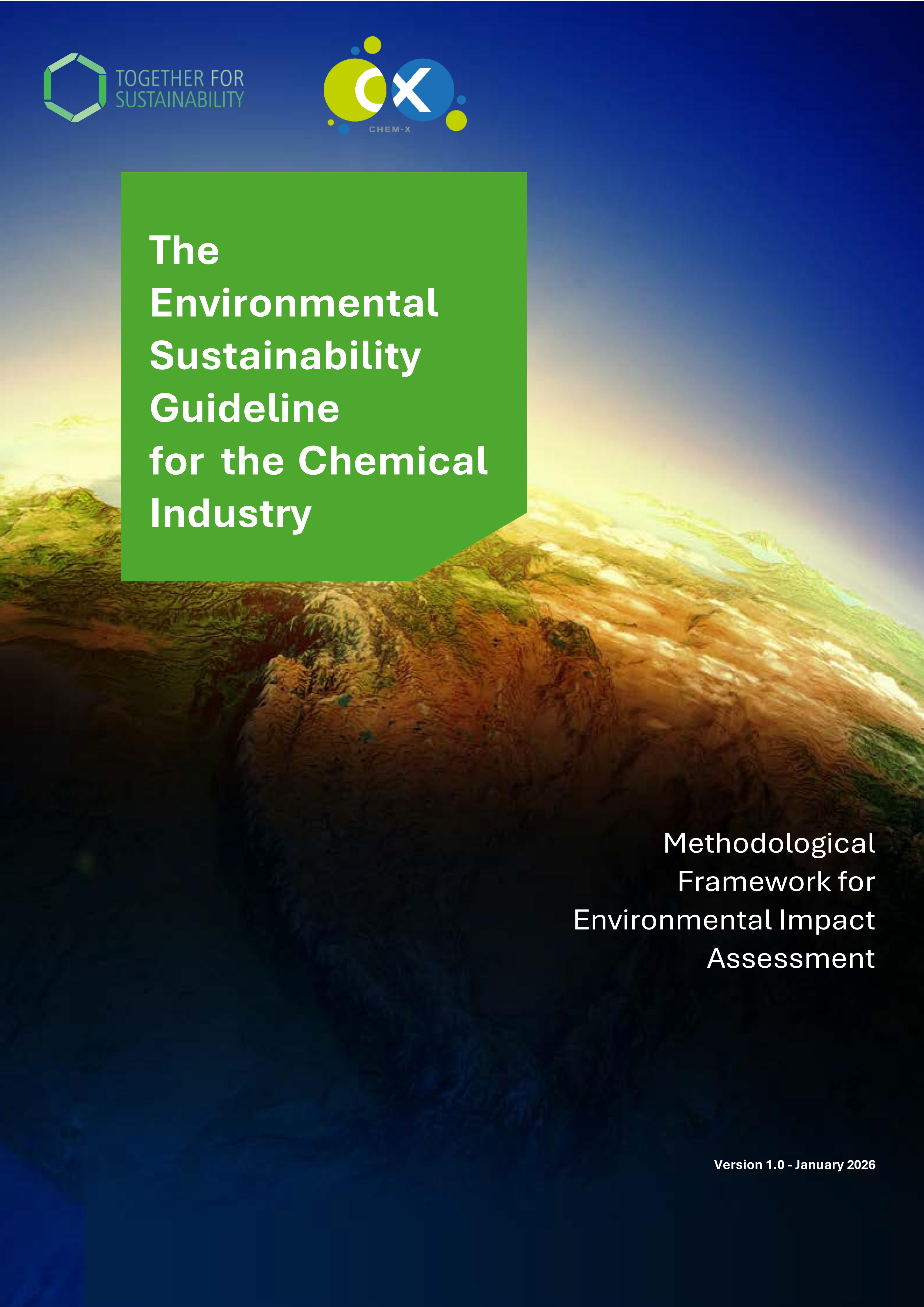

TOGETHER FOR SUSTAINABILITY

CHEM-X

The Environmental Sustainability Guideline for the Chemical Industry

Methodological Framework for Environmental Impact Assessment

Version 1.0 - January 2026

CHEM-X

Together for Sustainability
Chem-X consortium

The Environmental Sustainability Guideline for the Chemical Industry

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For more information,
please visit www.chem-x.de

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Note to the table of contents:

This document provides guidance on how to assess selected LCA impact categories (Module 1). The choice to address this specific set of impact categories in this first version of this Guideline document was based on a prioritization done by the working group. Following versions will contain additional impact categories.

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1. Introduction

The chemical industry is undergoing a pivotal shift in how it approaches sustainability. As Digital Material Passports (DMPs) and Digital Product Passports (DPPs) gain momentum as tools for improving transparency, traceability, and regulatory alignment, there's a growing recognition that focusing solely on carbon emissions is no longer sufficient. While carbon remains a critical metric, it represents just one dimension of a product's environmental footprint. To provide a more complete picture, DMP/DPPs must begin to incorporate a broader set of impact categories – such as water consumption, land use change, ecotoxicity, human health risks, resource depletion, and ozone layer degradation. These impacts span the entire life cycle of chemical products, from raw material extraction through production, use, and disposal.

Expanding the environmental scope of DMP/DPPs is not just a technical upgrade – it is a strategic necessity. Customers, regulators, and investors are increasingly seeking comprehensive data to guide procurement, evaluate sustainability claims, and manage risk. Without consistent reporting on these additional impact areas, DMP/DPPs risk falling short of their potential to drive meaningful change and innovation.

However, this expansion brings its own challenges. Today, companies differ widely in how they assess and report non-carbon impact categories, leading to fragmented data and limited comparability. To overcome this, the industry must work toward harmonized approaches – standardizing life cycle inventory datasets, impact assessment methods (such as ReCiPe, EF, CML or TRACI), and reporting formats. This alignment will not only improve data quality and interoperability but also enable benchmarking and foster collaboration across the sector.

A promising example of such alignment is the recently developed TfS (Together for Sustainability) PCF Guideline v3.0 (TfS Guideline), providing clear instructions for calculating and sharing Product Carbon Footprints (PCFs), with the goal of improving transparency across supply chains and enabling consistent reporting within the chemical sector. It outlines the methodology for PCF calculation and offers recommendations for sharing data, including key attributes. As the first and most highly regarded chemical industry-specific framework for PCFs, it empowers companies to generate high-quality, standardized data that aligns with ISO 14067 and the Greenhouse Gas (GHG) Protocol – setting a strong precedent for how other environmental impact categories can be addressed with similar consistency.

By building on this foundation and applying the same level of discipline to a wider range of environmental metrics, the chemical industry can unlock the full potential of digital product passports – not just as tools for compliance, but as drivers of innovation, accountability, and long-term sustainability.

2. About the Guidelines document

2.1. Background and context

Across the chemical industry and beyond there is an urgent need to measure, report, address and possibly improve environmental impacts considered within life cycle assessments (LCA). The environmental impacts of products usually do not arise within the scope of activities of a single manufacturer, but rather across several steps in the value chain. Therefore, a transparent and accurate exchange of product-level sustainability impact data along the supply chain is a key element to both inform consumer product choices and drive mitigation strategies toward climate resilience and responsible resource stewardship.

The TfS PCF Guideline (with its version 3.0 published in Dec 2024) has been broadly and globally recognized as valuable guidance for chemical manufacturers willing to assess the GHG emissions at product level. The guideline draws on the wealth of expertise and knowledge within the TfS member network to develop methodological guidelines for the chemical industry, while remaining fully compliant with existing generic standards including ISO Standards and the GHG Protocol. This guideline – the TfS Sustainability Metrics Guideline for the chemical industry – expands the scope of the TfS PCF Guideline v3.0 by covering additional environmental impacts that are addressed in Life cycle Impact assessments. This approach will benefit chemical manufacturers, their suppliers, and industry initiatives seeking to assess impact categories beyond global warming potential, serving as a practical drop-in methodology for the chemical sector. The Guideline has been developed within the publicly funded project Chem-X.

By applying this new Guideline, TfS members, companies in the chemical industry, and their value chain partners can holistically approach the integration of Life Cycle Impact Assessment (LCIA) of chemical products within their corporate data inventories.

This comprehensive guideline instructs companies on how to calculate and share the LCIA results of their own chemical products. It also provides guidance on using supplier-specific data, supporting transparency, and improving the environmental impact of the entire value chain.

About this version

Based on the TfS PCF Guidelines Version 3 published in 2024, including the related data model, this version adds new information on LCIA methodologies and the LCIA assessment for several defined impacts. Although this Guideline is separated from the TfS PCF Guideline v3.0, it does incorporate it as an integral chapter (see Chapter 3 for further details and guidance).

This document provides guidance on how to use and determine several LCA impact categories (Module 1). These impact categories include PCF (Chapter 4 referencing the TfS PCF Guideline v3.0, Resource Use, fossil (Chapter 5), Water Scarcity (Chapter 6), Acidification Potential (Chapter 7), Ozone Depletion Potential (Chapter 8) and Photochemical Ozone Creation Potential (Chapter 9). The choice to address this specific set of impact categories in this first version of this Guideline document was based on a prioritization done by the working group. Following versions of this Guideline will contain additional impact categories.

2.2. Description of the challenges

Developing sustainability guidelines involves navigating a complex and multifaceted landscape. Each sector —whether manufacturing, energy, or others— has unique considerations that must be addressed. This is especially critical for the chemical industry, which supplies products across numerous sectors. Because sustainability standards directly impact planetary health, community well-being, and long-term resilience, the responsibility and stakes are exceptionally high. This section revisits the core challenges through the lens of sustainability.

Sustainability brings together a diverse range of stakeholders—including industry leaders, environmental organizations, policymakers, community representatives, scientists, and the general public. Each group often holds distinct, and at times conflicting, priorities. For example:

- Businesses may focus on economic feasibility and operational efficiency;
- Environmental advocates might push for ambitious targets to protect natural resources and biodiversity;
- Policymakers balance legal, economic, and environmental outcomes for society;
- Communities may prioritize local impacts, such as jobs and health.

Reconciling these perspectives is complex, especially when interests appear at odds or when sustainability goals require trade-offs between short-term costs and long-term benefits.

Describing sustainability in precise terms is challenging. Concepts like "carbon-neutral," "circular economy," or "social responsibility" are nuanced and multi-faceted. Therefore, guidelines and standards must:

- Clearly define sustainability metrics (e.g., acceptable emission levels, resource efficiency, labor standards).
- Be understandable by stakeholders from different technical and cultural backgrounds.
- Address data collection and verification, ensuring claims are transparent and auditable.

Ambiguous language or technical loopholes can lead to misinterpretation or superficial compliance, ultimately undermining the purpose of the guideline or standard.

For a sustainability guideline or standard to be realistically implementable, it shall:

- Consider the economic impact on organizations, including small- and medium-sized enterprises.
- Ensure that monitoring and compliance do not demand unrealistic resources for many stakeholders.
- Deliver clear guidance, comprehensive training, and ongoing support to drive meaningful improvements rather than mere compliance.

If a guideline or standard sets overly ambitious targets, it may discourage participation or result in superficial compliance.

The relevance of indicators varies depending on the material being assessed. Mandatory elements are defined by the EU with category rules (PEFCR) at the material or product level. For final chemical industry products—which can differ significantly—general recommendations are therefore not feasible.

Assessing whether a sustainability guideline or standard delivers real-world benefits is crucial. Developing robust, science-based metrics for environmental impacts needs harmonized approaches and should establish mechanisms for independent monitoring and public reporting. In certain time frames, guidelines and standards must go for revision to consider current developments and to drive meaningful improvement. Continuous learning and adaptation in a consensus mode ensures the guideline or standard remains a force for positive change.

2.3. Objectives and purpose of the guidelines

Sustainability standards serve as a transparent assessment by which organizations can be assessed and held accountable. Key objectives in this area include the use of standards to provide concrete and measurable criteria for performance, making it easier to track progress and identify areas for improvement based on generic standards. Adherence to recognized standards strengthens the credibility and legitimacy of organizations in the eyes of investors, customers, regulators, and the wider public. Meaningful and established standards support third-party verification and certification processes offering independent assurance of compliance and performance, allow the exchange of data that were developed with a harmonized and commonly agreed approach, and allow performance tracking on product and company level.

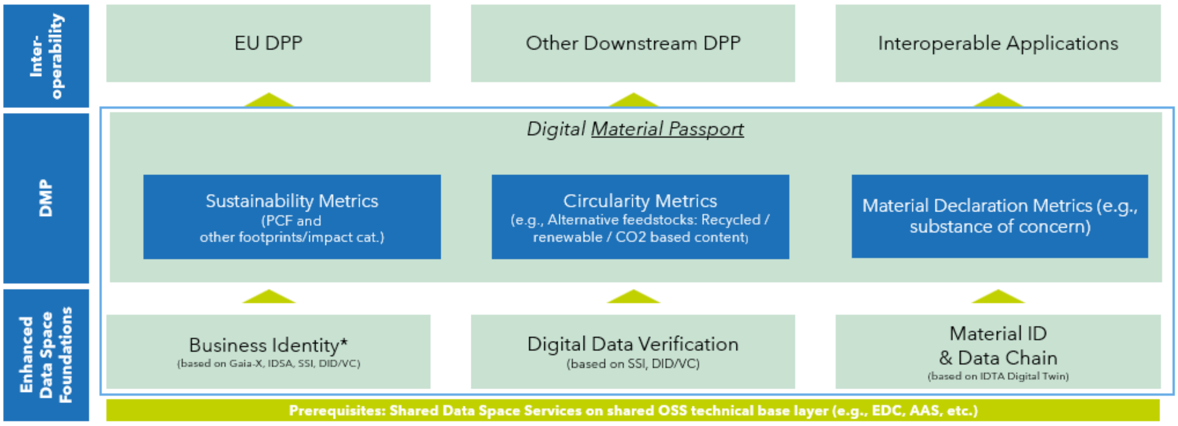
The proliferation of diverse sustainability initiatives across countries and industries can lead to confusion, duplication, and inefficiency. Well-defined sustainability standards aim to promote international consistency on information level and enable to facilitate cross-border collaboration and trade, ensuring that sustainability criteria are understood and accepted worldwide. Harmonization of standards helps avoid conflicting requirements and streamline compliance for multinational organizations enabling the sharing of best practices and lessons learned, thereby accelerating progress towards collective sustainability goals. Exchanging the data via a harmonized data approach gives more opportunities for data sharing and informs interested parties about product performance according to sustainability requirements.

This guideline delivers such a harmonized approach for the chemical industry and opens opportunities for other downstream sectors to select more sustainable products and receive meaningful information along their value chains. It is to be emphasized that the value of a harmonized approach for the definition, characterization and determination of key sustainability metrics is particularly relevant for chemical materials, as they constitute the input to over 95% of all manufacturing goods globally (ICCA 2019).

Therefore, the primary objective of this guideline is to ensure a consistent, practical, and accurate assessment of cradle-to-gate sustainability impacts for chemical inputs, regardless of their downstream application—whether in automotive, construction, textiles, packaging, personal and home care, pharmaceuticals, raw material extraction, or any other sector.

2.4. Link to Digital Material Passport (DMP) and Digital Product Passport (DPP)

DMPs and DPPs are structured digital records containing detailed product information from chemical production to end-of-life treatment, aiming at enhancing transparency, traceability, and sustainability within the industry. This Guideline document, developed in the frame of project Chem-X, defines the sustainability metrics' portion of the chemical DMP, which is designed to interoperate and enable the fulfillment of upcoming DPPs data requirements for regulated products shown in Figure 1.



* Includes positive list of supply chain due diligence and legal entity specific certificates

Figure 1: Chem-X DMP/DPP relations

This guideline aims to establish harmonized terminology, descriptions, and calculation methods for sustainability metrics in DMPs of chemical materials, regardless of their end-use application. Its purpose is to reduce costs and complexity for chemical sector companies seeking to generate and exchange sustainability data in line with regulated DPP requirements. Given that sustainability data is currently scarce and inconsistent across metrics, industries, regions, and products, this guideline represents a significant step toward enabling an effective and sustainable transformation throughout supply chains.

Beyond the above-mentioned methodological harmonization effort, it is not in the scope of this guideline to define or suggest regulatory must-have data points for upcoming regulated DPPs.

2.5. Methodology and reference to existing standards and guiding documents

This sectorial TfS Guideline within the Chem-X project for chemicals follows the international standards ISO 14040:2006/AMD 1:2020 and ISO 14044:2006/AMD 2:2020 for Life Cycle Assessment. Derived from these generic standards, the TfS PCF guideline v3.0 follows ISO 14067: 2018 for PCF. It also draws from other guidelines such as the GHG Protocol developed in recent years for PCF calculations. For PCF calculations, the Partnership for Carbon Transparency (PACT) Methodology and World Business Council for Sustainable Development (WBCSD) Life Cycle Assessments guidelines were considered as well. The TfS PCF Guideline v3.0 was developed in harmonization with Catena-X and the Global Battery Alliance (GBA).

This new guideline goes beyond PCF calculations, extending coverage to additional impact categories. Many elements from the TfS PCF Guideline v3.0 can also be applied to other impact metrics, as detailed in Chapter 3.

For characterization models and related aspects, the Environmental Footprint (EF) Guideline Version 3.1 issued by the EU Commission (2022) was referenced, as detailed in the chapters dedicated to individual metrics. The EF Guideline is expected to be updated in 2026 with Version 4.0. Once the new version is published, this document will be reviewed and revised accordingly. In addition to these standards, category-specific guidelines were also considered, such as ISO 14046 for water footprint. These category specific guidelines were cited in the respective metric chapters accordingly. While this guideline primarily builds on the ISO standard and EF guideline, we recognize the relevance of sector-specific frameworks such as EN 15804+ A2 for construction products, which applies similar principles for environmental information as EF guideline. These considerations have informed the Chem-X approach to ensure consistency with established practices across sectors.

2.6. Terminology

This guideline uses precise language to indicate which provisions of the standard are required, which are recommendations, and which are permissible or allowable options that companies may choose to follow. In this guideline, the terms defined by ISO International Standard are used; such as:

- The term “shall” is used throughout this guideline to indicate what is required for an LCI (Life Cycle Inventory).
- The term “should” is used to indicate a recommendation, but not a requirement.
- The term “may” is used to indicate an option that is permissible or allowable.
- The term “required” is used in the guideline to refer to requirements in the standard.
- “Needs,” “can,” and “cannot” may be used to provide guidance on implementing a requirement or to indicate when an action is or is not possible [GHG Protocol Corporate Value Chain (Scope 3) Standard].

Table 1 reports a summary of the terms used and what they indicate in this guideline.

Table 1: Terminology used in this guideline

Term	**Indicates**
Shall	Requirement
Should	Recommendation
May	Permitted or allowed
Can	Possible (for example, that an organization or individual is able to do something)

In summary, the terms defined by ISO International Standard are used:

- “Shall” indicates a requirement.
- “Should” indicates a recommendation.
- “May” is used to indicate that something is permitted.
- “Can” is used to indicate that something is possible, for example, that an organization or individual is able to do something.

In the ISO/IEC Directives, Part 2, 2021, 3.3.3, a requirement is defined as an “expression, in the content of a document, that conveys objectively verifiable criteria to be fulfilled and from which no deviation is permitted if conformance with the document is to be claimed.”

In the ISO/IEC Directives, Part 2, 2021, 3.3.4, a recommendation is defined as an “expression, in the content of a document, that conveys a suggested possible choice or course of action deemed to be particularly suitable without necessarily mentioning or excluding others.”

2.7. Literature

EU commission (2022), Environmental Footprint reference packages, European Platform on LCA | EPLCA; (accessed October 2nd 2025).

EU commission (2022), Advancing on comparability aspects for Product and Organisation Environmental Footprint, https://publications.jrc.ec.europa.eu/repository/handle/JRC130715; (accessed October 2nd 2025).

ICCA, (2019); The Global Chemical Industry: Catalyzing Growth and Addressing Our World’s Sustainability Challenges, https://icca-chem.org/wp-content/uploads/2020/10/Catalyzing-Growth-and-Addressing-Our-Worlds-Sustainability-Challenges-Report.pdf (accessed October 2nd 2025)

TfS PCF Guideline Version 3, The Product Carbon Footprint Guideline for the Chemical Industry (2024), https://www.tfs-initiative.com/app/uploads/2024/12/TfS-PCF-Guidelines-2024.pdf; (accessed October 2nd 2025)

3. Relationship and reference to the TfS PCF Guideline

LCIA methodologies are designed to address the scope of several impact categories in a consistent framework. This approach is followed by this Guideline as well, which builds on the TfS PCF Guideline v3.0.

