical relationships for processes producing more than one valuable product (functions) is to change the amount of one product produced while keeping the other products' production volume constant and observing how all other inputs and outputs change. Then the allocation of the inputs and outputs should reflect this quantitative change observed.

Suppose neither of the approaches can solve the multifunctionality problem. In that case, 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)<sup>2</sup>: 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.

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.
- For processes that co-produce CO<sub>2</sub>, the system expansion via avoided burden approach is applied. An avoided operation of the Direct Air Capture process is assumed for the avoided burden.
- For the steam cracking processes, allocation according to the official Product Category Rule (PCR), *Plastics Europe's recommendation on Steam Cracker allocation*<sup>3</sup>, is applied.
- For the chlor-alkali electrolysis processes, allocation according to the official Product Category Rule (PCR), *The Chlor-Alkali Process by Euro Chlor*<sup>4</sup>, is applied.
- For the MDI and TDI producing processes, allocation according to the official Product Category Rule (PCR), *Toluene Diisocyanate (TDI) & Methylenediphenyl*

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<sup>2</sup> 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.

<sup>3</sup> Life Cycle and Sustainability working group of PlasticsEurope, 2017. PlasticsEurope recommendation on Steam Cracker allocation.

<sup>4</sup> Euro Chlor, 2022. Chlorine (The Chlor-Alkali Process). An Eco-profile and Environmental Product Declaration of the European Chlor-Alkali Industry. Final report.

*Diisocyanate (MDI), Eco-profiles and Environmental Product Declaration of the European Plastic Manufacturers by ISOPA*<sup>5</sup>, is applied.

- In the TfS guideline, allocation according to the official Product Category Rules (PCR) from the Surfactant Life Cycle and Ecofootprinting Project by ERASM 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 or in the Supplier Carbon Footprints, the PCRs by ERASM are not implemented in this methodology.

### 2.2.5 Characterization method

Supplier Carbon Footprints are reported in terms of CO<sub>2</sub>-equivalent emissions (kg CO<sub>2</sub>-eq.). The calculation of CO<sub>2</sub>-equivalent emissions is based on “**Carbon Minds ISO 14067 (based on IPCC 2021) - climate change - global warming potential (GWP100)**” characterization factors.

The Carbon Minds ISO 14067 (based on IPCC 2021) method is an implementation of the latest IPCC 2021 characterization factors in compliance with ISO 14067 and the TfS guideline: All carbon footprints now calculated using IPCC 2021 characterization factors for the 100-year GWP, and also take into account biogenic CO<sub>2</sub>-removals and -emissions. Fossil greenhouse gas (GHG) emissions, biogenic GHG emissions, biogenic GHG removals, and GHG emissions and removals resulting from land use change can be accounted separately as required by ISO 14067 and the TfS guideline.

## 3. The life cycle inventory (LCI) model

The following sections illustrate the modeling approach used in the LCI model, from which Supplier Carbon Footprints are calculated.

### 3.1 Chemical plant level

Chemical plants represent the production of a given chemical in a specific production site. We collect information on the production location (site) for each chemical plant, the production volume, and the production technology used in the plant.

We define the term *production technology* as the production techniques used in a specific chemical plant to produce a particular chemical, including the reaction pathway, reactor technology, and separation steps. We use detailed technical models for each production technology to determine the raw material consumption, utilities (e.g. energy use), resource extractions, emissions, co-products, and wastes.

### 3.2 Integrated production site level

After chemical plants are modeled individually, we model interactions between plants within integrated production sites. As integrated production sites offer a range of

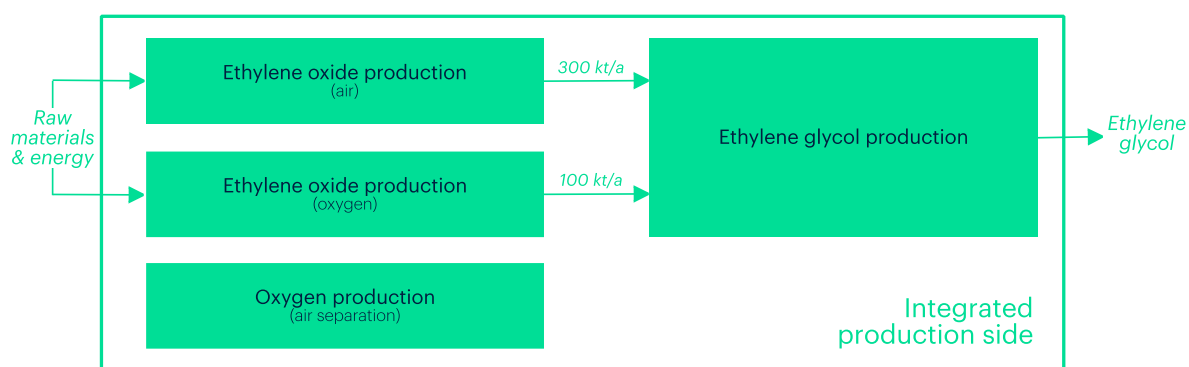
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<sup>5</sup> ISOPA, 2012. Toluene Diisocyanate (TDI) & Methylenediphenyl Diisocyanate (MDI). Eco-profiles and Environmental Product Declaration of the European Plastic Manufacturers.



efficiency savings (such as reducing transportation distances, energy integration, and the use of co-products), they are standard practice in the chemical industry and should be considered whenever possible.

In the LCI model, individual plants are summarized to integrated production sites based on their location. Production plants located in the same city are assumed to be in the same integrated production site. The modeling of integrated production sites allows us to account for plant-specific supplies of raw materials within an integrated production site, as shown in [Figure 2](#)



**Figure 2.** Modeling approach for plant-specific raw material supplies in integrated production sites.

[Figure 2](#) illustrates the modeling of raw material supplies based on a simplified example. The figure shows an integrated production site with four individual plants. Two plants produce ethylene oxide via the oxidation of ethylene. One plant uses oxygen from the air for oxidation; the other uses pure oxygen. For on-site air separation, a third plant delivers pure oxygen to the ethylene oxide production plant that requires it. The fourth plant processes ethylene oxide to produce ethylene glycol.

In this example, the technology mix used to produce ethylene oxide within the integrated production site is calculated according to the weighted average production from both ethylene oxide plants. 75% of the ethylene oxide production mix inside the integrated production site is produced using oxygen from the air for oxidation. The other 25% is produced using pure oxygen from the air separation process.

As a result of one of the main intentions behind integrated production sites is the reduction of transportation distance and the use of co-products, we assume that site-specific production technology mixes are used to satisfy demands for raw materials within integrated production sites. If the production volume of a specific chemical intermediate within the production site is insufficient to satisfy the entire demand of that site, the remaining demand will be met by the national consumption mix (cf. [Section 3.3](#)). The national consumption mix also delivers all inputs which are needed by any plant within an integrated site, but which are not produced inside of the integrated production site itself, e.g. the raw material and energy supplies of the ethylene oxide plants in [Figure 2](#)

### 3.3 National production and consumption mixes

After modeling all production plants and integrated production sites within a country, we calculate the average national production and consumption mixes. Carbon footprints for national production and consumption mixes are not included in the online tool but are modeled within the supply chains of plants (see previous section).

The production mix in a given country is calculated from the output of all chemical plants, which produce a given chemical in that country (cf. [Figure 3](#)). The production mix is calculated based on the country's proportional share of national production contributed by each chemical plant.

The national production mix of a chemical, however, does not necessarily reflect the consumption of that chemical in that country because parts of the amount consumed may be imported from other countries. Furthermore, parts of the national production may be exported to other countries. Consequently, the consumption mix is represented by the sum of a country's production mix, plus imported chemicals, minus exported chemicals, as illustrated in [Figure 3](#)

Production mixes are available for all countries where a specific chemical is produced. Consumption mixes are available for all countries that either produce a chemical and/or import it from other countries.