This chapter focuses on the communalities between the determination of PCF and other impact categories guiding the reader to refer to shared concepts to the respective sections covered in the TfS PCF Guideline v3.0. When it comes for example to system boundaries, declared unit, data source provisions, allocations in multi-output systems and several other topics, the approach developed for the Global Warming Potential impact category will apply also to other impacts. Therefore, we provide here the reader with guidance on how to transfer the application of rules specified for PCF to other metrics such as Acidification Potential, Water Footprint, Ozone Depletion Potential, etc.

Table 2 below provides a useful list of corresponding sections in the TfS PCF Guideline v3.0, describing methodological approaches valid also beyond PCF.

Table 2: Sections of the TfS PCF Guideline v3.0 with content applicable also to other impact categories than PCF and described in this Guideline.

Topic	**Section in TfS PCF Guideline v3.0**
Goal & Scope definition	5.1.1
System boundaries (incl. Geographic scope)	5.1.2
Declared Unit	5.1.3
Temporal scope	5.2.2
Cut-off criteria	5.2.3
Data types and sources	5.2.5
Multi-output process (allocation)	5.2.9
Data Quality and Share of Primary Data	5.2.11
Mass balance & CoC	5.2.10
Electricity	5.2.8

3.1. Goal and Scope: 5.1.1 in the TfS PCF Guideline v3.0

The scope of this guideline covers the so-called “cradle-to-gate” approach to calculate a Lifecycle impact up to the production stage of the company determining and declaring such an impact.

It is stated where the guideline defined specific rules for chemicals that are not reflected in detail in the current standards. The TfS PCF Guideline v3.0 is fully compliant with ISO 14040:2006/AMD 1:2020 and ISO 14044:2006/AMD 2:2020 for Life Cycle Assessment. For PCF calculations ISO 14067:2018 and the GHG Protocol Product Life Cycle Accounting and Reporting standard applies. The TÜV Rheinland as 3rd party certifier checked and validated the compliance of the TfS PCF Guideline v3.0.

It must be noted that a product assessment limited to only GHGs as described in the TfS PCF Guideline v3.0 has the benefit of simplifying the analysis and producing results that can be clearly communicated to stakeholders. However, the limitation of a GHG-only inventory is that potential trade-offs or co-benefits between environmental impacts can be missed. Therefore, the results of a GHG-only inventory should not be used to communicate the overall environmental performance of a product (GHG Protocol Product Standard 2011). To overcome these limitations, this guideline was prepared to cover more than one environmental impact category and to give users a more complete picture of the environmental impacts of a product.

3.2. System boundaries: 5.1.2 in the TfS PCF Guideline v3.0

The boundary of the guideline is a cradle-to-gate LCA, comprising all processes of extraction, manufacturing, and transportation, until the product leaves the factory gate. Downstream impacts from product use and end-of-life are in general excluded from a cradle-to-gate approach (Figure 5.2 in the TfS PCF Guideline v3.0) and Figure 2 in this document. The following activities shall be included in a cradle-to-gate calculation: all product related direct and indirect emissions of the production process, including fossil or biogenic removals, energy consumption from electricity, external heat and steam; fuel consumption like natural gas, biogas, utilities, manufacturing, inbound transportation, site-to-site transportation, treatment of process waste and wastewater treatment and all emissions of raw material consumption including catalysts that are consumed in the reaction (BASF SE 2021). Further information on included activities is provided in Table 5.1. of the TfS PCF Guideline v3.0.

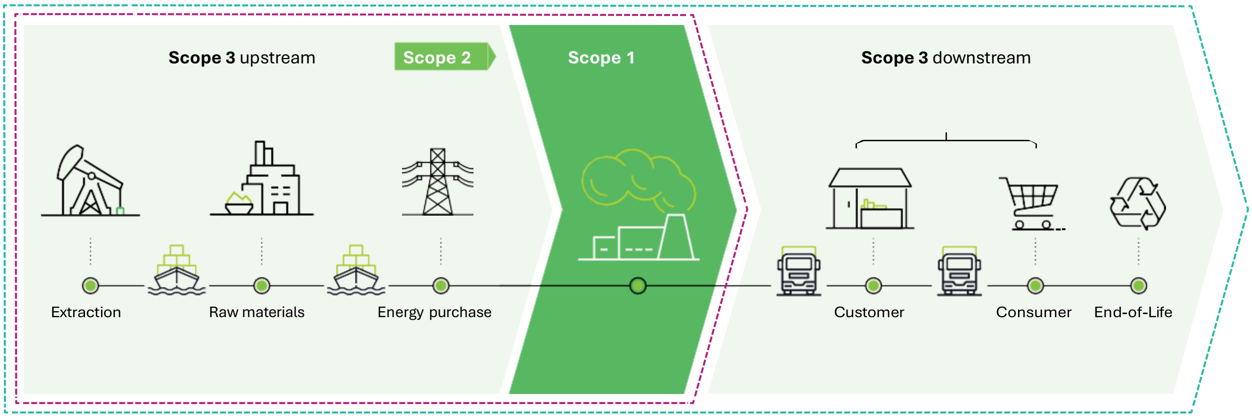


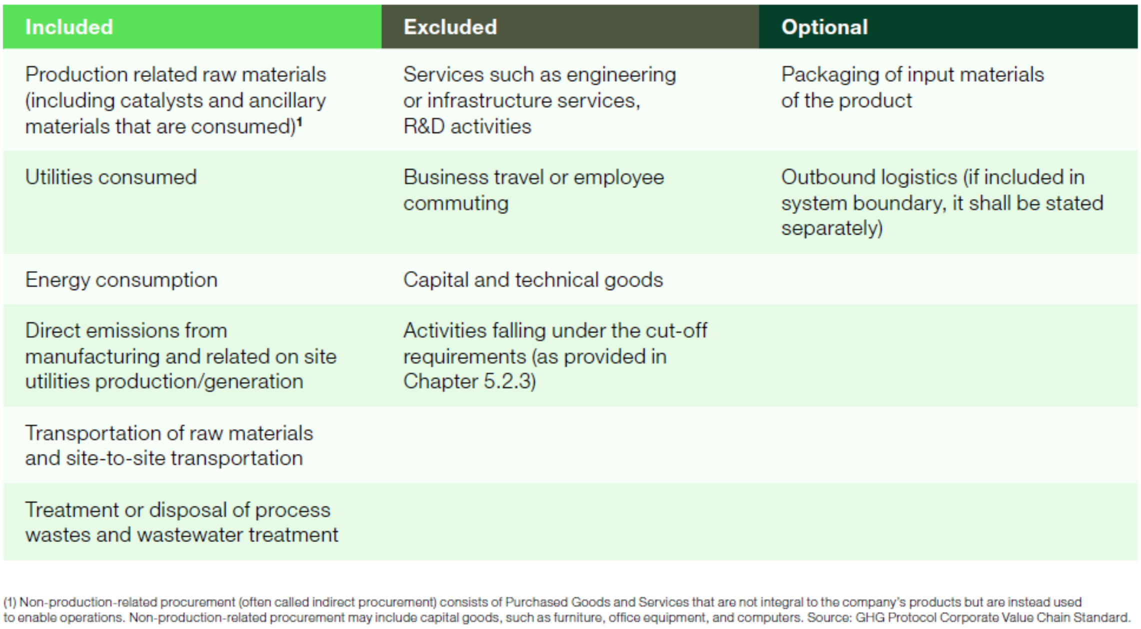
Figure 2: System boundary definition (Together for Sustainability, 2024)

As the guidance is product-related, the following activities shall not be included within the boundaries of a cradle-to-gate LCA: manufacturing of production equipment, buildings, infrastructure and other capital goods, business travel by personnel, travel to and from work by personnel, and research and development activities because generally they fall under cut-off criteria. However, infrastructure may be included when its relative impact exceeds these cut-off thresholds or is known to be significant for the technology in question. For example, according to the MLC Sphera online documentation, power plant construction and maintenance in electricity datasets are always included because its associated impacts do not meet the criteria for exclusion. Please also see Chapter 5.2.3 (TfS PCF Guideline v3.0) on requirements to cut off activities.

Outbound transportation of the product is in general excluded in a “cradle-to-gate” impact determination (see Figure 5.2 in the TfS PCF Guideline v3.0). Table 3 below gives an overview of activities and their inclusion in the assessment.

However, if it needs to be considered by customers’ requests, it should be calculated and reported separately (“Distribution stage”). Packaging of the product in question should be included. For many chemicals, the contribution of packaging to the LCA is negligible. This is for example the case for bulk chemicals which are delivered by a supplier to customer manufacturing sites. If packaging is included, it should be visible in the description of the Declared Unit (see 5.1.3 in the TfS PCF Guideline v3.0) and related reporting (see the data field “packaging included” in the data model).

Table 3: Activities to be included and excluded in the system boundaries and optional activities (Together for Sustainability, 2024)



Included	**Excluded**	**Optional**
Production related raw materials (including catalysts and ancillary materials that are consumed)[1]	Services such as engineering or infrastructure services, R&D activities	Packaging of input materials of the product
Utilities consumed	Business travel or employee commuting	Outbound logistics (if included in system boundary, it shall be stated separately)
Energy consumption	Capital and technical goods	
Direct emissions from manufacturing and related on site utilities production/generation	Activities falling under the cut-off requirements (as provided in Chapter 5.2.3)	
Transportation of raw materials and site-to-site transportation		
Treatment or disposal of process wastes and wastewater treatment		

(1) Non-production-related procurement (often called indirect procurement) consists of Purchased Goods and Services that are not integral to the company’s products but are instead used to enable operations. Non-production-related procurement may include capital goods, such as furniture, office equipment, and computers. Source: GHG Protocol Corporate Value Chain Standard.

The system boundary shall be the basis used to determine which unit processes are included within the LCA study. Where Product category rules (PCR) are used, their requirements on the processes to be included supersede those indicated above (see 5.2.4 in the TfS PCF Guideline v3.0).

The criteria, e.g., cut-off criteria (5.2.3 in the TfS PCF Guideline v3.0), used in establishing the system boundary, shall be identified and documented in the data model and the LCA calculation report.

It should be noted that when comparing the environmental performance of products, an LCA with cradle-to-grave boundaries should be used, to ensure impacts throughout the life-cycle of the product are considered.

3.3. Declared Unit: 5.1.3 in the TfS PCF Guideline v3.0

The Declared Unit (DU) describes the quantity of a product that is used as the reference unit in the quantification of the cradle-to-gate LCA. In case of chemical products, the Declared Unit is often defined as 1 kg of unpackaged product.

This TfS guideline deals exclusively with the use of a “Declared Unit” and does not address the use of a "Functional Unit", as it only covers cradle-to-gate LCA and thus does not include the full product life cycle. Declared unit is further described in ISO 14067 (ISO 2018).

The LCIA data is expressed in equivalents per Declared Unit. The equivalent unit is defined for every single impact category and can be extracted from every chapter describing the impact categories. Per impact category, the cumulated life cycle impacts shall be linked to the DU.

Standard unit should be LCIA equivalents per kg product preferably. For some specific products like gases (e.g., Hydrogen, LPG) the LCIA might be expressed per unit norm cubic meter of the product. Furthermore, some products are sold, based on a volume unit (like liter), or pieces (e.g.: automotive parts) and in that case the LCIA may be expressed in the respective unit. In these cases, conversion factors (densities with associated conditions) shall be provided by the supplier for conversion to kg which is required in the attributes list in the Data Model. A DU shall be intrinsic to the product in such a way that it could be independently measured and verified. Abstract or equivocal values, such as monetary amounts like Euro, shall not be used.

For processes, the LCIA may be expressed as, but not limited to, LCIA equivalents per ton of distilled product, per ton of treated wastewater or per ton of product in a crystallization process. Some sectors may use other units in the Declared Unit. Regardless of what is used, a sufficient physical transfer shall be communicated to be able to convert these units into kg.

The results of a LCIA linked to the Declared Unit should be reported as LCIA equivalents per Declared Unit with one decimal. However, for very small values (<0.1) it is recommended to report at least one significant figure.

The Declared Unit shall be consistent with the goal and scope of the LCIA study. The primary purpose of a Declared Unit is to provide a reference to which the inputs and outputs are related. Therefore, the Declared Unit shall be clearly defined and measurable. An example of a Declared Unit is typically referring to the physical quantity of a product, for example “1 kg of liquid laundry detergent with 30 percent water content”. The Declared Unit for which the LCIA of a product system is calculated is 1 kg of unpackaged product at factory gate, regardless of its state (solid, liquid, gas), as its specific density is considered (BASF SE 2021). If packaging is included (see 5.1.2), the Declared Unit is 1 kg of product packaged at the factory gate. 1 kg refers only to the product mass. The packaged product will weigh more than 1 kg.

$$\frac{\text{unit\_LCIA}^{1}\ \text{product (including packaging impact)}}{\text{kg product (excluding the mass of packaging)}}$$

Formula 1: Definition of Declared Unit.

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[1] unit_LCIA: unit used in the LCIA calculation, depending on the impact category. For example, Resource use, fossils = MJ; Water use (scarcity) = m^3

3.4. Temporal Scope: 5.2.2 in the TfS PCF Guideline v3.0

The time boundary of an LCIA refers to the time period for which the LCIA value is representative was derived from ISO 14067. The following time boundaries apply for the different types of data:

- Primary data (e.g. supplier specific data) used in the calculations should be as recent as practicable and not older than three years. The most recent full year (reporting or calendar year) should be applied as the time boundary for LCIA calculations, if representative of an average year of production. For production years that are not continuous or irregular, production data may be averaged for a longer time period to reduce variability due to revisions, turnaround, or other typical production conditions. When applying average production data in a PCF calculation, no more than the last three years of production (reporting or calendar year) shall be averaged and used in the calculation (BASF SE 2021), (PACT 2025).
- Secondary data used for all inputs and outputs should reflect the most recent activity data and/or the latest LCIs (Life Cycle Inventory) available. LCI data (e.g., from databases) used in the calculation of LCIAs shall be as recent as practicable and not older than ten years (BASF SE 2021). If older, appropriate, more recent proxies should be used instead. The data quality rating will be influenced by the choice of data.
- LCIAs shall have a maximum validity period of up to three years from the reference year of data collection if there have not been major changes to the production process (>20% impact from original LCIA result specific to PCF). It is recommended to use PCF as a guiding element but if there is a clear indication of other indicators differing more than 20% this change should be adopted. Companies may update their calculations on a more regular basis (e.g., annually). TfS decided that after three years or if the production process has changed significantly, LCIA values are no longer considered representative and shall be re-calculated. Once LCIA has been revised, the revised version will replace the original version and be valid for 3 years.
- The time boundary of the LCIA calculation is the reference year. The LCIA reference year and date of calculation/publication shall always be disclosed alongside the different values.

3.5. Cut-off criteria: 5.2.3 in the TfS PCF Guideline v3.0

In general, all processes, flows and activities that are attributable to the product system shall be included in an LCA (see 5.1.2 in the TfS PCF Guideline v3.0) (BASF SE 2021), (ISO 14067: 2018). There is in general no difference among the different impact categories concerning the cut-off criteria. Relevant impacts to the results are the important guidance on decisions if unit processes or inputs cut-off or not. If there are differences in cut-off depending on the impact categories and the cut-off shall be adjusted if needed. For example: If there is a unit process that generates a high level of Acidification but that is not relevant for GWP, the unit process shall not be excluded in the Acidification assessment.

The choice of elements of the physical system to be modelled depends on the goal and scope definition of the study, its intended application and audience, the assumptions made, data and cost constraints, and cut-off criteria. The models used should be described and the assumptions underlying those choices should be identified. The cut-off criteria used within a study shall be clearly understood and described (ISO 14040:2006 + Amd 1:2020).

The LCI data collection process shall aim for completeness. Where quantitative data is available, they shall be included. However, no undue effort should be spent on developing data of negligible significance concerning contributions to the LCIA results. If individual material or energy flows are found to be insignificant for results of a particular unit process, these may be excluded for practical reasons and shall be reported as data exclusions. If materials have a considerable upstream environmental footprint they shall be considered in the LCIA calculation, regardless of their relative contribution to the total mass of material flows. If the contribution is uncertain, an overview calculation should be done, and the results shall be included if significant.

Cut-off criteria specify the amount of material or energy flow or the level of significance of impacting the LCIA results associated with unit processes or the product system that may be excluded from an LCA study (derived from BASF SE 2021).

Furthermore, cut-offs may become necessary in cases where no data is available, where elementary flows are very small (below quantification limit), or where the level of effort required to close data gaps and to achieve an acceptable result becomes prohibitive.

If no data is available, but elementary flows are significant, data gaps should be closed in accordance with chapters 5.2.6 and 5.2.8. (in the TfS PCF Guideline v3.0).

Several cut-off criteria are used in LCA practice to decide which inputs are to be included in the assessment, such as mass, energy, and environmental significance (BASF SE 2021).

Requirements for LCIA cut-off criteria

1. All material inputs that have a cumulative total of at least 97% of the total mass inputs to the unit process shall be included. To generate LCIA with higher quality by improving the completeness of the calculation, 100% of total material inputs should be included.
2. All energy inputs that have a cumulative total of at least 97% of total energy inputs to the unit process shall be included. To generate an LCIA with higher quality by improving the completeness of the calculation, 100% of total energy inputs should be included. For most of the input materials, the mass & energy flow reflect the impacts to different impact categories accurately. But exceptions are possible. Where materials are used in a process that is considered or estimated to have a very high contribution to one of the addressed impact categories, the influence on the overall LCIA shall be evaluated and the cut-off kept below a defined threshold of the LCIA results per impact category. Such threshold is set at 3% for the Global Warming Potential impact category; for other impacts in the scope of this Guideline the same threshold shall be applied (except for water scarcity, please refer to the water scarcity section). The applied cut-off value for the given impact category shall be reported in the respective data field of the data model.
3. In cases where the input and influence on the results are unclear, an overall calculation should be made with generic figures to decide if a cut-off can be applied or not (iterative approach) (BASF SE 2021).
4. Some input material flows (for example catalysts containing metals of the platinum group, uranium, highly toxic materials, materials) that have a considerable high upstream environmental footprint shall be considered in the calculations, regardless of their relative contribution to the total mass of material flows, even if their mass input is < = 1% of the total mass. The LCIA calculations should at minimum consider the loss of material (e.g., the loss of catalyst) and assign an impact equal to the virgin material. If known, the efforts of recycling should be considered in addition. Otherwise known efforts, derived from other processes, can be used as a proxy.

3.6. Data types and sources: 5.2.5 in the TfS PCF Guideline v3.0

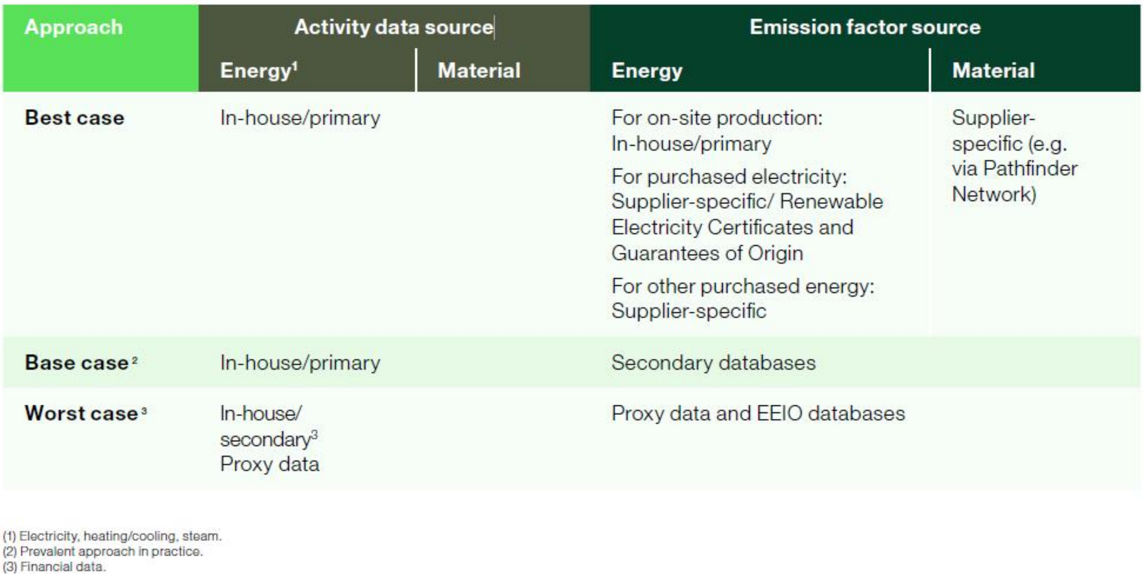
Data can have different levels of quality. Every LCIA calculation should be of the highest level of quality to be meaningful and applicable. High quality data are, for example emissions data that are verified under a governmental scheme such as the European Union-Emissions Trading SySTEM (EU-ETS) or other schemes. In a chemical reaction, several inputs are needed. Information about the inputs can be derived from different sources. The input from all sources shall be assessed with a quality rating system and data with the highest quality rates shall be used in the calculation of the impacts. For share of primary data and data quality rating, please refer to chapter 5.2.11. in the TfS PCF Guideline v3.0. In most cases, the same set of primary data is used in LCA modelling; however, both the primary data share and the data quality ratings may differ in some cases from one impact category to another. For example, if a practitioner receives PCF data from one supplier and uses acidification data from a database for the same product. Consequently, if that is the case, they should be reported separately for each impact category in the data model.