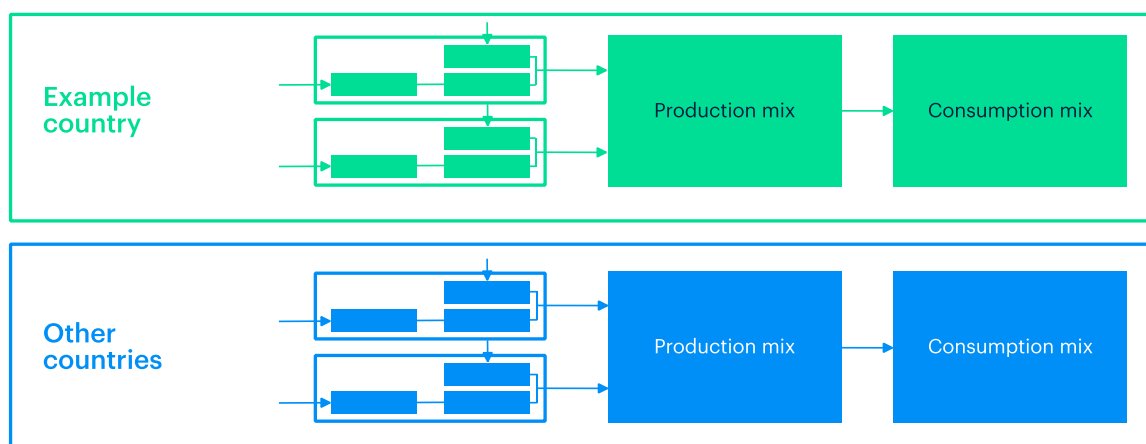


Figure 3. Determination of national production and consumption mixes based on plant-level data.

### 3.4 Specific modeling features

**Transportation.** Freight transportation has been considered for all internationally traded flows between two countries. We differentiate between two types of transportation: transportation by land and sea, and transportation by land.

**Trade data.** The LCI model includes bilateral trade flows between all regions considered. The model is built from data directly reported by each country to the United Nations Statistical Division. Data inconsistencies have been harmonized where needed.

*Waste incineration.* Waste incineration has been modeled based on a Life Cycle Inventory model developed by Doka (2003)<sup>6</sup>. We updated the model of Doka using primary data from hazardous waste incineration plants located in a chemical park.

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<sup>6</sup> Doka G. (2003) Life Cycle Inventories of Waste Treatment Services. ecoinvent report No. 13. Swiss Centre for Life Cycle Inventories, St. Gallen, 2009.

## 4. Data quality rating

This section describes the data quality indicators used to quantify the data quality of Supplier Carbon Footprints. Each dataset provides the data quality assessment according to two different data quality schemes:

- Data quality requirements according to Carbon Minds
- Data quality requirements according to the TfS guidelines

Is it up to the dataset user, depending on the requirements specified in their PCF methodology, to decide between using the data quality scheme from Carbon Minds or TfS.

### 4.1 Data quality requirements according to Carbon Minds

We specify the data quality of Supplier Carbon Footprints based on data quality indicators. These data quality indicators represent six data quality criteria: technological representativeness, geographical representativeness, time-related representativeness, completeness, reliability and methodological appropriateness, and consistency. For each criterion, five data quality levels exist, where level 1 represents the highest data quality and 5 the lowest. The definitions of the data quality criteria and quality levels are based on the Product Environmental Footprint (PEF) Guide by the Joint Research Center of the European Commission<sup>7</sup> except for the criterion "reliability". This criterion replaces the criterion "parameter uncertainty" specified in the PEF guide, which has not been assessed. [Table 2](#) shows the definition of each data quality criterion. [Table 3](#) gives an overview of the data quality assessment scheme for each data quality criterion and data quality level. Finally, [Table 4](#) shows the rating for plant- and supplier-specific carbon footprint data. The term *dataset* used in the tables below refers to the carbon footprint data including relevant metadata.

**Table 2. Definitions of data quality criteria according to Carbon Minds**

<b>Technological representativeness</b>	Chemicals can often be produced by different production technologies using different reaction pathways and plant designs. Technological representativeness is an indicator for the degree to which the dataset reflects the true population of interest regarding production technologies applied throughout the supply chain.
<b>Geographical representativeness</b>	Chemical production chains differ among regions. Geographical representativeness describes the degree to which the dataset reflects the true population of interest regarding geography.
<b>Time-related representativeness</b>	Technical, market, and trade data change over time. Time-related representativeness refers to the degree to which the dataset reflects the

<sup>7</sup>

<https://ec.europa.eu/environment/eussd/pdf/footprint/PEF%20methodology%20final%20draft.pdf>

	specific conditions of the system being considered regarding the time/age of the data.
<b>Completeness</b>	Completeness indicates to which degree relevant flows are covered by a specific dataset. Completeness refers to both technical flows and elementary flows throughout the production chain.
<b>Reliability</b>	Input data can be obtained from different sources, including measurements, detailed modeling, simplified process calculations, and assumptions. This quality indicator rates the reliability of a dataset based on the underlying data sources.
<b>Methodological appropriateness and consistency</b>	Methodological consistency is crucial for comparable results. Therefore, all Supplier Carbon Footprints are compiled based on the same, consistent methodology described in this document if not stated otherwise. This quality indicator assesses the consistency of the methodology applied, as well as its appropriateness.

**Table 3. Assessment scheme for the determination of data quality criteria and quality levels according to Carbon Minds.**

Quality level	1 - Very good	2 - Good	3 - Fair	4 - Poor	5 - Very poor
<b>Technological representativeness</b>	All relevant production technologies are considered for the main product under study, and for all major raw materials, e.g., complete production and consumption mixes are used where needed.	Production of one or more raw materials is not modeled based on all relevant production technologies and only the market dominant production technology is considered.	Production of up to 50% of the raw materials is modeled based on a production technology that is industrially relevant but not the dominant production technology in the market.	Production of more than 50% of the raw materials is modeled based on a production technology that is industrially relevant but not the dominant production technology in the market.	Production of the main product or one or more major raw materials is based on a technology that is known not to be representative.
<b>Geographical representativeness</b>	Data on the production of the main product and all major raw materials is fully representative of the respective region by	Data on the type of production technology and all major raw materials is (partly) based on the market dominant technology.	Data on the production technology for the main product is representative; generic process data is used for each production	Data on the production of the main product and all major raw materials is fully representative of the respective region by	Data on the type of production technology and all major raw materials is (partly) based on the market dominant technology.

	including site-specific mixes, production mixes and consumption mixes. Fossil feedstock and energy supplies are rarely based on larger regional averages (e.g., European average for a specific country).	Fossil feedstock and energy supplies are partly based on larger regional averages (e.g., European average for a specific country).	technology; supply of most raw materials (incl. chemical intermediates ) is based on larger regional averages that include the region under study but are not fully representative.	including site-specific mixes, production mixes and consumption mixes. Fossil feedstock and energy supplies are rarely based on larger regional averages (e.g., European average for a specific country).	Fossil feedstock and energy supplies are partly based on larger regional averages (e.g., European average for a specific country).
<b>Time-related representativeness</b>	Representativeness has been checked and confirmed within the last 3 years.		Representativeness has been checked and confirmed within the last 3 years. Minor changes are known, but the dataset is still considered to be partly representative.		Data for substantial parts of the production chain is known to be outdated.
<b>Completeness</b>	All process data has been measured or modeled at a high level of detail, including all technical and elementary flows	All technical flows and major elementary flows have been measured or modeled at a high level of detail. Potential data gaps have been closed based on additional modeling or calculations	Only major technical and elementary flows are considered. It is possible that some relevant flows are missing	Only some of the major technical and elementary flows are considered. Larger data gaps are likely.	Completeness has not been specified.
<b>Reliability</b>	The dataset is fully based on measurements at all relevant production	The dataset is based on detailed process simulations. Potential data	The dataset is based on simplified process calculations considering	The dataset is based on qualified estimates or stoichiometric calculations,	The process data is based on non-qualified estimates.

	sites (primary data). The results have been verified. <sup>8</sup>	gaps are closed through thermodynamic calculations. The results have been verified. <sup>3</sup>	the underlying stoichiometric reaction. Default values are used for energy supplies and conversion efficiencies.	where energy supplies and conversion efficiencies are neglected.	
<b>Methodological appropriateness and consistency</b>	3 <sup>rd</sup> party verification of the compliance with a defined methodology following ISO 14040/14044 based on (at least) spot checks.	Dataset is compliant with a clearly defined methodology based on ISO 14040/14044.	Requirements specified in ISO 14040/14044 are mainly met.	Requirements specified in ISO 14040/14044 are only partly met.	Methodological appropriateness and consistency are not specified.