The most recent databases at point of calculation should be used. Moreover, the database version use shall be transparently indicated in the data model. For the PCF calculation for example, there was a significant change in the datasets in 2023/2024 connected to increased methane emissions from the extraction processes of oil and gas. Therefore, we put a requirement of using database versions as e.g. ecoinvent V3.10, Sphera MLC 2024.1 or Carbon Minds cm.chemicals database Version 2.00, July 2023, or later versions of these databases.

The use of different databases should be avoided as much as possible, to ensure higher quality. If this is not possible, the user shall make clear the databases used, and in which way data from different databases have been mixed and clearly report the Data Quality Rating (DQR) as described in the TfS PCF Guideline v3.0. Overall, the most conservative approach is recommended. The methodology for assessing DQR is further described in Chapter 3.10 of this guideline.

In the TfS PCF Guideline v3.0, Primary and Secondary data definitions are provided. They are valid in the same way for LCIA calculations and shown in Table 4.

Table 4: Data hierarchy for energy and material inputs regarding primary, secondary and proxy data (Together for Sustainability, 2024)



Approach	Activity data source		Emission factor source	
	Energy[1]	Material	Energy	Material
Best case	In-house/primary		For on-site production: In-house/primary For purchased electricity: Supplier-specific/ Renewable Electricity Certificates and Guarantees of Origin For other purchased energy: Supplier-specific	Supplier-specific (e.g. via Pathfinder Network)
Base case[2]	In-house/primary		Secondary databases	
Worst case[3]	In-house/ secondary[3] Proxy data		Proxy data and EEIO databases	

(1) Electricity, heating/cooling, steam.
(2) Prevalent approach in practice.
(3) Financial data.

Data gaps

Data gaps exist when there is no primary or secondary data that is sufficiently representative of the given process in the product's life cycle. For most processes where data are missing, it should be possible to obtain sufficient information to provide a reasonable estimate. Therefore, there should be few, if any, data gaps. The data quality rating will indicate that there are data gaps existing which were filled by proxy data. The section in the TfS PCF Guideline v3.0 gives additional guidance on filling data gaps with proxy data and estimated data. Table 5.2 in the TfS PCF Guideline v3.0 gives a summary and an overview.

Proxy data

Proxy data are data from similar processes that are used as a stand-in for a specific process. Proxy data can be extrapolated, scaled up, or customized to represent the given process. Companies may customize proxy data to resemble the conditions of the process studied more closely in the product's life cycle if enough information exists to do so. Data can be customized to better match geographical, technological, or other metrics of the process. Identifying the critical inputs, outputs, and other metrics should be based on other relevant product inventories or other considerations (e.g., discussions with a stakeholder consultant) when product inventories do not exist.

Examples of proxy data include:

- Using data on polyethylene plastic processes when data on the specific plastic input (e.g., HDPE) is unknown. Depending on the specific assessment, the processes under study and the contribution to the overall sustainability metric, using polyethylene data as a proxy for polypropylene might be sufficient as well.
- Adapting an electricity grid emission or impact factor for one region to another region with a different generation mix.
- Adapting a generic data set of a precursor for one process to another, similar process for Ethylamine or Diethylamine.

- Customizing the process of another product to match the studied process, e.g. by changing the amount of material consumed to match a similar process in the product studied.
- Data from proxy might differ in quality related to the different environmental impacts addressed.

Customizing the environmental impacts of a generic process to match the supplier specific results provided for one environmental category. For example, if a supplier provides PCF data for Ethanol but no other impact category, an industrial average model can be used as a proxy for Ethanol and modified to match the PCF given by the supplier.

Estimated data

When a company cannot collect primary data or integrate meaningful secondary data or proxy data to fill a data gap, companies shall estimate the missing data to determine the significance of its contribution to the LCIA result. If processes are determined to be insignificant based on estimated data, the process may be excluded from the inventory results (cut-off criteria).

Where possible, sensitivity analysis shall be performed. Additionally, DQR shall also be reported transparently.

3.6.1. Data Granularity

Highly granular data significantly enhances the precision and credibility of environmental assessments. They enable more accurate allocation, hotspot identification, and interpretation of impacts across life cycle stages. Best practices emphasize collecting data at the **process level**, where flows are directly linked to specific operations. However, when such detail is unavailable, **structured disaggregation methods** should be applied using transparent documentation and justified assumptions.

When detailed **mass**, **energy**, or **water** flow data are not available at the process level, broader datasets (e.g., site-level, department-level, or corporate-level) may be used and systematically disaggregated. Below are practical cases and methodologies applicable across all three flow types.

Case 1: Only Site-Level Data Available

Scenario: A production site includes multiple distinct processes (e.g., Process A and Process B), but only aggregate mass, energy, or water data is available at the site level.

Approach: Disaggregate site-level data to individual processes using relevant allocation criteria. Recommended proxies include (but are not limited to):

- Process-specific intensity data from design specifications or engineering models
- Historical usage patterns or expert input
- Production volumes or throughput

Example: If Process A consumes twice the energy per unit of output compared to Process B, and both produce equal volumes, allocate energy as follows:

- Assign 2 parts energy to Process A
- Assign 1 part energy to Process B

This proportional allocation provides a rational approximation and must be clearly documented, including all assumptions and sources.

Case 2: Flow Estimation Based on Energy or Mass Balance

If direct flow data (mass, energy, or water) is missing, estimates can be derived from:

- Mass or energy balances, which often yield more accurate results (e.g., steam requirements, material conversion rates, heat losses)
- Process-specific benchmarks from literature, industry databases, or technical standards

Example: A beverage facility lacks measured data for water used in bottle rinsing. Industry literature suggests 1.5 liters per bottle rinsed. This can be used as a proxy and scaled based on production data.

Case 3: Shared Utilities or Services

In facilities where flows are shared across multiple units (e.g., central steam generation, compressed air systems, water treatment), allocation should be based on:

- Utility loads per process (e.g., heating or cooling demand, material throughput)
- Engineering estimates of consumption per unit
- Operating time or production intensity

Case 4: Only Corporate-Level Data Available

Scenario: Flow data is only available at the corporate or group level, aggregating multiple sites, products, and geographies. This is common in multinational corporations reporting in sustainability disclosures or environmental databases.

Approach: Allocate corporate-level mass, energy, or water data down to the product system or site of interest using auxiliary data. Recommended allocation bases include:

- Publicly reported site-level environmental intensity indicators (if partially available)
- Production volume of individual facilities
- Sales volume by product line

Considerations: Combine corporate-level water data with production and product-level activity data and clearly disclose the uncertainty and assumptions involved in this top-down allocation.

The examples provided above are intended as guiding suggestions to support consistent and credible disaggregation of mass, energy, and water flows. However, practitioners may encounter unique scenarios not explicitly covered in this guideline. In such cases, applying alternative or more suitable practices is acceptable, provided that all assumptions, data sources, and reasoning are transparently documented. Where possible, sensitivity analysis shall be performed. Additionally, the DQR shall also be reported transparently.

3.7. Electricity and thermal energy: 5.2.8.1 in the TfS PCF Guideline v3.0

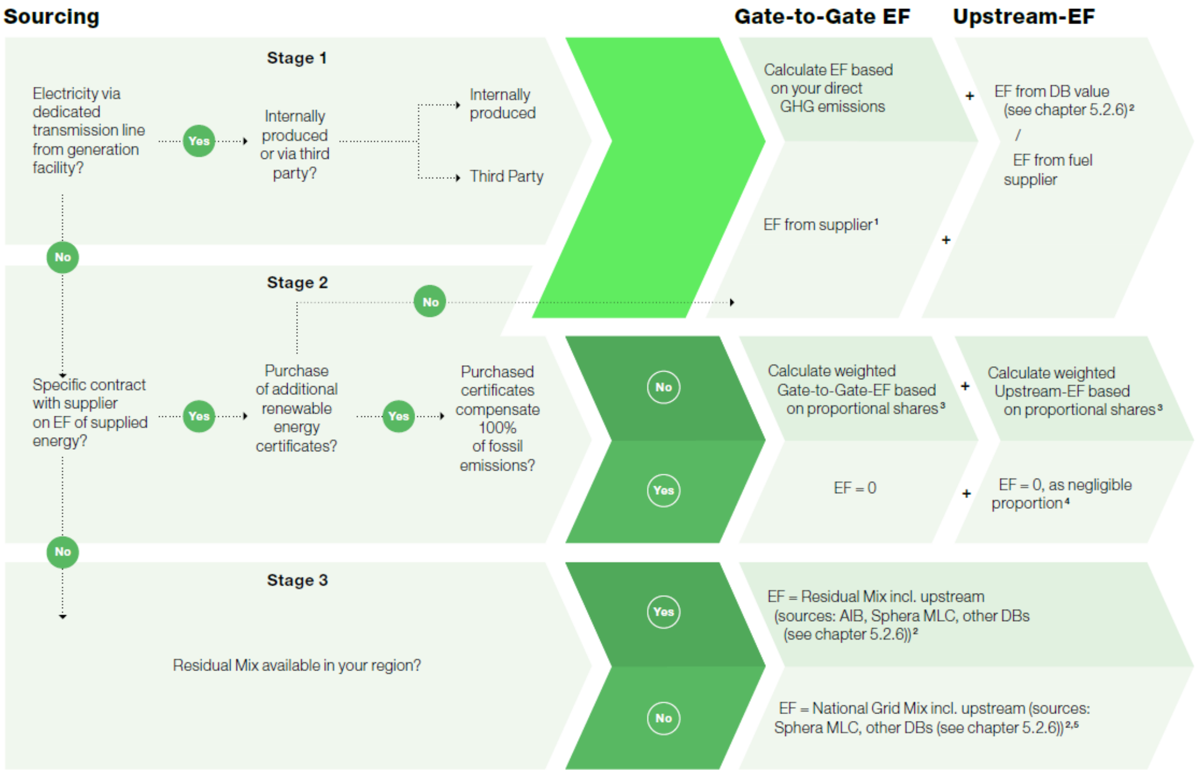
This chapter provides guidance on how to account for the emissions associated with the use of electricity and thermal energy such as steam, heat and cooling.

The emissions associated with the use of energy shall include:

- Upstream emissions from the energy supply system (e.g. the mining and transport of fuel to the energy generator or the growing and processing of biomass for use as a fuel).
- Emissions during the generation of electricity or thermal energy, including losses during transmission and distribution.
- Downstream emissions (e.g. the treatment of waste as ashes arising from the operation of coal fired power plants).

Please follow the decision tree in Figure 3 to determine your options on GHG emissions of procured electricity. Start in the top left corner of stage 1. Exception: If your company has sold energy attribute certificates for received electricity via a contractual instrument to a third party, start at stage 3.

Further details regarding the inclusion of impact from Electricity and Thermal energy use are described in chapter of the TfS PCF Guideline v3.0 Chapter 5.2.8.1 Electricity and thermal energy and is valid for other impact categories including Global Warming Potential.



(1) If the Emission Factor (EF) from supplier is not available, directly move to stage 3.

(2) If no access to Upstream EF data, please apply 20% of the IEA value instead and add it to the Gate-to-Gate EF.

(3) After receiving the individual energy mix from your supplier, multiply the EFs corresponding to their energy source with their proportional share of the energy mix while also taking the partly compensated fossil emissions by purchased certificates into account (e.g.: energy mix: 20% renewable energy (RE), 80% fossil energy (FE); purchased certificates: an amount to compensate 50% of fossil emissions
= EFWeighted= 0.2 × EFRE+ 0,5*(0.8 × EFFE)+ 0,5*(0.8 ×EFRE)).

(4) If impacts including upstream emissions lie within the cut-off range (s. chapter 5.2.3), apply EF = 0. Otherwise, please use an appropriate DB value: Values from databases consider the full life cycle and also contain emissions from the construction stage (Sphera MLC or other DBs (see chapter 5.2.6)).

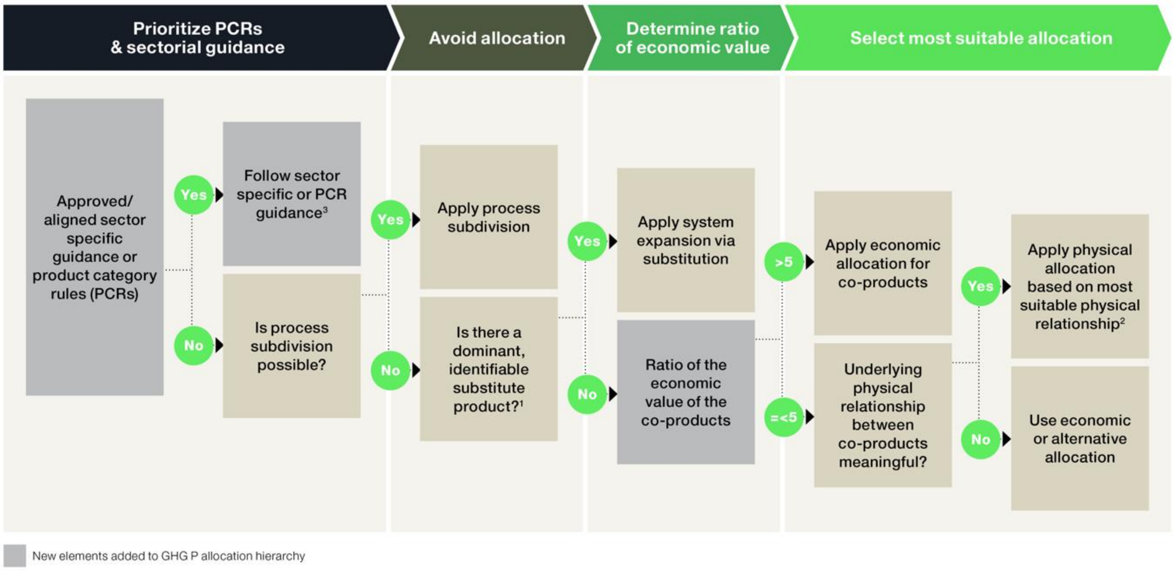
(5) Alternatively, IEA-Data can be implemented if additional Upstream EFs from DBs (Sphera MLC or other DBs (see chapter 5.2.6)) are added.

Figure 3: Decision tree on selection of emission factors for externally sourced electricity (Together for Sustainability, 2024)

3.8. Multi-output Processes: 5.2.9 in the TfS PCF Guideline v3.0

This chapter is about allocating inputs and impacts in multi-output situations, i.e., when a process delivers more than one product, referred to as co-products. The term co-product also includes energy products such as steam or electricity, or any other product which is defined as co-product and not as waste. Herein *energy* is understood as direct energy e.g., from exothermal reactions (PACT Methodology). Materials that are identified as waste following the decision tree in Figure 5.7 in the TfS PCF Guideline v3.0, Chapter 5.2.8.4, shall be excluded from the attribution of environmental burdens. Impacts from treatment processes shall be linked to the process, where the waste was generated.

Leaning on hierarchies described in the GHG Protocol Product Standard, ISO 14040:2006, ISO 14044: 2006, ISO 14067: 2018, PACT Methodology and the European Commission Environmental Footprint recommendations, the following steps shall be applied to attribute impacts in multi-output situations (see Figure 5.16 in the TfS PCF Guideline v3.0 and Figure 4 below).



(1) System expansion via substitution should only be used if there is a dominant, identifiable displaced product and production path for the displaced product based on sector consensus.
(2) In doubt. mass allocation should be prioritized. but there are instances where other allocation factors may be more suitable (e.g. volume for gases. energy content for energy).
(3) Sector specific guidance or PCRs shall be used if approved and required as Drop-in standards by TfS for Chemical Industry. by Catena-X for other automotive industry supplying sectors or by WBCSD pathfinder for sectors other than those covered by TfS and Catena-X.

Figure 4: Decision tree to show allocation rules and reduce assessment burden downstream (Together for Sustainability, 2024)

1. The approach described in published and accepted PCR, Industry Association projects, directives as e.g. REDII where available, for corresponding product systems shall be applied (see 5.2.4 Standards used in the TfS PCF Guideline v3.0, along with the list of TfS approved PCRs for chemical-specific product systems published on the landing page[2]). When more than one PCR exists for a product or product category, priority shall be given to allocation rules as described in chapter 5.2.9.3. in the TfS PCF Guideline v3.0.
2. Multi-output situations shall be avoided by using process subdivision, whenever possible. The common process shall be disaggregated into sub-processes that separately produce the co-products. Process subdivision may be done through submetering specific process lines and/or using engineering models to model the process inputs and outputs (GHG Protocol Product Standard).
3. If the multi-output situation cannot be avoided by subdivision, a system expansion shall be applied. System expansion refers to expanding the system by including the co-products into the system boundary and communicate LCIA results for the expanded system (PEF GUIDE 2012). System expansion and substitution can be a means of avoiding allocation. The product system that is substituted by the co-product is integrated into the product system under study. In practice, the co-products are compared to other substitutable products, and the environmental burdens associated with the substituted product(s) are subtracted from the product system under study (ISO 14044: 2006). System expansion by substitution (further referred to as “substitution”) is only acceptable if the Declared Unit stays as defined in chapter 5.1.3. in the TfS PCF Guideline v3.0. Substitution, as described in chapter 5.2.9.1 in the TfS PCF Guideline v3.0, shall be applied to attribute impact to co-products in multi-output situations if all the following apply:

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[2] https://www.tfs-initiative.com/pcf-guideline

   a. The co-products are generated in the process additionally but are not the main products of the process. Main products are defined as products that the process is operated for and optimized to produce. Additionally, the economic values of the main products are generally significantly higher than for the co-products.
   b. The co-product directly replaces an alternative product with a dedicated production process on the market. The production of this alternative product is reduced through provision of the co-product.
   c. Data about the impact of the alternative production process is available to calculate the LCIA of the alternative product.
   d. There is consensus for a production path of the displaced product agreed by TfS. TfS maintains and publishes a positive list of processes and product systems on the landing page[3].

4. In all other cases companies shall allocate the impact to co-products following the allocation rules described in chapter 5.2.9.3. in the TfS PCF Guideline v3.0. The applied approach to solving multifunctionality shall always be stated and justified.

TfS is aligned with PACT Methodology, Catena-X, GBA on the allocation hierarchy and thus the allocation approach as described in a PCR might be prioritized before system expansion and substitution. Since the PCR is ranked very high, it will overrule other approaches.

3.9. Mass balance & Chain of Custody (CoC): 5.2.10.5 in the TfS PCF Guideline v3.0

Chain of custody is an administrative process by which information about materials is transferred, monitored, and controlled as those materials move through supply chains (ISO 22095:2020). Mass balance is a chain of custody (CoC) model (ISO 22095:2020) used in multiple industries where it is not practical to maintain physical segregation of alternative and conventional feedstocks during processing. Mass balance helps enable a transition to a sustainable and circular economy by enabling the efficient co-processing of alternative materials in existing large-scale assets and complex supply chains. The alternative materials are not limited to bio-based feedstocks but could also consist of chemically recycled feedstocks, waste feedstocks, or CO_2-based materials.

Mass balance is especially important to many companies in the chemical industry that are transitioning to the use of waste-based materials and bio-based materials as feedstocks. This transition aims to reduce the usage of virgin fossil-based materials and help solve the global plastic waste dilemma through recycling.

Mass balance ensures that the quantity of output material is balanced with (does not exceed) the input of material and is appropriately adjusted for yields and conversion factors.

Co-processing of alternative and conventional materials results in the production of materials of mixed origin, which are not distinguishable in terms of composition or technical properties. Mass balance allows alternative content to be attributed to individual outputs, creating value from the use of alternative inputs. Large integrated assets cannot be transitioned immediately, and mass balance provides a critical bridge.

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[3] https://www.tfs-initiative.com/pcf-guideline

Since certain sectors, customers or regulatory frameworks may not support all possible chain-of-custody models and their attribution methods, the economic operator shall transparently communicate about it via the information model. This enables the customer to choose the desired product offering.