**Table 4. Data quality rating according to Carbon Minds**

Quality level	Rating	Justification
<b>Technological representativeness</b>	1	All relevant production steps within the chemical industry are represented based on plant-level data covering between 95% and 100% of worldwide production capacities. The production of crude oil, naphtha, and natural gas is represented by data for production and consumption mixes from Ecoinvent (e.g., a specific European country or European average).
<b>Geographical representativeness</b>	1	The model is based on representative information on which production technology is used in the individual chemical plants throughout the supply chain. Detailed technical process data is used for each production technology. Country-specific fossil feedstock supplies are applied whenever possible. Otherwise, larger regional averages are used. Fossil feedstock, energy, and electricity supplies are modeled based on data from the Ecoinvent database using the cut-off system model. Trade balances are based on data directly reported by each country to the United Nations Statistical Division and partly modified to correct errors or increase consistency.
<b>Time-related representativeness</b>	1	Representativeness is checked on an annual basis, and updates are carried out for all data points that have been identified not to be representative based on the quality ratings specified here.

<sup>8</sup> Verification can be carried out, e.g., by on-site checking, by additional modelling, through mass, energy, and elementary balances or by cross-checking with other sources.

<b>Completeness</b>	1	All technical flows and major elementary flows have been determined based on detailed process modeling. Checks have been performed as discussed in the previous sections. Mass and elementary balances have been calculated for every chemical process to identify and subsequently close potential data gaps. Trade balances are based on data directly reported by each country to the United Nations Statistical Division and transformed into a harmonized physical trade model.
<b>Reliability</b>	2	Chemical process data has been obtained from detailed process simulations. Data gaps have been closed based on additional modeling. All process data has been verified through mass and elementary balances and – whenever possible - cross-checked with other sources.
<b>Methodological appropriateness and consistency</b>	1	All Supplier Carbon Footprints are based on the methodology specified in this document. The application of the methodology leads to high levels of consistency. The methodology is 3rd party certified and spot checks of data have been performed as part of the certification (see <a href="#">Section 6</a> ).

## 4.2 Data quality requirements according to TfS

In addition to the data quality requirements developed by Carbon Minds, we additionally specify the data quality of Supplier Carbon Footprints based on data quality indicators according to the product carbon footprint guideline for the chemical industry developed by the Together for Sustainability (TfS) initiative. According to TfS, these data quality indicators represent five data quality criteria: Technological representativeness (TeR), Geographical representativeness (GeR), Time-related representativeness (TiR), Completeness (C), and Reliability (R). For each criterion, three data quality levels exist, where level 1 represents the highest data quality and 3 the lowest. [Table 5](#) shows the definition of each data quality criterion. [Table 6](#) gives an overview of the data quality assessment scheme for each data quality criterion and data quality level. Finally, [Table 7](#) shows the rating for plant- and supplier-specific carbon footprint data. The term *dataset* used in the tables below refers to the carbon footprint data including relevant metadata.

Additionally, the Data Quality Rating (DQR) is calculated to provide a quantitative information of the overall quality of the data and the resulting Product Carbon Footprint (PCF). The DQR of the unit process is based on the five data quality criteria, as specified in the formula below:

$$DQR_{\text{unit process}} = \frac{\text{TeR} + \text{GeR} + \text{TiR} + \text{C} + \text{R}}{5} \quad (1)$$

According to TfS, the total DQR of a dataset and its respective PCF is calculated from the sum of the PCF-based shares of the individual DQRs of the unit process inputs and the unit process itself, as specified in the formula below:



$$DQR_{total} = \frac{\sum_i DQR_{total,input\ i} \cdot PCF_{input\ i} \cdot UnitConsumption_{input\ i}}{PCF_{total}} + \frac{DQR_{unit\ process} \cdot PCF_{unit\ process}}{PCF_{total}} \quad (2)$$

In this version of Supplier Carbon Footprints, the calculation of the DQR is simplified by a conservative estimate: The DQR of the unit process is assumed to be representative for the total DQR of the process. For Supplier Carbon Footprints, this estimation is appropriate. It is planned to eliminate this simplification and fully implement [formula 2](#) in future versions of Supplier Carbon Footprints.

**Table 5. Definitions of data quality criteria according to Together for Sustainability**

<b>Technological representativeness</b>	The degree to which the data reflects the actual technology(ies) used.
<b>Geographical representativeness</b>	The degree to which the data reflects the actual geographic location of the activity (e.g. country or site).
<b>Time-related representativeness</b>	The degree to which the data reflects the actual time (e.g. year) or age of the activity.
<b>Completeness</b>	The degree to which the data are statistically representative of the relevant activity. Completeness includes the percentage of locations for which data is available and used out of the total number that relate to a specific activity. Completeness also addresses seasonal and other normal fluctuations in data.
<b>Reliability</b>	The degree to which the sources, data, collection methods and verification procedures used to obtain the data are dependable
<b>Data Quality Rating (DQR)</b>	The DQR is calculated to provide a quantitative information of the overall quality of the data and the resulting Product Carbon Footprint. In simple terms, the DQR is an average of the five data quality criteria described above.

**Table 6. Assessment scheme for the determination of data quality criteria and quality levels according to Together for Sustainability**

Quality level	1 – Good	2 – Fair	3 – Poor
<b>Technological representativeness</b>	Same technology	Similar technology (based on secondary data)	Different or unknown technology
<b>Geographical representativeness</b>	Same country or country subdivision	Same region or subregion	Global or unknown

<b>Time-related representativeness</b>	Data from reporting year	Data less than 5 years old	Data more than 5 years old
<b>Completeness</b>	All relevant sites for specified period	<50% of sites for specified period or >50% of sites for shorter period	Less than 50% of sites for shorter time period or unknown
<b>Reliability</b>	Measured activity data	Activity data partly based on assumptions	Non-qualified estimate
<b>Data Quality Rating (DQR)</b>	Overall good quality by considering all five data quality criteria described above.	Overall fair quality by considering all five data quality criteria described above.	Overall poor quality by considering all five data quality criteria described above.

**Table 7. Data quality ratings according to Together for Sustainability**

Quality level	Rating	Justification
<b>Technological representativeness</b>	1	All relevant production steps within the chemical industry are represented based on plant-level data covering between 95% and 100% of worldwide production capacities. The production of crude oil, naphtha, and natural gas is represented by data for production and consumption mixes from Ecoinvent (e.g., a specific European country or European average).
<b>Geographical representativeness</b>	1	The model is based on representative information on which production technology is used in the individual chemical plants throughout the supply chain. Detailed technical process data is used for each production technology. Country-specific fossil feedstock supplies are applied whenever possible. Otherwise, larger regional averages are used. Fossil feedstock, energy, and electricity supplies are modeled based on data from the Ecoinvent database using the cut-off system model. Trade balances are based on data directly reported by each country to the United Nations Statistical Division and partly modified to correct errors or increase consistency.
<b>Time-related representativeness</b>	1	Representativeness is checked on an annual basis, and updates are carried out for all data points that have been identified not to be representative based on the quality ratings specified here.
<b>Completeness</b>	1	Production plants with different technologies covering in total between 95% and 100% of worldwide production capacities are considered for a time period of one year. Furthermore trade balances are considered. Additionally, all technical flows and major elementary flows have been determined based on very detailed and sophisticated process modeling. Checks have been performed as discussed in the previous sections. Mass and elementary balances have been calculated for every chemical process to identify and subsequently close potential data gaps.

<b>Reliability</b>	2	Chemical process data has been obtained from detailed process simulations. Data gaps have been closed based on additional modeling. All process data has been verified through mass and elementary balances and – whenever possible - cross-checked with other sources.
<b>Data Quality Rating (DQR)</b>	1.2	The DQR is calculated to provide a quantitative information of the overall quality of the data and the resulting Product Carbon Footprint. In simple terms, the DQR is an average of the five data quality criteria described above. As a result, the DQR of the core layer is 1.2 due to the average good data quality.

## 5. Updates

Supplier Carbon Footprints will have a full data update once per year to ensure an up-to-date representation of climate impacts. Furthermore, the database will be recertified by TÜV Rheinland Energy GmbH on an annual basis.

## 6. Review and certification

The cm.chemicals database methodology document<sup>9</sup>, upon which Supplier Carbon Footprints are based, was reviewed and certified by TÜV Rheinland against ISO 14040/44/67 and the Together for Sustainability (TfS) guideline for PCF calculations. The present document summarizes the parts of the cm.chemicals methodology that are relevant for the calculation of Supplier Carbon Footprints. The verification includes annual monitoring and recertification by TÜV Rheinland Energy GmbH.

More information on the review is available at Certipedia:

[https://www.certipedia.com/quality\\_marks/0000081021?locale=en](https://www.certipedia.com/quality_marks/0000081021?locale=en)



<sup>9</sup> <https://www.carbon-minds.com/cm-chemicals-methodology.pdf>