The following requirements shall apply for the usage of mass balance chain of custody in determination of LCA calculations:

1. The mass balance shall follow a transparent certification standard, and the conformance to the certification shall be verified by an independent and qualified third party. Different certification systems have different requirements which are in scope of this guideline.
    a. The certification system shall have clear chain of custody rules, traceability requirements, defined boundaries, guidelines for marketing claims, include safeguards against double-counting, and shall identify the type of sustainable raw material throughout the supply chain. Different certification systems have different requirements which practitioners can follow to be in line with this guideline.
    b. To attribute environmental characteristic (specified characteristics) of a sustainable input [4] (feedstock, fuel, energy, etc.) to a product of interest to generate a mass-balanced LCIA, a mass balance certification for the product shall be completed. The certification confirms the total required amount of feedstock, considering all losses.
    This amount of feedstock can be substituted with chosen sustainable feedstocks following the rules of the chain of custody certification schemes (for example, ISCC PLUS, REDcert[2], UL ECVP 2809, RSB Advanced Materials, FSC, RSPO, or equivalent).
    The section in the TfS PCF Guideline v3.0 considers a possible chain of custody certification scheme, the mass-balancing, in detail. The chain of custody certification scheme allows a variety of system boundaries (e.g., process, plant, site, multi-site) and attribution methods.
    Upcoming standards that shall be used are ISO/FDIS 13662 that defines Mass balance requirements in detail and ISO 14077 that describes the calculation of LCA with CoC models as basis.
2. The LCA of the manufacturing process in which the mass balance attribution occurs shall be in conformance with ISO 14044 [ISO 14044: 2006]. The study shall document how the material flow and attributions were calculated. For the LCIA calculation, the system boundaries for the fossil and the mass-balanced product shall follow the standards mentioned in section 5.2.4. in the TfS PCF Guideline v3.0.

All other requirements defined in the TfS PCF Guideline v3.0 shall apply. The examples are generic and can be used in an LCIA context as well.

In the TfS-Chem X “Circularity Guideline” more details related to CoC models can be found.

So far mass-balance credit transfer is not addressed in this guideline.

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[4] e.g. circular, bio or low carbon feedstocks are examples for sustainable feedstocks.

3.10. Process Data Quality and Share of Primary Data: 5.2.11 in the TfS PCF Guideline v3.0

Primary Data Share

To create visibility on the share of primary data in LCIA calculations, the Primary Data Share (PDS) in each dataset shall be determined (and shared) (PACT Methodology). PDS score may differ among the several impact categories, depending on the data input used respectively. The calculation and reporting of a PDS will become mandatory for PCF issued from 2027 onwards, giving companies sufficient time to prepare. So far, for other impact categories it is recommended to do it on a voluntary basis

More details listed in the data exchange format, particularly regarding when this field will become mandatory.

The PDS can be assessed by calculating the proportion (%) of the total impact per impact category in impact equivalents, e.g. H^+ eq, NMVOC eq etc. that is derived by using primary data in the cradle-to-gate system boundary (see Formula 2 belowFormula).

See glossary for definitions of primary and secondary data.

$$\mathrm{PDS}_{\mathrm{DU}} = \Sigma\ (|\mathrm{IC}i| * \mathrm{PDS}i)\ /\ \Sigma\ |\mathrm{IC}i|$$

Formula 2: Calculation approach of the PDS (Primary Data Share)

Where:

- DU is the Declared Unit
- $\mathrm{PDS}_{\mathrm{DU}}$ is the primary data share of $\mathrm{LCIA}_{\mathrm{DU}}$, in % (0-100%)
- i is any input or output of a process, except the DU
- $|\mathrm{IC}i|$ is the absolute value of the Impact Contribution of i to $\mathrm{LCIA}_{\mathrm{DU}}$, in kg LCIA e/DU
- $\mathrm{PDS}i$ is the Primary Data Share of contributor i, in % (0-100%)

Process Data Quality

During the data collection process, companies shall assess the data quality of LCIA contributors (emission factors and/or direct emissions data) by using the data quality indicators (DQIs). The data quality of each LCIA shall be calculated and reported.

If data with higher quality exists in-house than available in secondary databases (for example, in-house emission factors for fuel) and is used for calculations, the adequacy of such in-house data shall be reviewed and reported in a DQR following the criteria outlined in chapter 5.2.11 of the TfS PCF Guideline v3.0 more in detail. Data sourced from verified emission factor databases (see chapter 5.2.6 in the TfS PCF Guideline v3.0) shall be reported in a DQR as well, addressing its representativeness, relevance, and correct application to the product in question as well. The calculation and reporting of a DQR will become mandatory for PCF issued from 2027 onwards, giving companies sufficient time to prepare. For other impact categories it is recommended to do it on a voluntary basis.

Assessing data quality during data collection allows companies to make data quality improvements more efficiently than when data quality is assessed after the collection is complete. Additionally, understanding the quality of the data allows companies to identify key secondary data sources that should be improved or replaced with primary data for companies to be able to track the impact of emissions reduction plans more accurately.

The requirements of this guideline were harmonized with PACT Methodology, Catena-X and GBA. Three DQIs are required for the assessment of data quality

The process starts by assessing the technological, geographical, and temporal representativeness of emission factors and direct emissions data only for each impact contributing material. Emission factors can be contained in, or derived from, company-specific or secondary datasets, for which the same matrix should be used to assess the quality of this data. Direct emissions data can be derived as explained in chapter 5.2.8.5 (in the TfS PCF Guideline v3.0) and should also use the same matrix proposed for emission factors. The rationale behind this approach is described in the TfS PCF Guideline v3.0.

The quality indicators are summarized in Tables 5.14-5.16 (in the TfS PCF Guideline v3.0). Data quality rating criteria shall follow the approach outlined in Section 5.2.11.2 of the TfS PCF Guideline v3.0. The quality levels of TeR, GeR and TiR are expressed in five categories, from 1 to 5, where 1 is the optimum result in each indicator. The representativeness (technology, geography, and temporal/time-related) characterizes the degree to which the processes and products selected depict the system analyzed.

- **Technological Representativeness (TeR)**: the degree to which the data reflects the actual technology(ies) used in the process.
- **Geographical Representativeness (GeR):** the degree to which the data reflects actual geographic location of the processes within the inventory boundary (e.g., country or site).
- **Temporal/Time Representativeness (TiR):** the degree to which the data reflects the actual time (e.g., year) when the process was assessed.

The general calculation of data quality ratings is shown in the following formula:

$$\mathrm{DQR}i = (\mathrm{TeR}i + \mathrm{GeR}i + \mathrm{TiR}i)\ /\ 3$$

Formula 3: Calculation approach of the DQR (Data Quality Rating)

DQR of product(s) obtained from a process with one or more input materials:

$\mathrm{DQR}_{\mathrm{DU}} = \sum (|\mathrm{IC}i| * \mathrm{DQR}i) / \sum |\mathrm{IC}i|$, for $|\mathrm{IC}i| \geq 0.05 \sum |\mathrm{IC}i|$

Where:

- DU is the Declared Unit
- $\mathrm{DQR}_{\mathrm{DU}}$ is the data quality of $\mathrm{LCIA}_{\mathrm{DU}}$, in range 1-5
- i is any input or output of a process, except the DU
- $|\mathrm{IC}i|$ is the absolute value of the Impact Contribution of i to $\mathrm{LCIA}_{\mathrm{DU}}$, in kg LCIAe/DU
- $\mathrm{DQR}i$ is the Data Quality of contributor i, in range 1-5

Note: $\mathrm{DQR}_{\mathrm{DU}}$ is a linear combination of $\mathrm{DQR}i$. $\mathrm{DQR}i$ is based on the assessment of $\mathrm{TeR}i$, $\mathrm{GeR}i$ or $\mathrm{TiR}i$ and will yield the respective value of a $\mathrm{DQR}i$ for DU.

The DQR_{DU} shall be calculated for the output of e.g., 1kg or 1t, as defined in the Declared Unit.

Both the primary data share and the data quality ratings may differ from one impact category to the other: consequently, they will be reported separately for each impact category in the data model.

Data quality is handled in many LCA as support in the interpretation phase. Different approaches exist and they are discussed in several publications. Some examples of application and further reading can be found in literature as well (Edelen 2016), (Lewandowska 2021) and (Kölsch 2023).

3.11. Literature

Edelen, A., Ingwersen, W.W., Guidance on Data Quality Assessment for Life Cycle Inventory Data, (2016), Report number: EPA/600/R-16/096, EPA/600/R-16/096 | June 2016 | www.epa.gov/research; (accessed on 18 December 2025).

GHG Protocol Product Standard, (2011), Product Life Cycle Accounting and Reporting Standard; https://ghgprotocol.org/product-standard; (accessed on 18 December 2025).

ISO 14040:2006+Amd 1: 2021, (2020), Environment Management-Lifecyle Assessment-Principles and Framework

ISO 14044:2006+Amd 2: 2020, (2020), Environment Management-Lifecyle Assessment-Principles and Framework

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4. GHG emissions / PCF (Global Warming Potential)

For the impact category Global Warming Potential and the rules of determining the product carbon footprint it shall be referred to the TfS PCF Guideline available on the landing page[5].

According to the TfS PCF Guideline v3.0, the GHGs that shall be accounted for are identified within the GHG Protocol titled "Required Greenhouse Gases in Inventories: Accounting and Reporting Standard Amendment". The list includes Carbon dioxide (CO_2), Methane (CH_4), Nitrous oxide (N_2O), Hydrofluorocarbons (HFCs), Perfluorinated compounds, Sulphur hexafluoride (SF_6), Nitrogentriflouride (NF_3), Perfluorocarbons (PFCs), Fluorinated ethers (HFEs), Perfluoropolyethers (e.g. PFPEs), Chlorofluorocarbon (CFCs) and Hydrochlorofluorocarbon (HCFCs). The GHG emissions shall be aggregated as CO_2-equivalents and should not be reported separately for individual gases.

The 100-year GWP characterization factors (GWP100y) according to the Intergovernmental Panel on Climate Change (IPCC) shall be used in the PCF calculations, based on the IPCC's Sixth Assessment Report (AR6).

These factors include climate carbon response for non-CO_2 gases. If in future there will be updates, TfS will update the guideline accordingly to follow the latest version.

According to ISO 14067, biogenic removals from CO_2 uptake during biomass growth shall be included in the PCF calculation. Additionally, all biogenic emissions (e.g. methane emissions from manure application etc.) and further emissions from relevant processes, such as cultivation, production and harvesting of biomass shall be included in the PCF [ISO 14067: 2018]. Furthermore, the biogenic carbon in products, fossil and biogenic GHG emissions and removals shall be reported. GHG emissions and removals from land use should be reported. Biogenic carbon in waste streams shall also be correctly reflected.

Removals of CO_2 into biomass shall be characterized in the PCF calculation as —1 kg CO_2/kg CO_2 when entering the product system, while biogenic CO_2 emissions shall be characterized as +1 kg CO_2e/kg CO_2 of biogenic carbon (ISO 14067: 2018). As referred to in Chapter 5.3.2, the PCF, that considers biogenic emissions and removals, shall be reported as PCF (including biogenic CO_2 removal).

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[5] https://www.tfs-initiative.com/pcf-guideline

5. Resource Use, fossils

5.1. General Description

Potential risks and impacts to the environment associated with chemical production and chemical products should be analyzed critically and in detail. One of the indicators selected by the TfS Chem X project was the “Resource Use, fossils”. This impact category was defined in earlier approaches when a characterization factor (CF) was applied as abiotic depletion potential (ADP_{fossil}). That relates to earlier versions of the ADP indicator, where minerals and metals as well as fossil fuels were assessed with a characterization model.

However, several limitations of ADP_{fossil} have been identified leading to the decision not using it anymore in EF:

- Resource Availability Uncertainty: The global reserves and extraction rates of fossil fuels are subject to significant uncertainty and fluctuation. This makes it challenging to provide a reliable, universally applicable depletion indicator.
- Limited Environmental Relevance: The environmental impacts associated with fossil fuel use extend beyond resource depletion, including greenhouse gas emissions, air pollution, and ecosystem damage.
- Lack of Policy Alignment: Modern environmental policies, especially in the European Union, focus on reducing overall fossil fuel consumption due to climate change concerns, rather than solely on resource scarcity.

Given these limitations, the EF methodology has shifted toward directly assessing fossil fuel use, typically measured in terms of energy content (e.g., megajoules of fossil energy used). This category does not apply to a characterization model as in EF, therefore energy content and energy use are the focus without referring to an environmental characterization model. In this sense, it is more a reporting element and does not address further impacts such as ecological degradation, biodiversity loss, and social impacts in extraction regions. That may be addressed in other impact categories.

The approach does not address other effects associated with resource depletion, is related to EF and therefore aligned with upcoming regulatory frameworks (e.g., ESPR).

In this chapter, we describe the resource use of fossil fuels.

When conducting an environmental assessment, “Resource Use, fossils” is assessed within most LCAs and derived mainly from Product Environmental Footprint (PEF). Although many practitioners or experts perceive “Resource Use, fossils” as an economic issue rather than an environmental one.

Upstream methane emissions and other extraction-related losses are reflected both in climate-related impact categories and in the ‘resource use, fossil’ indicator, as incorporated in current LCA databases.

5.1.1. Issues of Concern

Fossil fuels are finite resources. The continued extraction of coal, oil, and gas depletes reserves that have taken millions of years to form. As these resources become scarcer, their extraction grows more difficult and environmentally damaging, prompting concerns about long-term energy security and sustainability.

The combustion of fossil fuels releases significant amounts of GHGs, notably carbon dioxide, which drives global climate change. This warming effect alters weather patterns, raises sea levels, and threatens biodiversity. Air pollution from burning coal, oil, or natural gas also produces particulate matter, nitrogen oxides, and sulfur dioxide, which can degrade air quality and harm respiratory health.

Moving away from fossil fuels toward cleaner energy sources presents technical, economic, and social hurdles. Many industries, communities, and nations are deeply tied to fossil fuel infrastructure, making the shift to renewables complex and, at times, contentious. The chemical industry is rather unique, as it is currently doubly reliant on fossil raw materials, both for energy use and as a feedstock for the synthesis of the key chemical building blocks upon which chemical manufacturing is based on. In the future, fossil fuels will play a less important role. But the carbon in fossil feedstock might be more relevant for the chemical industry.

5.1.2. Key Components of Potential Impact

The depletion of abiotic resources was defined in different ways: a) decrease in the amount of the resource itself, b) decrease in world reserves of useful energy/exergy, or c) an incremental change in the environmental impact of extraction processes at some point in the future (Hauschild, 2011)), (Van Oers & Guinée 2016), (Finnveden et al. 1996), (Heijungs et al. 1997).

Following methodological discussions in EF, fossil fuels were categorized as a distinct type of resource, not comparable to minerals. Consequently, the method was changed to assess fossil fuels in terms of energy consumption without the application of a characterization model, as opposed to being linked with a specific resource characterization model. Therefore, it is termed as “Resource Use, fossils” instead of abiotic depletion, this term will be used for the remainder of the document.

Fossil fuels are used in industry, making it an important energy source. Therefore, it is considered in the category “Resource Use, fossils”.

5.1.3. Regulatory Compliance

Due to European regulatory schemes (e.g., Green Deal), there is a demand to shift from fossil resources to renewables.

5.1.4. Importance for the Chemical Industry

The chemical industry uses a wide range of fossil fuels. They play a crucial role in the chemical industry as important precursors. They are used as raw materials (feedstocks) to produce a wide range of chemicals, including plastics, fertilizers, pesticides, fibers, and personal care products. The chemical industry is one of the big consumers of fossil fuels and is responsible for roughly 3% of global anthropogenic CO_2 emissions (Our world in data, 2020), that are mainly derived from the use of fossil fuels and motivates the industry to reduce the use of them. In addition, among energy intensive industries, the chemical industry is one of the most challenging to defossilize due to the abundance of cheap fossil fuel-feedstocks. Among energy intensive industries, the chemical industry is one of the most challenging to reduce the use of their fossil fuel-feedstocks. They are not only used as fuel but also as building blocks of products. In this sense, the term “defossilization” not the best term to address.

Due to European regulatory schemes, such as the European Green Deal, there is a strong demand to shift from fossil resources to renewables. The Green Deal aims for climate neutrality, prioritizing the decarbonization of the energy system and building a power sector largely based on renewable sources. The Renewable Energy Directive sets ambitious targets for increasing the share of renewables in the energy mix. Complementary initiatives like the Fit for 55 package and the REPowerEU Plan further accelerate this transition by reducing fossil fuel dependency and promoting clean energy deployment. These policies are supported by substantial investments, signaling a systemic shift toward renewables.

Even though the impact category “Resource Use, fossil” does not consider the reserves of the different fossil resources, the assessment of "Resource Use, fossil" delivers valuable information for the transition of the chemical industry to a more sustainable use of fossil resources, as they are limited. It is therefore essential to use them in a responsible manner to enable future generations to access these feedstocks when other sources are not available. Renewables feedstocks normally have a much lower "Resource Use, fossil" compared to fossil feedstocks, as their inherent feedstock energy is derived from renewable sources, that do not count for "Resource Use, fossil".

Unlike other energy-intensive industries, the chemical industry cannot be made fully sustainable directly with renewable electricity and green electricity-based hydrogen (e-hydrogen). Therefore, alternative carbon feedstocks, such as biogenic materials, recycled materials or captured CO_2, must be developed to reduce the use of fossil resources in the production of large volume organic chemicals.

Fossil fuels are essential for various processes, including heating, generating steam, and providing raw materials for chemical production. The environmental impact of fossil fuel extraction and the importance of considering "Resource Use, fossil" in environmental assessments is a key element to be more sustainable in the future.

5.2. Methodology of Characterization

In van Oers & Guinée (2016) and van Oers et al. (2002), resource depletion was considered an environmental problem, while recognizing that views differ regarding this topic. The problem was defined as the decreasing natural availability of abiotic natural resources, including fossil energy resources, elements, and minerals.

The Lower Heating Value (LHV) is a crucial property for energy and fuel calculations, indicating the amount of heat released by a fuel during combustion, without accounting for the latent heat of vaporization of water. PEF 3.1 refers to the PEF Guide, version 3.1 (European Union 2021), which provides standardized factors for energy calculations and environmental assessments.

The authoritative LHV values from PEF 3.1 are available in the official PEF documentation, which should be consulted for precise and regulatory-compliant data. Including uranium in the list of fuels ensures that assessments and comparisons encompass all significant energy sources in modern energy systems.

In order to facilitate improved communication between the two communities in the future, it is recommended to use the terms 'resources' and 'reserves' in a consistent manner. In the next chapter only the chosen EF method is described more in detail, whereas the description of other impact assessment methods as Exergy, Swiss Ecoscarcity and EDIP 1997 can be found in the in the Appendix 11.1.1.

5.2.1. Chosen Method: EF

Based on comprehensive LCIA method evaluations, the abiotic depletion potential for fossil fuels (ADP fossil fuels) by van Oers et al. (2002) as implemented in the CML method is recommended to assess Resource use of fossil fuels in LCA for chemical industry products and materials. The CML method allows for global applicability across diverse regions and markets. Its widespread adoption by international standards and industry guidelines, such as the EF method by the European Commission makes it the preferred choice for harmonization efforts across the chemical sector and beyond (Hauschild, 2011). The scope of this impact category specifically addresses fossil fuels and non-renewable energy carriers, with the CML method (2016) demonstrating methodological stability as it is based on the LHV of fossil resources without requiring frequent updates. In contrast to related methods using the Higher Heating value such as Cumulative Energy Demand- non renewables (CED-non renewables) (Frischknecht et al. 2015), focus on LHV represents the amount of energy that can practically be recovered from fossil fuels in industrial applications.

ADP fossil is not used anymore in the EF context, so we will use the new term “Resource use, fossil” in this guideline.

Resource use fossil as an environmental impact category reflects the potential depletion of fossil resources due to their extraction and use, but it is not a physical property of the product itself.

For fossil-based products, the “Resource use fossil” value typically exceeds the product’s LHV, because it accounts not only for the fossil content embedded in the product but also for the upstream fossil resource consumption throughout the pre-chain. However, due to allocation rules applied in multi-output processes, it is possible that the calculated Resource use fossil for a specific product is lower than its LHV. This does not imply an error but reflects the chosen allocation method, which shall be applied uniformly across all impact categories.

In such cases, besides Resource use fossil also the LHV can be reported. A comment should be included to explain why the Resource Use Fossil is lower than the LHV, ensuring transparency and enabling accurate modelling in downstream processes*.

Additionally, for products with partial or full biogenic content, the Resource use fossil may be significantly lower than the LHV, since biogenic inputs do not contribute to fossil resource depletion.

Importantly, the total Resource use fossil across all outputs of a process should reflect the actual fossil resource demand. If allocation results in a lower Resource use fossil for one by-product, it will be correspondingly higher for the other by-product(s), maintaining consistency at the process level*.

How to accurately report:

*Proposed text for a comment in the data exchange format: 'Note that the "Resource use, fossil" value is lower than the LHV of the product. This may be due to e.g. allocation effects and/or due to biogenic content in the product'.

Formula

Based on all the choices described above, the characterization model can be described. The characterization model is based on the LHV of fossil fuels. The method has been made operational for fossil fuels (actually: the energy content of fossil fuels). The assessment reflects the use of fossil fuels. It shall be expressed in Megajoule (MJ). In accordance with the general structure of the LCIA, the impact category indicator results for the impact category of "Resource use, fossils" is calculated by multiplying LCI results, extractions of fossil fuels (in MJ) by the CFs. It is calculated as outlined in the following formula to calculate the "Resource use, fossils" for all fossil materials and inputs:

$$\text{Kg fossil fuel} * \text{LHV (MJ/kg)} = \text{MJ}$$

Formula 4: Calculation approach of "Resource use, fossils"

$$\text{“Resource use, fossils”} = \sum (I_{i\text{-Resource use, fossil}} \times \text{LHV}_{i\text{- Resource use, fossil}})\ [\text{MJ per kg}]$$

Formula 5: Equation for "Resource use, fossils" calculation

Where:

- $I_{i\text{-Resource use, fossil}}$ = Input of fossil materials (e.g., Oil, gas, coal, lignite, ...)
- $\text{LHV}_{i\text{- Resource use, fossil}}$ = Lower heating value (LHV) per fossil input

The impact of "Resource use, fossils" is, therefore, expressed in MJ per kg.

Characterization Factor in EF Method

The LCI flows and the respective CFs for the "Resource use, fossils" category are based on the van Oers et al. (2002) model, extracted from EF 3.1 and are presented in Table 5. In case of missing CFs, these values can be used. Specific CFs shall be addressed and used in LCA studies, because these values can differ depending on the quality of the fuel used as well as their regional specifications. The Table 5 shows an overview of existing average numbers for the assessment of the midpoint category "Resource use, fossil":

*Table 5: Overview of average LCI flows recommended**

Flows	CFs (MJ/kg)
Brown coal (Lignite)	12
Hard coal	25
Crude oil	42
Natural gas	49
Peat	8.4
Pit gas	40
Pit methane	49
Uranium**	546,000
Uranium oxide	332,000

*Note: Different CFs values were identified for the LCI flows from EF 3.1 depending on the LCA software used. It is recommended to use the latest EF version proposed by the LCA software provider.

**Uranium is included here because, despite not being a conventional combustible fuel, it is a primary energy source in nuclear power generation. Its energy content is not measured by LHV in the traditional sense, as its energy is released through nuclear fission rather than combustion. However, for the purposes of standardized energy comparisons in environmental assessments and lifecycle analyses, the energy released by uranium through fission can be quantified and is sometimes referenced in terms comparable to heating values. This allows for a more comprehensive comparison across all major energy carriers, ensuring that analyses can account for the vast energy potential of nuclear fuels just as they do for fossil fuels and renewables. It was decided in the Technical advisory board of the EU commission to keep it on the list and to generate a kind of LHV which allows a combination with conventional fossil fuels.

The full list of LCI flows (incl. respective CFs) can be found under the following link: EF 3.1.

EF 3.1 provides regionalized CFs for “Resource use, fossil” for relevant elementary flows, when using impact assessment method package for EF 3.1 provided by example Sphera MLC. However, depending on the LCA database or software provider (e.g., ecoinvent, openLCA), also only averages may be included in their impact assessment method for calculation (like the water footprint with AWARE methodology, see Chapter 0). Averages should be used to increase consistency. The goal for the future should remain to switch from average to more regionalized CFs.

5.2.2. LCI Flows

Table 6 shows a few examples of LCI flows for “Resource use, fossil”.

Table 6: Description of relevant LCI flows concerning Resource use, fossil

LCI Flow	**Description of Flow**
Brown Coal (Lignite)	Brown coal, or lignite, is a type of soft coal that is low in carbon content and high in moisture. It is primarily used for electricity generation in power plants due to its high-water content and lower energy density compared to harder coals. In the chemical industry, lignite can be converted into synthetic natural gas and other chemicals through gasification processes.
Hard Coal	Hard coal, also known as bituminous coal, has a higher carbon content and energy density than lignite. It is widely used in electricity generation and in the production of coke for steel manufacturing. In the chemical industry, it serves as a feedstock for various chemical processes, including the production of chemicals like methanol and ammonia.
Crude Oil	Crude oil is a liquid fossil fuel composed of hydrocarbons and is a primary source for fuels and petrochemicals. In the chemical industry, crude oil is refined into various products such as gasoline, diesel, and feedstocks for producing plastics, fertilizers, and other chemicals.
Natural Gas	Natural gas is a fossil fuel primarily composed of methane. It is used for heating, electricity generation, and as a feedstock in the chemical industry. Natural gas is crucial for producing ammonia (via the Haber process) and methanol.
Peat	Peat is an accumulation of partially decayed organic matter found in wetlands. It is primarily used as a fuel in some regions and can be processed into biofuels. In the chemical industry, peat can be converted into activated carbon and other chemicals, although its use is less common compared to other fossil fuels.
Pit Gas	Pit gas refers to gases released during the extraction of coal, primarily methane. It is often captured and used as a fuel source for heating or electricity generation. In the chemical industry, pit gas can be utilized as a feedstock for producing chemicals or energy.
Pit Methane	Pit methane, like pit gas, is methane released from coal mines. It is typically harnessed for energy production and can also be used in chemical processes. Its capture and utilization help reduce GHG emissions from mining operations.
Uranium	Uranium is a heavy metal used as fuel in nuclear reactors. In the chemical industry, it is primarily involved in the production of nuclear energy.
Uranium Oxide	Uranium oxide is a compound of uranium used as fuel in nuclear reactors. It is typically processed from uranium ore and is essential for the nuclear fuel cycle. In the chemical industry, uranium oxide plays a crucial role in energy production through nuclear fission.

The full list of LCI flows (incl. respective CFs) can be found under the following link: EF 3.1.

5.3. Assessment Examples

Figure 5 provides some assessment examples for Resource use, fossils. Following the Formula 5, all "Resource use, fossils" are calculated. For electricity as an example, the efficiency of a factor 3 was used, meaning that 3 MJ primary energy is needed to generate 1 MJ of electricity. This number can vary significantly depending on energy generation technology. For the transfer to kWh which is often used as well, the factor is 3.6. For steam production an efficiency of 90 % is considered and the energy content of 1 kg steam is considered as 2.5 MJ / kg. This varies as well, depending on the production technology and the pressure of steam.

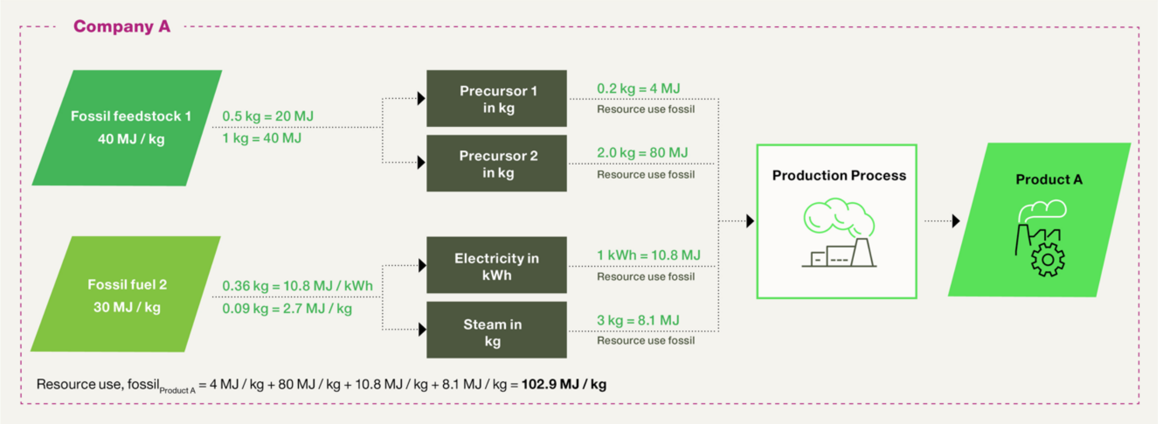

Figure 5: Assessment example for Resource use, fossils

5.4. Literature

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6. Water Scarcity

6.1. General Description

Water is an indispensable resource for life and a critical input for numerous industrial processes, including chemical production. The sustainable management of water resources has become a significant concern, considering the increasing demand and the impact of water scarcity on the environment and society. Water scarcity is an important impact category in LCA and is being increasingly included in environmental assessments

Comparable to the Product Carbon Footprint which is an LCA study focusing on only one environmental impact, a water footprint (ISO 14046:2014) is defined as metric(s) that quantifies the potential environmental impacts related to water within LCA. If water-related potential environmental impacts have not been comprehensively assessed, then the term “water footprint” can only be applied with a qualifier. A qualifier is one or several additional terms used in conjunction with the term “water footprint” to describe the impact category/categories studied in the water footprint assessment, e.g. “water scarcity footprint”, “water eutrophication footprint”, “non-comprehensive water footprint”[6]. This chapter delves into the concept of water scarcity within the framework of LCA and its application in the chemical industry. Water scarcity as described in this guideline is considered a non-comprehensive water footprint.

6.1.1. Issues of Concern

According to ISO 14046 water scarcity is defined as the extent to which demand for water compares to the replenishment of water in an area, e.g. a drainage basin, without considering the water quality.

According to Joint Research Centre (JRC), water scarcity assesses water use impacts by considering both consumption and regional water stress levels (JRC, 2018). The Figure 6 shows the relation between Water use, Consumptive Water and Water Scarcity. The water scarcity can therefore be calculated by multiplying the inventory data of water consumption with the CF of the country. Relevant CFs are defined by different LCIA methodologies.

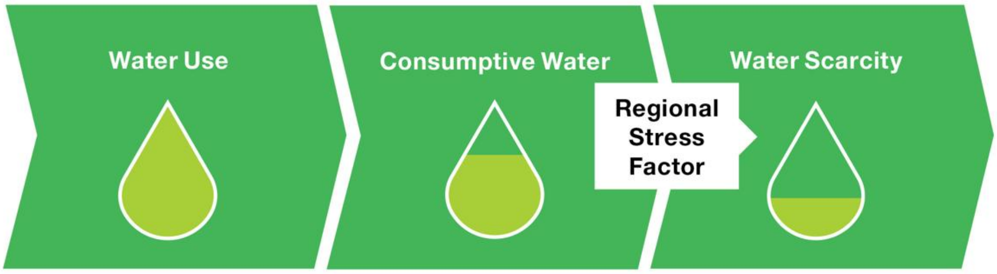

Figure 6: Definition of water scarcity footprint

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[6] The principle of comprehensiveness implies to consider all environmentally relevant attributes or aspects of natural environment, human health and resources related to water, including water availability and water degradation.

According to ISO 14046:2014, Consumptive Water Use refers to the volume of freshwater withdrawn and not returned to the same watershed. Water consumption can be because of evaporation, transpiration, integration into a product, or release into a different drainage basin or the sea. Change in evaporation caused by land-use change is considered water consumption (e.g. reservoir).

The environmental impact of water consumption largely depends on the availability of water in a given country where the process is located. Using water in areas with plentiful resources typically has different consequences than in countries facing water scarcity. These differences are captured through water stress indicators from countries where water is used in the life cycle of a product. This assessment method focuses exclusively on the quantity of water used.

6.1.2. Key Components of Potential Impact

Water scarcity can have significant effects on ecosystems (destruction of aquatic habitats and effects on biodiversity), human health (malnutrition and infectious diseases) and natural resources (depletion of water reserves for future generations).

Integrating water scarcity into environmental assessments is crucial for promoting sustainable water management practices. It allows for a comprehensive understanding of how water resources are utilized and helps in the development of policies and strategies that balance water use with conservation. This can include initiatives such as efficient irrigation techniques, water recycling programs, and the promotion of water-saving technologies.

Water scarcity issues in many countries or regions are getting very important nowadays. Changes in precipitation patterns, increased evaporation rates, and the frequency of extreme weather events can all influence water availability.

When water is diverted from rivers, lakes, or aquifers for consumptive purposes, the reduced water availability can impact aquatic habitats, alter water temperature, and affect the quality of the remaining water. These changes can threaten the survival of fish and other aquatic organisms, disrupt breeding and feeding patterns, and lead to the degradation of wetlands and riparian zones (EU commission 2025).

6.1.3. Regulatory Compliance

Water scarcity represents critical global challenges in sustainable resource management, prompting the European Union and other jurisdictions to establish regulatory frameworks aimed at preserving freshwater availability and promoting responsible water use. The Water Framework Directive (WFD 2015) provides a comprehensive basis for water resource protection, requiring Member States to assess and manage water quantity alongside quality, and to ensure sustainable abstraction and use of water bodies to achieve “good status”. In parallel, the Groundwater Directive (European Union, 2006) complements these efforts by regulating groundwater abstraction and preventing overexploitation, thereby safeguarding long-term water availability.

To address agricultural pressures on water resources, the Common Agricultural Policy (CAP) incorporates water-related conditionalities and incentives for efficient irrigation practices, drought-resilient cropping systems, and water-saving technologies. These measures align with broader EU goals for climate adaptation and resource efficiency.

Globally, water scarcity has driven policy responses such as the U.S. WaterSMART Program, which promotes water conservation and reuse in drought-prone regions, and the UN Sustainable Development Goal 6, which calls for universal access to clean water and sustainable water management. These initiatives reflect growing recognition of water footprint as a key environmental indicator in LCA, especially in countries facing hydrological stress.

6.1.4. Importance for the Chemical Industry

The chemical industry uses significant amounts of water, with applications ranging from chemical synthesis to cooling and cleaning. The sector's water use is broadly categorized in Table 7. More information can be found in CORDIS - EU research results (EU 2016).

Table 7: Water usage categories within chemical industries

Category	**Description**	**Example**
Chemical Synthesis	Water is a crucial reactant and solvent in many chemical processes. It facilitates reactions, dissolves reactants, and helps in the separation and purification of products.	In the production of ammonia through the Haber process, water is used to generate hydrogen via steam reforming natural gas.
Heating and Cooling Systems	Cooling and heating are vital for maintaining operational safety and efficiency in chemical plants.	Water is used in cooling towers, as heat exchangers, and in other cooling systems to dissipate heat generated during exothermic reactions and mechanical operations.
Cleaning and Maintenance	Water is essential for cleaning equipment, maintaining hygiene standards, and preventing contamination between production batches.	High-purity water is often required to meet stringent quality standards.
Waste Treatment	The chemical industry generates various effluents that require treatment before discharge or reuse.	Water is used in the treatment processes, including dilution, neutralization, and biological treatment.
Steam generation and condensation	Steam in the chemical industry refers to steam that is produced on-site or off-site, which is then used for heating, power generation, or driving equipment.	Typically, freshwater is used to produce steam. A closed circuit helps to recover steam condensate. However, any loss of steam condensate should be replaced with fresh water.
Evaporation	Some chemical processes produce water vapor, which is water evaporated from the process. In addition, evaporation can be used for cooling. Evaporated water is usually not directly emitted back to the water body / basin where the water initially comes from	While using the spray drying process, for example by producing dispersible polymer powder, water vapor occurs which sometimes evaporates without further use.
Water in products	The chemical industry also produces aqueous based products via emulsion-based polymerization. The water contained in products as raw material usually is consumptive water.	Aqueous dispersion, solutions,

Note: The table contains non-exhaustive list of examples for water scarcity and therefore might not cover all categories relevant for the water scarcity application.

6.2. Methodology of characterization

This section outlines the approach used to characterize water use impacts in accordance with international standards and best practices. It begins with relevant ISO guidance, followed by the rationale for selecting the Environmental Footprint (EF) method as the primary LCIA methodology for water footprint. Finally, it explains how the EF method is applied in practice to quantify the water footprint.

6.2.1. Chosen method: EF

ISO 14046:2014 outlines the principles, requirements, and guidelines for conducting a water footprint assessment within the framework of environmental LCA. ISO 14046 uses ISO 14040:2006 and ISO 14044:2006 as normative references and applies all general principles of these standards

The ISO standard addresses both consumptive water use, and water-related impacts, such as water scarcity. It emphasizes the local context of water availability and scarcity, recognizing that the same quantity of water use can lead to different impacts depending on the location.

Although ISO 14046 does not prescribe a specific LCIA method for water-related impacts, it provides a conceptual framework for applying scientifically validated models. These models typically use data on water availability and withdrawals to quantify water scarcity level, which is usually done with the geographical resolution on water basin and country level.

To support alignment with international best practices and ensure regionally sensitive assessments, the AWARE (Available WAter REmaining) method was developed in accordance with ISO 14046 (Boulay, et al. 2018). It also serves as the basis for the water scarcity indicator used in the EF method developed by the European Commission. While water scarcity category in EF is derived from AWARE, it includes modifications to the original CFs to improve the differentiation of countries and to align with the European Union's policy goals and data quality standards.

Choosing the EF method over the standalone AWARE approach supports greater consistency with other environmental impact categories assessed under the EF framework and facilitates broader acceptance and comparability of results. Given its widespread application in product-level environmental assessments and alignment with both ISO standards and European guidance, EF provides a robust and harmonized basis for evaluating water scarcity impacts in life cycle assessments.

These models are based on the pre-selected methods reported in the ILCD Handbook (Hauschild et al., 2011).

Furthermore, it's the only available compilation of characterization methods covering the whole breadth of 16 impact categories, and which is subject to a scientifically maintained cross consistency check (through JRC).

In the Environmental Footprint (EF) method, Water Scarcity is represented as Water Use. This should not be mixed with simple water consumption that ignores local water stress levels.

The EF indicator follows ISO 14046 standards and measures how water use in a specific country may limit availability for other users—both people and ecosystems. It reflects the potential impact of water scarcity at the midpoint level.

Formula

The EF method calculates Water Scarcity impact using the following formula:

$$\text{Water Scarcity [m}^3\text{ world eq.]} = \text{Consumptive Water Use [m}^3\text{]} \times \text{EF water scarcity CF [m}^3\text{ world eq./m}^3\text{]}$$

Formula 6: Equation for "Water Scarcity" calculation

Where:

- Consumptive Water [7]Use refers to the volume of freshwater withdrawn and not returned to the same watershed (e.g., via evaporation, incorporation into products, or transfer to other basins or the sea).
- EF CFs are applied based on the geographic origin (Country level) of water use.

The resulting unit, m^3 world equivalent, facilitates comparison across different countries and systems.

Remark: water that is generated in a chemical reaction contribute negatively to consumptive use and reduces the consumptive water use of a process if this water is captured and transferred to a watershed.

Characterization Factor in EF Method

In the EF method, each country is assigned a CF that reflects its relative water scarcity, normalized against the global average. A CF of 1 represents the global average water scarcity level. In practice, CFs range from 0 (no scarcity) to well above 1, even reaching values near 100 in extremely stressed countries. These CFs are determined using hydrological models such as WaterGAP3 and account for water availability, sectoral demand, and environmental flow needs.

Official EF CFs are maintained by the European Platform on Life Cycle Assessment (EPLCA) and are available as part of the EF LCIA method documentation:

- EF reference package spreadsheet can be downloaded from https://eplca.jrc.ec.europa.eu/LCDN/developerEF.html
- CFs can be assessed by geographically defined countries, ensuring as much as possible accurate assessments.
- Practitioners can integrate CFs directly or use them via LCA software platforms that support the EF method.

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[7] In some sources, this may be referred to as blue water consumption. However, we adopt the ISO terminology for consistency with international standards

It should be noted that water scarcity can vary significantly within a country. Companies can choose a more specific CF if the source of this CF is referenced. Although this is a slight deviation from the EF method, it is important to allow increased specificity where available.

Selection Guidance

In the spreadsheet “Cradle to Grave Template with EI 3.10 Emission Factors”, tab “lciamethods_CF”, CFs are provided for specific water flows and countries. Notably, the same specific values may appear as either positive or negative, depending on whether the water flow represents an input or output for that country. This approach ensures that the water mass balance is maintained across the modeled product system.

To correctly select and apply the appropriate CFs in each calculation, the following considerations are important:

- For practitioners using standard background databases available on the market as sources of secondary data, CFs are typically pre-selected and applied within the datasets. However, these background databases may carry uncertainties regarding the country and flow-specific granularity of CF application. In the absence of primary data, such limitations are acknowledged, and these datasets are treated as the best available solution.
- For practitioners modeling foreground processes, it is essential to know the country associated with each individual inflow and outflow of water.
- If all water flows pertain to the same country, net consumptive water use can be calculated and multiplied by the positive CF provided by the EF method for that country.
- However, if the origin and/or destination of water flows differ across countries, it is critical to apply the correct CF based on both the flow name and corresponding country. This ensures an accurate water balance and appropriate characterization of water use across the product system.

6.2.2. LCI Flows

Calculating water scarcity is a critical aspect of understanding and managing water usage in various processes and products. LCI flows play a pivotal role in this calculation, as they provide the necessary data on the inputs and outputs associated with water use.

To assess water scarcity impacts, LCI data should ideally be collected with spatial resolution, preferably at the watershed or basin level. However, in alignment with the EF method, which applies country-level CFs, this document focuses on the collection of annual, country-specific water use data. This approach is deemed as adequate to achieve scale in the water scarcity assessment at current levels of data availability.

If water is qualified as freshwater, it typically contains less than 1 000 mg/l of dissolved solids and is generally accepted as suitable for withdrawal and conventional treatment to produce potable water. If the water quality is changed from freshwater to brackish water (1 000 mg/l to 30 000 mg/l) or to seawater (concentration of dissolved solids greater than or equal to 30 000 mg/l), this is considered as consumptive water use.

In Table 8 the key LCI flows needed for the calculation of a water footprint, along with precise examples, are shown:

Table 8: Checklist of Water Flows for Consumptive Use Assessment (Aligned with EF method – country-level resolution)

Water Use Element	**Examples**	**Data Required**	**Contributes to Consumptive Use?**[8]
Water input from environment[6, 7]	River, lake, groundwater withdrawal	Source type, country, volume	**No**
Water from water supply system	Municipal supply	Supplier, country of withdrawal, volume	**No**
Water incorporated into product[9,10]	Water contained in final product	Estimated or measured volume	**Yes**
Evaporation	Boiling, drying, cooling towers	Estimated volume	**Yes**
Water lost via drift or leaks	Open systems, faulty pipes	Estimated volume	**Yes**
Water transformed, chemically bound or contained	Chemical reactions (consumed or produced), incorporated in waste	Volume, transformation description	**Yes**
Return to same country*	Discharge to surface or sewer	Volume, water quality, receiving country	**No**
Return to a different country	Discharge across borders (e.g., via pipeline)	Volume, receiving country	**Yes**
External wastewater treatment	Sent off-site for treatment	Volume, treatment type, discharge country	**Possibly**, depends on final quality[6]
Onsite recycled/reused water	Cooling systems, process loops	Volume reused	**No**
Stormwater harvested	Rainwater used in processes	Volume used, purpose	**No**
Incidental water uses	Firefighting or spills		**Possibly**[11]

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[8] Water generated during chemical reactions in a process reduces overall consumptive use (negative consumptive use), as it adds to the available water rather than depleting it.

[9] if fully returned in usable quality

[10] Note on water quality:

- If return water is degraded to the point that it is no longer usable, it is functionally lost and should be counted as consumptive.
- If water undergoes adequate on-site or off-site treatment before discharge, it is considered returned in usable form and thus non-consumptive.
- If water is discharged with pollutants exceeding regulatory or ecological thresholds, it may be considered fully consumptive (in practice, partial consumptiveness is generally not accounted for in LCA databases).

[11] Incidental water uses, such as firefighting or spills, are excluded from LCI unless they are frequent, systemic, and materially significant at the product level.

6.2.3. Data Granularity

Water Balance and Cut-off Criteria

To ensure data consistency and completeness, a water balance check should be performed across the system boundaries. The relative difference between total water inputs and outputs should not exceed 5% in absolute value, which is considered acceptable based on best practice in water footprinting. Flows below this threshold are considered negligible and are excluded only if they have no significant influence on the overall results. All exclusions should be transparently documented and justified to maintain methodological robustness.

As a best practice, conservative assumptions and adjustments may be applied to water flow data to correct imbalances (>5%) and ensure a closed water balance (section 6.2.4.1.1).

Corrective Considerations for Surplus Water Outputs

In cases where the water balance shows more water output than input, a discrepancy may exist that warrants further investigation. While such imbalances may arise from measurement errors or data gaps, they can also result from physical or chemical phenomena that are not always captured in initial flow inventories. The following corrective approaches outline common causes and recommended methods for resolution.

Case 1: Water Formation Through Chemical Reactions

In certain processes, water is generated as a byproduct of chemical reactions (e.g., condensation reactions, neutralizations, or combustion). This additional water may appear in the output flows (e.g., wastewater, steam, or emissions), leading to an apparent surplus relative to measured inputs.

Recommended Action: Perform a stoichiometric analysis of the relevant chemical reactions to quantify the amount of water produced. If the calculated water formation aligns with the imbalance, it is considered a valid explanation. The result should be documented and included as an internal source of water in the inventory.

Case 2: Water Content in Raw Materials

Some input materials may contain inherent moisture (e.g., wet biomass, slurries, agricultural products) that are not initially accounted for as a separate water input. This moisture can be released during processing and counted as part of water output (e.g., in evaporated or discharged streams).

Recommended Action: Review the moisture content of raw material inputs and estimate the corresponding water mass using material specifications or literature data. Adjust the water input inventory accordingly to account for this internal water source.

Case 3: Rainwater Entering Water Output Flows

In some cases, rainwater may unintentionally be included in measured water outputs, particularly in outdoor or open-system facilities where stormwater enters wastewater drains, surface runoff collection systems, or treatment infrastructure. This can result in apparent excess output water volumes relative to the reported input water, thus distorting the water balance.

This is particularly relevant in methodologies such as the EU PEF, where rainwater is not characterized with any water scarcity impact factor. Including rainwater in output flows without adjusting the inventory can lead to misinterpretation of results, specifically:

- Artificially high output volumes that appear to "offset" consumptive water use.
- Incorrect attribution of negative water scarcity impacts (credits).
- Recommended Action: Identify if the water output streams include rainwater contributions.
- Estimate the volume of rainwater using local precipitation data, catchment area dimensions, and runoff coefficients.
- Deduct the calculated rainwater volume from the water output inventory.

Example: If a facility discharges 5,000 m^3 of water annually and 500 m^3 is estimated to originate from rainwater collected on impermeable surfaces, only 4,500 m^3 should be reported as water output for water scarcity impact modeling.

Corrective Considerations for Surplus Water Inputs

In situations where the water balance indicates a higher total water input than output, this suggests that certain water losses or transformations have not been fully captured in the system inventory. These imbalances must be addressed to ensure consistency and to avoid underestimating water consumption or misleadingly low water scarcity impacts. The following are common causes and corrective measures for surplus water inputs.

Case 1: Unaccounted Water Evaporation or Transpiration

Water losses due to evaporation (e.g., from cooling towers, open tanks, cleaning processes) or transpiration (e.g., from agricultural crops) may not always be measured directly and can lead to an apparent deficit in water outputs. These flows are considered consumptive uses and must be accounted for in the output inventory to maintain an accurate water balance.

Recommended Action: If there is more input water than output water, consider scaling up the average water output, such as evaporated water and/or wastewater, in proportion to your average water outputs.

- Identify processes where evaporation or transpiration likely occurs.
- Add the estimated water vapor as an elementary flow to air in the water output inventory.

In a chemical plant, 1,000 m^3 of water is input, and only 850 m^3 is accounted for in discharge and product incorporation. The missing 150 m^3 is likely lost through evaporation in the unit process. This volume should be added as water vapor output to air, closing the water balance and ensuring accurate accounting of consumptive use.

Case 2: Water Incorporated into Byproducts or Waste Streams

In some cases, water may leave the system via byproducts, residues, or waste that was not originally considered part of the product system. If water content of these streams is not well defined by the water inventory, they can result in unaccounted water losses.

Recommended Action:

- Review whether any moisture-containing byproducts (e.g., sludges, organic waste, co-products) are leaving the system unaccounted for.
- Estimate water content using material specifications or standard moisture content values.
- Adjust the output inventory to reflect this water flow.

Water Loss Estimation

Water losses through evaporation commonly occur in cooling and heating systems, including cooling towers and steam generation processes (section 6.1.4). Due to the inherent difficulty in accurately measuring water vapor emissions, precise quantification is often challenging. In situations where actual evaporation rates are unknown or unavailable, it is considered best practice to apply estimated default values to account for evaporative water losses, ensuring consistency and conservatism in the water balance. However, these default evaporation rates are suggested, but the LCA practitioner is not limited to use if better estimates are available.

Table 9: Default water loss estimation when primary data is missing. Estimations are based on expert judgement.

Input flow	**Default consumption rate**
Water for steam production, closed system	5% of input value
Cooling water (approx. 20ºC), (Closed circuit with cooling tower)	2% of input value
Cooling water (approx. 5ºC), (closed circuit without cooling tower)	1% of input value
Process water	7% of input value
Cleaning water	30% of input value

Cleaning Water: stream of water used to clean equipment, reactors, pipelines, containers, and production areas.
Process Water: is the water used directly in chemical manufacturing operations to enable, carry out, or influence chemical reactions and process conditions.
Cooling Water: is water used to remove excess heat from chemical processes, equipment, or utilities in order to maintain safe operating temperatures, ensure process stability, and protect equipment integrity. It does not participate in the chemical reaction itself; instead, it serves as part of the thermal management system.
Water for Steam Production: is water that is treated and supplied generate steam used as a thermal utility in chemical manufacturing.

6.3. Assessment Examples

This example shows how to estimate the water scarcity impact of producing 1 ton of solvent at a chemical plant in Spain (gate-to-gate[12] system boundary).

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[12] The calculation is performed gate to gate to facilitate the understanding of practitioners. Therefore, the same procedure should be performed for the supplied material and energy (suppliers water consumption) and being summed up with this gate-to-gate calculation to entail the cradle to gate calculation needed for the product level water scarcity.

Water balance from site inventory:

Table 10: Example water scarcity

Input		
Water flow	**Volume [m^3]**	
Cooling tower	5.0	
Process water	3.0	
Boiler water for steam	2.0	
Cleaning water	1.0	
Output		
Cooling water returned to network	4.0	9.5 m^3
Process water returned to river	2.8	
Steam condensate to network	1.8	
Cleaning water returned to river	0.9	
Evaporation	0.9	
Water lost via drift or leaks	0.4	
Water bound in product	0.2	

Water balance:
Total water inputs = 5.0 m^3 + 3.0 m^3 + 2.0 m^3 + 1.0 m^3 = 11.0 m^3
Total water outputs = 4.0 m^3 + 2.8 m^3 + 1.8 m^3 + 0.9 m^3 + 0.9 m^3 + 0.4 m^3 + 0.2 m^3 = 11.0 m^3

Step 1: Calculate Consumptive Water
Consumptive water = Total water inputs – Total water returned to environment (except the sea) = 11.0 m^3 – 9.5 m^3 = 1.5 m^3

Step 2: Obtain EF CF
From EF 3.1 environmental footprint reference packages, obtain CF for Spain:
CF = 77.7 m^3 world eq./m^3

Step 3: Calculate Water scarcity
Water scarcity Impact = consumptive water use x CF = 1.5 m^3 x 77.7 m^3 world eq./m^3 = 116.6 m^3 world eq. per ton solvent

6.4. Literature

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7. Acidification Potential

7.1. General Description

7.1.1. Issue of Concern

Acidification refers to the process by which acidic substances are introduced into the environment, leading to a decrease in pH levels. This phenomenon is primarily caused by the emissions of sulfur dioxide (SO_2), nitrogen oxides (NO_x), and ammonia (NH_3), which can result from various chemical processes, industrial activities (e.g., fuel and coal combustion) as well as agricultural activities (e.g., through fertilizers) (Gade et al., 2021). When these compounds are released into the atmosphere, they can react with water vapor to form sulfuric acid, nitric acid, and other acidic compounds, leading to acid rain and other forms of acid deposition. Acidification potential (AP) refers to the compounds that are precursors to acid rain. Acidification occurs with substances varying in their acid formation potential. This guideline emphasizes terrestrial acidification as it represents the initial stage of preceding ocean acidification.

Acidification has a wide range of negative effects on both natural and human environments, and it is regarded as a regional effect. It is caused by the release of protons in terrestrial or aquatic ecosystems. The acidifying substances are only contributing to acidification if the anion is leached out from the system. Organic acids predominantly are mineralized and do not leach to the system; accordingly, they are not regarded as contributors to acidification. In certain areas, acidification leads to increased mobility of heavy metals and aluminum. Acid rain, resulting from airborne acidifying substances, can affect ecosystems hundreds of kilometers from original emission sources. Acidic deposition on land, either direct or via acidic precipitation, initiates significant changes in soil chemistry. Primary effects include a decrease in soil pH, altered bioavailability of essential plant nutrients (like calcium and magnesium), or enhanced leaching of critical nutrients. Premature shedding of leaves and needles, disruption of photosynthesis, impaired plant growth and development, and reduced overall ecosystem health and resilience are only some negative aspects of acidification (Zhang et al., 2023). A shift in soil pH might also cause leaching of ecotoxic minerals and metals, e.g., Aluminum (III) or heavy metal ions, ultimately leading to a decrease of biodiversity and bio-productivity in affected areas. While this also affects agricultural plant growth, acidification has negative implications for food safety as well. (Chen et al., 2013) Besides affecting plant growth (Shi et al., 2021), acid rain can also corrode buildings, monuments, and other infrastructure, leading to economic losses. (Pawłowski, 1997) The hydrological transport of acidifying compounds creates significant impacts on aquatic environments, e.g., due to lowering the pH in water bodies. (Baker & Christensen, 1991) So, acidification can harm fish and other aquatic organisms by disrupting their reproductive processes and causing physiological stress. (Gade et al., 2021; Baker & Christensen, 1991) Furthermore, it can negatively impact human health, particularly respiratory health, due to increased exposure to harmful pollutants (UNECE, 2012; EEA, 2024).

Considering that the economic benefits of improved air and water quality outweigh the costs of reductions measures, there is ample reason to reduce N emissions, both from agriculture and from traffic and industrial sources (de Vries, 2021). High NO_2 concentrations can lengthen and worsen common viral infections and cause severe damage to the lungs (Spannhake et al., 2002) as well as asthma (Achakulwisut et al., 2019).

The release of acidifying substances represents a significant environmental concern that necessitates inclusion in comprehensive environmental assessments within the framework of digital product passports. Systematic evaluation of AP delivers multiple benefits. These include identification of emission hotspots throughout product lifecycles, which supports the development of targeted soil and plant protection strategies.

7.1.2. Key Components of Potential Impact

The substances normally considered as contributors to acidification are: sulfur dioxide (SO_2), sulfur trioxide (SO_3), nitrogen oxides (NO_x), hydrogen chloride (HCl), nitric acid (HNO_3), sulfuric acid (H_2SO_4), phosphoric acid (H_3PO_4) (note: the anion does not leach and the contribution to acidification is in practice equal to zero), hydrogen fluoride (HF), hydrogen sulfide (H_2S) and ammonia (NH_3). Although the list of acidification contributors is long, not all of them are considered in LCIA methods. Usually SO_x, NO_x and NH_3 are considered as the main contributors to the formation of acid rain. HCl, for example, while being an acid, does not typically contribute to the same atmospheric processes that lead to acidification as these other compounds do.

7.1.3. Regulatory Compliance

There are no existing specific regulations dealing with acidification pollutants, but with general air pollutants as The National Emissions reduction Commitments (NEC) Directive (2016/2284/EU) (EU, 2024), which sets 2020 and 2030 emission reduction commitments for five main air pollutants (EU, 2016), namely NO_x, Non-Methane Volatile Organic Compounds (NMVOCs), NH_3, SO_2 and $PM_{2.5}$. The directive transposes the reduction commitments for 2020 agreed by the EU and its Member States under the revised Gothenburg Protocol (UNECE, 2012) for the Convention on Long-range Transboundary Air Pollution (LRTAP Convention). The more ambitious reduction commitments agreed for 2030 are designed to reduce the health impacts of air pollution by half compared with 2005. Further, it requires Member States to draw up National Air Pollution Control Programs that should contribute to the successful implementation of air quality plans established under the EU's Air Quality Directive. (EEA, 2024)

It is particularly critical to deliver on the 2030 targets related to air pollution under the zero-pollution action plan (EC, 2021): to reduce the number of premature deaths caused by air pollution by 55% and to reduce the area of EU ecosystems where air pollution threatens biodiversity by 25%, in both cases compared to 2005 levels. To achieve these targets, it will be vital that EU Member States meet their respective emission reduction commitments set for 2020-2029 and for 2030 onwards under the NEC Directive. The biggest challenge for the period 2020-2029 is reducing ammonia emissions: 10 Member States need to cut their 2021 emission levels to fulfil their 2020-2029 reduction commitments. The agriculture sector is the principal source, responsible for 93% of total ammonia emissions. Since 2005, ammonia emissions have only slightly decreased in many Member States and in some cases have increased. (EEA 2025) Regarding **NH_3**-emissions, five Member States already met their 2030 emission reduction commitments in 2021. 13 Member States need reductions under 10% and 8 need emissions to fall by between 10% and 30%. Regarding **NO_x** emissions, four Member States met their emission reduction commitments for 2030. However, 23 Member States will need to reduce emissions, of which 1 Member State will need to reduce them by more than 50%, 6 Member States by more than 30% and 15 Member States need a reduction of up to 30% (Figure 7) (EEA 2025).

Figure 7: Number of Member States that had met their national emission reduction commitments for the five main pollutants for 2030 (EEA 2025).

The updated Directive on industrial and livestock rearing emissions is in force, revising the former Industrial Emissions Directive. (EEA, 2025) In line with the Zero Pollution ambition of the European Green Deal (EC, 2019), the revised Directive will result in less emissions from large industrial installations. Under the Industrial Emissions Portal Regulation (IEPR), industrial operators for these sites are required to report on significant emissions and the use of resources (EC, 2026). The EU aims to improve transparency in data reporting by collecting and disseminating information on the amounts of industrial pollutant releases, off-site transfers of waste and pollutants in wastewater, the consumption of energy, water and key raw materials. This modernized law will help guide industrial investments necessary for Europe's transition towards a cleaner, carbon-neutral, more circular, and competitive economy. By 2050, the implementation of the revised Directive is expected to reduce emissions of key air pollutants ($PM_{2.5}$, SO_2, NO_x and NMVOC) by up to 40% compared to 2020 levels. It is the first EU environmental law to enshrine the right of people to seek compensation for damage to their health caused by illegal pollution (EC, 2024).

In the United States, the Clean Air Act (CAA) provides the legal framework for addressing air pollution, including acid rain. The Acid Rain Program, established under Title IV of the CAA, requires significant reductions in sulfur dioxide and nitrogen oxides emissions from power plants and other industrial sources. (Lattanzio 2022)

7.1.4. Importance for the Chemical Industry

The chemical industry, being an energy intensive sector, is one big emitter of SO_2 and NOx (Figure 8) (EEA 2025) that react in the atmosphere producing acid rain.

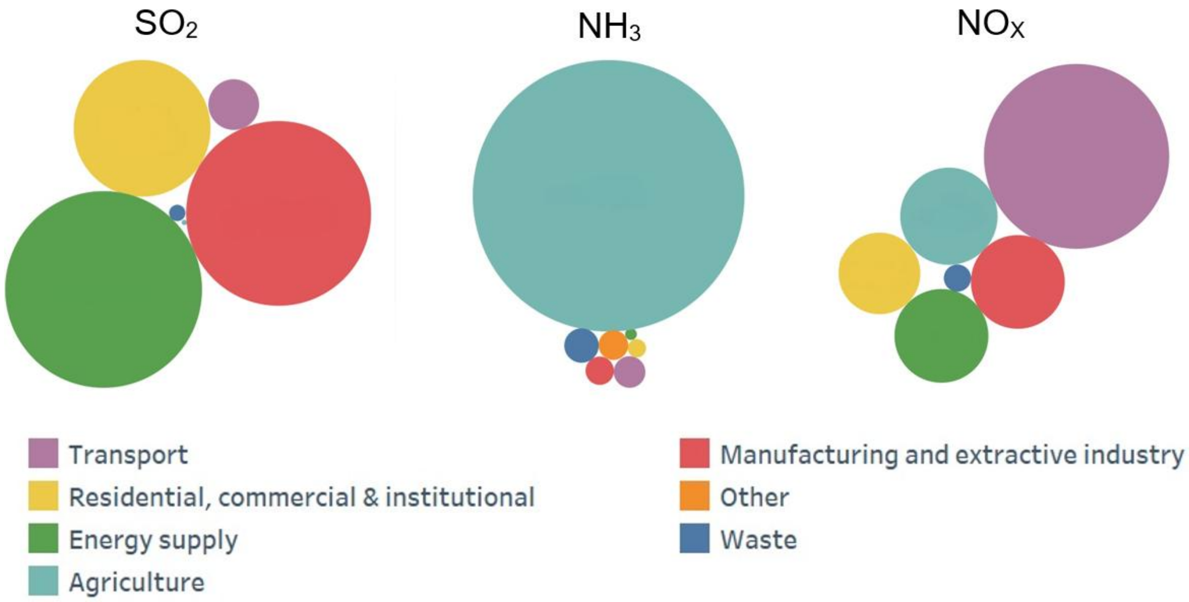

Figure 8: Sectors and activities contributing to emissions of the five regulated air pollutants in EU Member States in 2023 (EEA 2025).

The chemical industry supports company and product related transparency on emissions and related impacts while having its own mitigation targets in place. Product related impacts on acidification are not only dependent on safe production and processing but also on safe transport, use, and end-of-life handling. Understanding and controlling acidification is essential for reducing acid rain formation and complying with environmental regulations. Chem-X developed a sustainability data model with an acidification information data model to be useable in a digital product passport.

Acidification is a significant environmental issue in the chemical industry, and there are several applications where it is particularly relevant. These processes can be categorized as follows in Table 11.

Table 11: Processes directly or indirectly related to acidification relevant in the chemical industry (not exhaustive list)

Processes	**Example**
Production of Sulfuric Acid	Sulfuric acid is widely used in the chemical industry for various applications, including fertilizer production, mineral processing, and chemical synthesis. The production process can lead to acidification due to the release of sulfur dioxide (SO_2) and other acidic compounds
Nitric Acid Manufacturing	Nitric acid is another important chemical used in fertilizers, explosives, and other industrial processes. Its production involves the oxidation of ammonia, which can result in the emission of nitrogen oxides (NO_x) that contribute to acidification.
Petrochemical Industry	The refining of petroleum and the production of petrochemicals can lead to acidification through the release of sulfur compounds and other acidic pollutants.
Metal Plating and Surface Treatment	Processes such as electroplating and surface treatment often use acidic solutions, which can lead to acidification if not properly managed.
Waste Treatment and Disposal	The treatment and disposal of industrial waste, especially hazardous waste, can result in acidification if acidic substances are not neutralized before disposal.

7.2. Methodology of Characterization

The prevailing LCIA characterization models emphasize terrestrial acidification, as it often occurs prior to aquatic acidification when inland water is acidified after the attenuation of the acid neutralization capacity of its watershed. (Hauschild et al., 2011). Several LCIA methods can be used to assess the terrestrial acidification potential (tAP) in LCA. These LCIA methods can differ due to their underlying characterization model, considered elementary flows or other aspects (Hauschild et al., 2011). Brief descriptions of existing LCIA methods and their considered AP characterization models are given below for the chosen EF method and for the other LCIA methods see the Appendix 11.3.1. These models are based on the pre-selected methods reported in the ILCD Handbook (Hauschild et al., 2011), while methods not compatible with LCA and outdated methods are excluded (Jungbluth 2025).

7.2.1. Chosen Method: EF

Based on the LCIA method comparisons (see Appendix 11.4.1 11.3.1), the LCIA method EF 3.1 (or any updated version) is recommended to assess AP in LCA for products / materials especially intended for the European market. As recommended by the ILCD Handbook (Hauschild et al., 2011), EF 3.1. uses the **Accumulated Exceedance** (AE) method (Seppälä et al., 2006) as default method for midpoint evaluation of acidification as currently used in the EF Method. The AE method provides country-specific CFs for acidification and terrestrial eutrophication in Europe (Seppälä et al., 2006). It uses the European Monitoring Centre for Air Pollution (EMEP) model along with a critical load database to determine atmospheric transport and deposition to land

and major water bodies. AP is expressed as Accumulated Exceedance, with an implicit dose-response curve of 1. An updated publication (Posch et al., 2008) revised the AE factors using the 2006 EMEP Eulerian model, which includes deposition data across various land cover types and the latest critical load database (Hettelingh et al., 2007) covering approximately 1.2 million ecosystems. The AE model is utilized in the EF LCIA method for assessing the Product Environmental Footprint (PEF), which includes guidelines for modeling this impact category. (Hauschild et al., 2011)

The EF method, developed by the European Commission, provides a comprehensive framework for evaluating the environmental performance of products throughout their life cycle. In terms of acidification, the EF method includes specific guidelines for modelling and assessing this impact category. The method uses CFs to translate emissions into potential acidification impacts, considering various substances such as SO_2, NO_x, and NH_3.

Formula

The following formula shows how to calculate the AP:

$$\text{Acidification Potential} = \sum(E_{i\text{-}AP} \times CF_{i\text{-}AP}) \ [\text{mole of } H^+ \text{ eq. per kg}]$$

Formula 7: Equation for Acidification Potential calculation

Where:

- $E_{i\text{-}AP}$ = Emission of the relevant substance for acidification (e.g., SO_2, NO_x, NH_3)
- $CF_{i\text{-}AP}$ = Characterization factor for the respective acidifying substance

Where: $E_{i\text{-}AP}$ *and* $CF_{i\text{-}AP}$ *are, respectively, the mass and the* $CF_{i\text{-}AP}$ *of the acidifying substance. The impact of AP is, therefore, expressed in mole of* H^+ *eq. per kg.*

Characterization factors in EF method

In Table 12, the average CFs for Acidification, which help to quantify the extent to which each emission contributes to acidification, are presented. The impact of acidification is often expressed in SO_2 equivalents (SO_2-eq), meaning that different acidifying substances are converted based on their effect relative to sulfur dioxide (SO_2), which is used as the standard reference. Some LCA methodologies, such as the Environmental Footprint (EF) method, express acidification in moles of atomic hydrogen (mol H^+ eq).

Table 12: EF 3.1 Acidification average characterization factors, expressed in mole of H+ eq. per kg emissions to air (EF 3.1)

Flow	**CF [mole of H^+ eq. per kg]**
Ammonia	3.02
Nitrogen dioxide	0.74
Nitrogen monoxide	1.13
Nitrogen oxides	0.74
Sulphur dioxide	1.31
Sulphur oxide	1.31
Sulphur trioxide	1.05

Link to download the CFs for Acidification can be found under the following link: EF 3.1.

The approach fulfils scientific-based standards, and it has been well received by stakeholders. The method includes atmospheric and soil fate factors that are sensitive to the emission scenario, and it distinguishes between the loading of sensitive and non-sensitive areas. This method generates Average Default CFs, or a consistent set of CFs for each continent, if complemented by regional/continental models that are consistent with each other and expert estimates of soil sensitive areas (Hauschild 2011). The EF approach ensures consistency and comparability across different products and industries, enabling stakeholders to identify and implement effective mitigation strategies.

Selection Guidance

Generally, EF 3.1 provides regionalized CFs for the AP relevant elementary flows. However, depending on the database used (e.g., ecoinvent, Sphera MLC, CarbonMinds), the AP is only assessed using averages provided by EF (like the water footprint with AWARE methodology, see Chapter 6.2.10). Averages should be used to increase consistency. The goal for the future should remain to switch from average to more regionalized CFs.

7.2.2. LCI Flows

Table 13 shows a few examples of LCI flows for acidifying substances.

Table 13: Description of relevant LCI flows concerning Acidification.

LCI Flow	Description of Flow
Ammonia	Ammonia (NH_3) is primarily produced through agricultural activities, particularly from livestock waste and the application of nitrogenous fertilizers. It can also be emitted during the combustion of fossil fuels and biomass.
Nitrogen Dioxide	Nitrogen dioxide (NO_2) is generated from combustion processes, particularly in vehicles and power plants. It is formed from nitrogen oxides (NO_x) during high-temperature combustion.
Nitrogen Monoxide	Nitrogen monoxide (NO), also known as nitric oxide, is produced during combustion processes, especially in internal combustion engines and industrial processes. It is one of the primary nitrogen oxides emitted.
Nitrogen Oxides	Nitrogen oxides (NO_x) are a group of gases that includes both nitrogen monoxide (NO) and nitrogen dioxide (NO_2). They are emitted from vehicle exhaust, industrial processes, and power generation, primarily during combustion.
Sulphur Dioxide	Sulphur dioxide (SO_2) is mainly produced from the burning of fossil fuels, particularly coal and oil, in power plants and industrial facilities. It can also be emitted from volcanic eruptions.
Sulphur Oxide	Sulphur oxides refer to a group of gases that includes both sulphur dioxide (SO_2) and sulphur trioxide (SO_3). They are primarily generated by the combustion of sulphur-containing fuels and industrial processes.
Sulphur Trioxide	Sulphur trioxide (SO_3) is produced during the oxidation of sulphur dioxide (SO_2) in the atmosphere or during industrial processes, particularly in the manufacture of sulfuric acid.

The full list of LCI flows (incl. respective CFs) can be found under the following link: EF 3.1.

7.3. Assessment Examples

Example: Fertilizer Production

Consider the production of ammonium nitrate fertilizers, which involves the reaction of ammonia (NH_3) with nitric acid (HNO_3). This process releases significant amounts of nitrogen oxides (NO_x) and ammonia, both of which contribute to acidification. To assess the Terrestrial Acidification Potential within LCA, the following steps are taken:

- Inventory Analysis: Data is collected at each stage of the fertilizer production process, including the extraction of raw materials, synthesis of ammonia, production of nitric acid, and the final reaction to form ammonium nitrate. Emissions are measured and recorded, focusing on NO_x and NH_3 released during these processes.

- Impact Assessment: Using characterization models like EF 3.1, the AP of the emissions are calculated. CFs for NO_x and NH_3 are applied to quantify their contribution to acidification, expressed in mole of H^+ eq. per kg. See simplified calculation example in Table 14.
- Mitigation: The results of the impact assessment highlight the stages with the highest AP. To mitigate these impacts, the company might implement Selective Catalytic Reduction systems to reduce NO_x emissions, optimize the ammonia synthesis process to minimize NH_3 release, and explore alternative raw materials or production methods. Additionally, research into more sustainable fertilizer formulations, such as controlled-release fertilizers, can reduce acidifying emissions.

Table 14: Simplified *example for the calculation of the Acidification Potential to produce a fertilizer.*

	Emission flows [g/t]	**CF**	**Result [H^+ eq./t]**
NH_3 Production			
NH_3 emission	14	3.02	42.28
NO_x emission	2,200	0.74	1,628
SO_2 emission	1,800	1.31	2,358
Nitric acid process			
NH_3 emission	20	3.02	60.40
NO_x emission	500	0.74	370
SO_2 emission	1	1.31	1.31
Ammonium nitrate process			
NH_3 emission	30	3.02	90.60
NO_x emission	100	0.74	74
SO_2 emission	10	1.31	13.10
Total			
NH_3 emission			193
NO_x emission			2,072
SO_2 emission			2,372
			4,637

7.4. Literature

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8. Ozone Depletion Potential

8.1. General Description

8.1.1. Issues of Concern

The ozone layer acts as Earth's sunscreen, filtering out ultraviolet (UV) radiation that can cause skin cancer, cataracts, and other health problems, as well as damage aquatic ecosystems and terrestrial plant life. Without this protective layer, life on Earth would be exposed to significantly higher levels of UV radiation, leading to severe ecological and health consequences. Any significant depletion of this protective layer can lead to increased UV exposure, resulting in adverse effects on human health and negative impacts on ecosystems and agriculture. In this context, the ozone depletion potential (ODP) is a critical environmental impact category assessed in LCA, as it measures the potential of various substances to destroy ozone and consequently deplete the ozone layer. The ODP of a substance is a metric for determining the relative strength of that chemical's ability to destroy ozone (WMO, 2022).

Ozone (O_3) is formed when oxygen molecules (O_2) are split by UV light into individual oxygen atoms, which then combine with O_2 to form O_3. This process occurs naturally and is balanced by the natural breakdown of ozone molecules shown in Figure 9. However, human activities have introduced substances that disrupt this balance, leading to ozone depletion. Besides ozone-depleting substances (ODS)[13] , the subsequent release of reactive halogen gases, especially chlorine and bromine, after breaking down by UV light in the stratosphere has a big impact on ODP (WMO, 2022). These released atoms then react with ozone, causing it to break down into oxygen molecules, thus thinning the ozone layer. Although, any substance that can destroy ozone in the stratosphere (NO, OH, Cl, or Br) is an ODS, in the Montreal Protocol only volatile compounds containing Cl or Br are classified as ODSs (UNEP, 2020).

Figure 9 illustrates the explanations from Oever et al. (2024) and of Baird and Cann (2012a, 2012b).

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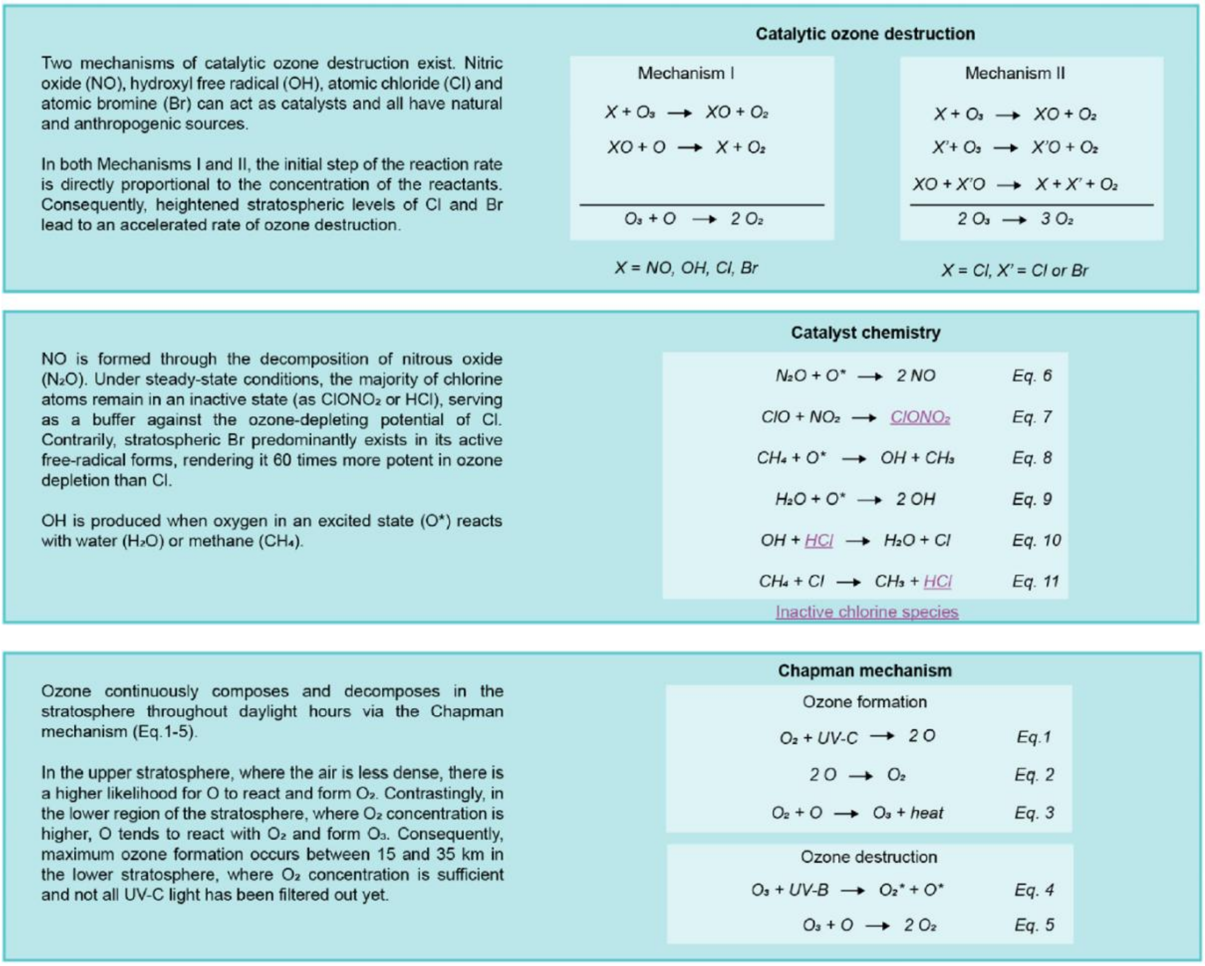
[13] Ozone-depleting substance (ODS) refers to gases containing either chlorine or bromine that are released to the atmosphere because of human activity and are controlled under Annexes A, B, C, or E of the Montreal Protocol. These include, among other CFCs, CCl_4, CH_3CCl_3, halons, CH_3Br and HCFCs. These ODSs typically have sufficiently long atmospheric lifetimes to reach the stratosphere after being emitted at the surface. Methyl bromide is the shortest-lived of the controlled substances and has natural and anthropogenic sources. Other substances contribute chlorine and bromine to the atmosphere but are not controlled under the Montreal Protocol for various reasons. (WMO, 2022)



Catalytic ozone destruction

Two mechanisms of catalytic ozone destruction exist. Nitric oxide (NO), hydroxyl free radical (OH), atomic chloride (Cl) and atomic bromine (Br) can act as catalysts and all have natural and anthropogenic sources.

In both Mechanisms I and II, the initial step of the reaction rate is directly proportional to the concentration of the reactants. Consequently, heightened stratospheric levels of Cl and Br lead to an accelerated rate of ozone destruction.

Mechanism I

$X + O_3 \rightarrow XO + O_2$

$XO + O \rightarrow X + O_2$

$O_3 + O \rightarrow 2\,O_2$

$X = NO, OH, Cl, Br$

Mechanism II

$X + O_3 \rightarrow XO + O_2$

$X' + O_3 \rightarrow X'O + O_2$

$XO + X'O \rightarrow X + X' + O_2$

$2\,O_3 \rightarrow 3\,O_2$

$X = Cl,\ X' = Cl$ or Br

Catalyst chemistry

NO is formed through the decomposition of nitrous oxide (N_2O). Under steady-state conditions, the majority of chlorine atoms remain in an inactive state (as $ClONO_2$ or HCl), serving as a buffer against the ozone-depleting potential of Cl. Contrarily, stratospheric Br predominantly exists in its active free-radical forms, rendering it 60 times more potent in ozone depletion than Cl.

OH is produced when oxygen in an excited state (O*) reacts with water (H_2O) or methane (CH_4).

$N_2O + O^* \rightarrow 2\,NO$	Eq. 6
$ClO + NO_2 \rightarrow ClONO_2$	Eq. 7
$CH_4 + O^* \rightarrow OH + CH_3$	Eq. 8
$H_2O + O^* \rightarrow 2\,OH$	Eq. 9
$OH + HCl \rightarrow H_2O + Cl$	Eq. 10
$CH_4 + Cl \rightarrow CH_3 + HCl$	Eq. 11

Inactive chlorine species

Chapman mechanism

Ozone continuously composes and decomposes in the stratosphere throughout daylight hours via the Chapman mechanism (Eq.1-5).

In the upper stratosphere, where the air is less dense, there is a higher likelihood for O to react and form O_2. Contrastingly, in the lower region of the stratosphere, where O_2 concentration is higher, O tends to react with O_2 and form O_3. Consequently, maximum ozone formation occurs between 15 and 35 km in the lower stratosphere, where O_2 concentration is sufficient and not all UV-C light has been filtered out yet.

Ozone formation

$O_2 + UV\text{-}C \rightarrow 2\,O$	Eq.1
$2\,O \rightarrow O_2$	Eq. 2
$O_2 + O \rightarrow O_3 + heat$	Eq. 3

Ozone destruction

$O_3 + UV\text{-}B \rightarrow O_2^* + O^*$	Eq. 4
$O_3 + O \rightarrow 2\,O_2$	Eq. 5

Figure 9: Summary of stratospheric ozone chemistry (Oever et al., 2024).

In Figure 10, substances having a positive effect on the ozone layer (marked with a plus-sign) and ODS (marked with a minus-sign) are illustrated, including other impacts resulting from ODP (GHG = greenhouse gas, VSLS = very short-lived substance). Moreover, the arrows show if the substances are generally considered in (LCIA) methods. The Figure shows effects on the Ozone Layer, with Illustrations by Francesco Gavardi (Oever et al., 2024).

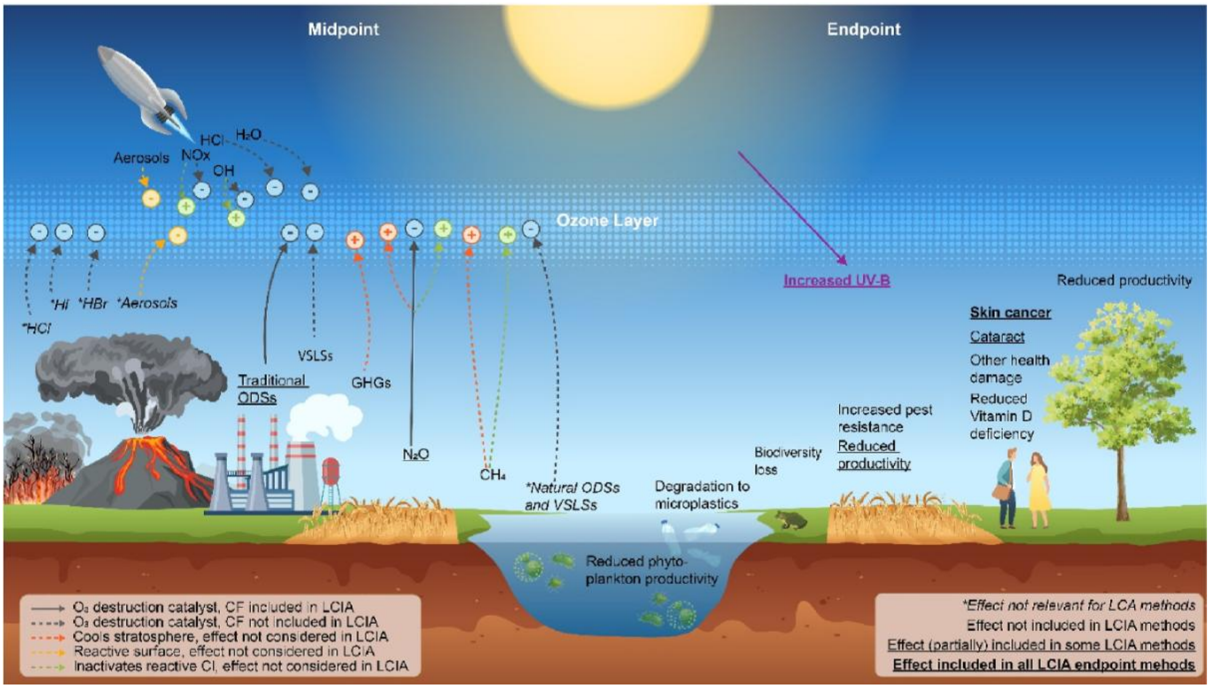


Figure 10: Summary of limitations and challenges related to midpoint and endpoint characterization (Oever et al., 2024).

ODP is seen as the second-least important impact category for human health in specific LCIA methods (Andreasi et al., 2023; Fazio et al., 2018; Sala and Cerutti, 2018), due to the existing reports proving a recovering of the ozone layer (WMO, 2022). However, potential ozone layer threats caused by new technologies in the space sector must be considered. (Oever et al., 2024) Additionally ODP remains important for other sectors as the agricultural sector due to fertilizer-related N_2O emission and the chemical industry, as data gaps between ODS consumption reports and atmospheric measurements point to potential leakage issues from ODS serving as precursors or intermediates (WMO, 2022). The importance of ODP for the chemical industry is described in more detail in the next chapter.

8.1.2. Key Components of Potential Impact

Some of the ODS are the following:

- Chlorofluorocarbons (CFCs)
- Halons (e.g., bromine-containing halons)
- Methyl-bromide (CH_3Br)
- Carbon Tetrachloride (CCl_4)
- Methyl Chloroform (CH_3CCl_3)
- Hydrochlorofluorocarbons (HCFCs)

These substances were commonly used in refrigeration, air conditioning, foam blowing, and as solvents until their harmful effects on the ozone layer were discovered. ODS can be also found in aerosol products, portable fire extinguishers, insulation boards, panels, pipe covers, and pre-polymers (UNEP, 2020).

8.1.3. Regulatory Compliance

Recognizing the significance of ODP has led to international efforts to control and eliminate the use of high-ODP substances. The most notable of these efforts is the Montreal Protocol, an international treaty signed in 1987 aimed at phasing out the production and consumption of ozone-depleting substances. The Montreal Protocol has been successful in reducing the emission of ODS, and it has been amended several times to include more substances and accelerate phase-out schedules.

Over the years, many other national and international regulations have been developed to limit ODP substances. Compliance with these regulations is essential for the industry to avoid penalties and trade restrictions. Accurate LCA, including ODP metrics, helps companies adhere to these regulations and demonstrate their commitment to environmental protection. (S.O. Andersen et al., 2018).

The Montreal Protocol has led to significant reductions in the concentrations of high-ODP substances in the atmosphere. This has contributed to the gradual recovery of the ozone layer, with projections suggesting that the ozone layer could return to pre-1980 levels by the middle of the 21st century, if current regulations are maintained (S.O. Andersen et al., 2018).

8.1.4. Importance for the Chemical Industry

The chemical industry has been a contributor to ozone depletion through the production of synthetic ODS. The discovery of the Antarctic ozone hole in the 1980s prompted global concern, leading to the adoption of the Montreal Protocol in 1987, which mandated the phase-out of ODS. In response, industry has evolved significantly, developing safer alternatives. Regulations and national legislation have significantly restricted the production and use of high ODS, but calculating ODP of chemical substances remains crucial for the chemical industry as it directly influences environmental sustainability, regulatory compliance, innovation and market advantage. The chemical industry plays a pivotal role in environmental sustainability. Understanding ODP is vital for gauging the environmental impact of various chemicals and for formulating strategies to preserve and restore the ozone layer (WMO, 2022).

The chemical industry uses products or applications potentially affecting the ozone layer, which are categorized and presented in Table 15.

Table 15: Categories directly or indirectly related to Ozone depletion relevant for the chemical industry

Category	Example
Refrigeration and Air Conditioning	CFCs and HCFCs have been extensively used as refrigerants in cooling systems.
Aerosols	CFCs were commonly used as propellants in aerosol sprays.
Foam Blowing Agents	CFCs and HCFCs have been used in the production of foam insulation and packaging materials.
Fire Suppression Systems	Halons have been used in fire extinguishers and fire suppression systems.
Solvents	CFCs and other ODS have been used as solvents in cleaning and degreasing applications.

8.2. Methodology of Characterization

Several LCIA methods can be used to assess the ODP in LCA. Brief descriptions of existing LCIA methods and their considered characterization models are given below for the chosen EF method and for the other LCIA methods see the Appendix chapter 11.4.1.

8.2.1. Chosen Method: EF

Based on the LCIA method comparisons presented in the chapter above, the LCIA method EF 3.1 (or any updated version) is recommended to assess ODP in LCA for products / materials. Besides the reason that EF 3.1 is the recommended LCIA method by the European Union, EF 3.1 is up to now the only LCIA method, compared to all the others, that is based on the WMO (2014) publication. It is expected that the ODP impact category will further be maintained by the EU and consequently the new version of WMO (2022) will be updated, too.

Formula

The ODP is a metric used to quantify the relative ability of a chemical to destroy stratospheric ozone. It is defined as the ratio between the change in global ozone resulting from a given mass of the substance and the change produced by the same mass of CFC-11 ($CFCl_3$), which serves as the reference compound. (WMO, 2022)

To allow comparison of the potential impacts of different gases on the ozone layer, emissions are multiplied by their respective ODP characterization factors and expressed as ODP-normalized emissions.

Formula 8 (adapted from Oever et al. 2024) to calculate the ODP is as follows:

$$\text{Ozone Depletion Potential} = \sum(E_{i\text{-}ODP} \times CF_{i\text{-}ODP})\ [\text{kg CFC-11-eq. per kg}]$$

Formula 8: Equation for Ozone Depletion Potential calculation

Where:

- $E_{i\text{-}ODP}$ = Emission of the relevant ozone depleting substance (e.g., CFC-11, Halons, Carbon Tetrachloride (CCl4))
- $CF_{i\text{-}ODP}$ = Characterization factor for the respective ozone depleting substance

Where: $E_{i\text{-}ODP}$ and $CF_{i\text{-}ODP}$, are, respectively, the mass and the $CFi_{\text{-}ODP}$ of the ozone depleting substance. The impact of ODP is, therefore, expressed in kg CFC-11-eq. per kg.

Characterization Factors in EF Method

The ODP factors for a selection of substances are listed in Table 16. The reference substance for ODP calculation is trichlorofluoromethane (CFC-11), which has an ODP of 1.0. Other substances are compared to CFC-11 to determine their ODP values: substances with an ODP greater than 1.0 have a higher potential to destroy ozone molecules than CFC-11, while those with values below 1.0 are less harmful by comparison.

Table 16: Selected ODP characterization factors for some substances (retrieved from EF 3.1)

Substance	**Characterization Factor (CFC-11 eq.)**
CFC-11	1.0
Halons	3-10
Carbon Tetrachloride (CCl4)	1.2
Methyl Chloroform (CH3CCl3)	0.8
HCFC-22	0.055
HCFC-123	0.02

Links to download the CFs for Ozone Depletion can be found under the following link: EF 3.1.

Selection Guidance

As this is a global impact category, no selection is needed.

8.2.2. LCI Flows

Table 17 shows a few examples of LCI flows for ODP.

Table 17: Description of relevant LCI flows concerning Ozone Depletion

Flow	Description of Flow
CFC-11	CFC-11 (trichlorofluoromethane) is primarily produced as a refrigerant and aerosol propellant. It was widely used in foam-blowing agents and as a solvent in industrial applications. Its production has been largely phased out due to its ozone-depleting potential.
Halons	Halons are a group of brominated compounds used mainly in fire extinguishers. They are produced during the manufacturing of specific fire suppression systems and have significant ozone-depleting effects.
Carbon Tetrachloride (CCl_4)	Carbon tetrachloride is produced as a solvent and in the manufacture of other chemicals. It was historically used in dry cleaning and as a refrigerant, but its production has been reduced due to its harmful environmental impact, particularly in ozone depletion.
Methyl Chloroform (CH_3CCl_3)	Methyl chloroform was primarily used as an industrial solvent for degreasing and cleaning. Its production has decreased significantly due to its classification as an ozone-depleting substance.
HCFC-22	HCFC-22 (hydrochlorofluorocarbon) is used as a refrigerant in air conditioning and refrigeration systems. It is produced as a transitional replacement for CFCs, but its use is being phased out due to its potential to harm the ozone layer.
HCFC-123	HCFC-123 is primarily used as a refrigerant in commercial air conditioning systems. It is produced as a replacement for CFCs and is less harmful to the ozone layer, but it is still being phased out under international agreements.

The full list of LCI flows (incl. respective CFs) can be found under the following link: EF 3.1.

8.3. Assessment examples

Case Study: The Transition from CFCs to HFCs in Refrigeration

A significant example of the importance of ODP in the chemical industry is the transition from CFCs to HFCs in the refrigeration industry (IRP 2025). CFCs, once widely used as refrigerants, were found to have a high ODP and were major contributors to ozone depletion. In response to the Montreal Protocol, companies invested in research and development to find alternatives with lower ODP (Adams 2025), (Bhatti 2023).

One successful outcome of this effort is the adoption of HFCs, which have significantly lower ODP. A notable problem is the transition by the company to new systems, which has developed new refrigeration systems using HFCs. These systems not only comply with international regulations but also offer improved energy efficiency and reduced environmental impact. This transition not only helped to preserve the ozone layer but also demonstrated the chemical industry's capability to innovate and adapt in response to environmental challenges.

Chemical industry example

A simplified example of the general calculation process for chemicals is shown in Figure 11. The mass flows derived from a bill of materials shall be linked with the relevant LCI and the ODP flows in the LCI to generate the LCI for the process. Linked to the CFs (see Table 16) the single ODP flows can be calculated and aggregated to the CFC-11eq total result.

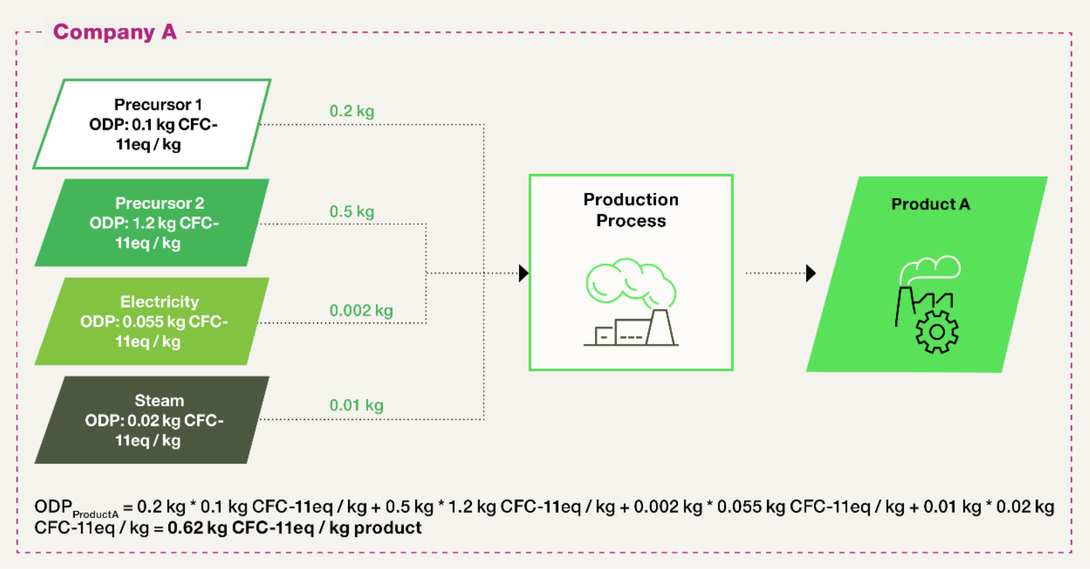


Figure 11: Simplified example of an ODP calculation for a chemical process with ODP mass emission flows.

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9. Photochemical Ozone Creation Potential

9.1. General Description

9.1.1. Issue of Concern

Photochemical Ozone Creation Potential (POCP) describes the ability of a chemical compound to form ground-level ozone in the presence of sunlight and nitrogen oxides (NO_x). POCP is commonly used to evaluate the relative ability of various organic compounds to create photochemical smog. High POCP values indicate that a compound significantly contributes to ozone formation.

Tropospheric ozone is a secondary pollutant and is not directly emitted. The formation occurs locally through photochemical reactions initiated by solar radiation, which cause the oxidation of NMVOCs in the presence of nitrogen oxides (NO_x) (Preiss, P. 2015). NMVOCs are released using solvents, domestic activities and natural sources, such as forests. Figure 12 shows an example of activities emitting Volatile Organic Compounds (VOCs) and NO_x as the main contributors to ozone formation (Donzelli G., Suarez-Varela M.M. 2024). This document focuses primarily on NMVOCs due to their direct role in ozone formation. Figure 12 illustrates the human activities that mostly contribute to VOC and NO_x emissions, highlighting that coal combustion and diesel vehicles emissions have the biggest impact. The graphic Figure 12 illustrates the human activities that mostly contribute to VOC and NO_x emissions, highlighting that coal combustion and diesel vehicles emissions have the biggest impact.

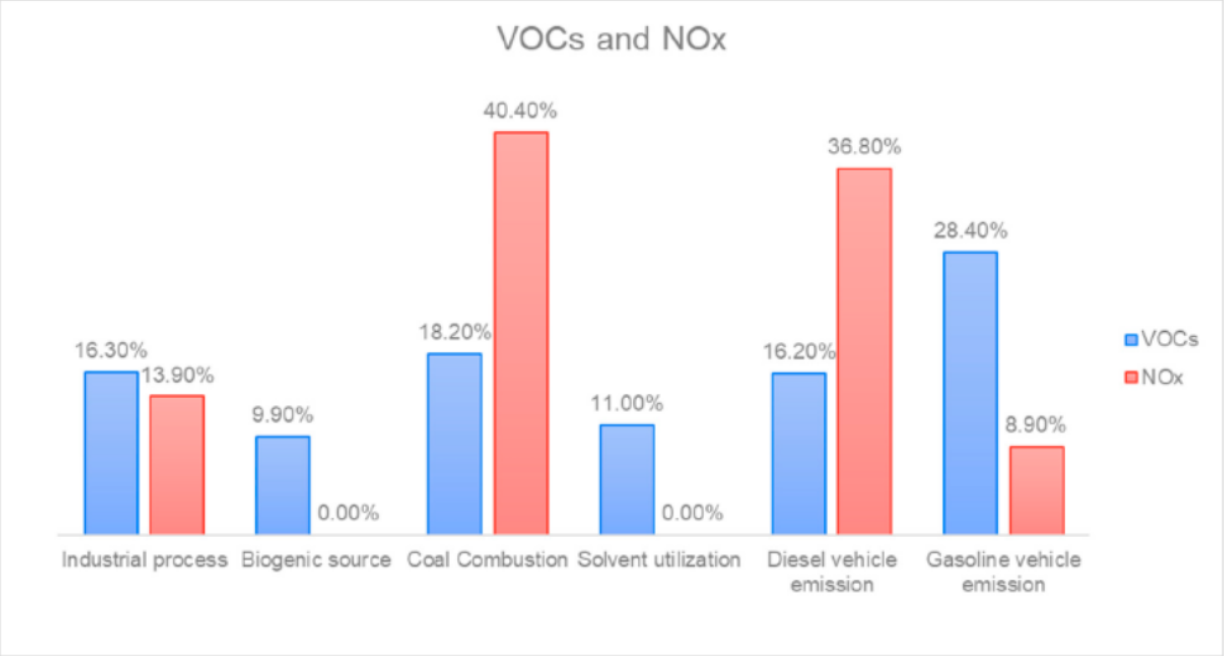

Figure 12: Representation of the six main sources of VOCs and NOx in a typical industrial city in China (Donzelli G., Suarez-Varela M.M. 2024).

The interaction between NMVOCs and NO_x is non-linear and strongly depends on meteorological factors and the background concentration of these compounds. This process is typical of sunny and warm days and is one of the main causes of ground-level ozone pollution (Preiss, P. 2015). This negatively affects air quality and generates major consequences on:

- Human health: Ozone irritates the respiratory system, worsens conditions such as asthma and increases the risk of premature mortality, especially among vulnerable populations (Donzelli G., Suarez-Varela M.M. 2024)
- Ecosystems (flora & fauna): Ozone reduces photosynthesis, damages leaves, and decreases crop yields. This leads to biodiversity loss and compromises ecosystem services, ultimately impacting human well-being and food security (Emberson, L. 2020).
- Materials: Ozone accelerates the deterioration of materials exposed to air, including rubber, plastics, and surface coatings. While often not part of LCIA, this degradation can lead to substantial economic costs due to increased maintenance needs and shortened product lifespans (Preiss, P. 2015)

Assessing the POCP of a product is a crucial aspect of LCA. It enables the identification of the environmental impacts (i.e., on air quality and human health) and supports strategies for mitigation (Holland R., et al, 2025). Additionally, since POCP is partly driven by anthropogenic activities (i.e., transportation, industrial processes, energy production), it is closely monitored by policymakers aiming to reduce its impact (Donzelli G., Suarez-Varela M.M. 2024).

9.1.2. Key Compounds of Potential Impact

High concentration of ozone is formed due to release of NO_x (comprising of nitric acid (HNO_3) and nitrogen dioxide (NO_2)) and VOCs because of incomplete combustion. The reactivity of VOCs plays a crucial role in ozone formation. Recent studies have shown that reactive VOCs tend to decrease with altitude due to oxidation, while oxygenated VOCs accumulate at higher altitudes, influencing ozone production rates differently across atmospheric layers. Additionally, the balance between VOCs and NO_x concentrations governs the efficiency and rate of ozone formation, with variations leading to different photochemical regimes. While VOCs and NO_x are the primary precursors, other compounds such as carbon monoxide (CO), methane (CH_4) and Peroxyacetyl Nitrate (PAN) also contribute towards the formation of ozone.

Understanding the roles and interactions of these compounds is essential for developing effective strategies to mitigate ground-level ozone pollution and its associated health and environmental impacts.

9.1.3. Regulatory Compliance

POCP is also an important topic for regulatory Compliance. Governments and environmental agencies have established strict regulations to control VOC emissions and reduce ground-level ozone. The chemical industry must monitor and manage POCP to comply with these regulations and avoid penalties (Kim, M.-G. *et al.*, 2023).

- In the United States, the Clean Air Act and the National Ambient Air Quality Standards (NAAQS) regulate ozone precursors. Facilities must develop State Implementation Plans (SIPs) and apply Best Available Control Technology (BACT) to limit emissions (U.S. Environmental Protection Agency [EPA]).

- In the EU, the Industrial Emissions Directive 2010/75/EU (European Union, 2010) establishes emission limit values for VOCs. Additionally, the VOC Solvents Emissions Directive 1999/13/EC (European Union, 1999), now incorporated into the Industrial Emissions Directive (IED), specifically regulates emissions from solvent use. Complementing these source-control measures, EU legislation has also addressed the impacts of VOCs through their role in ozone formation: the earlier Council Directive 92/72/EEC on air pollution by ozone introduced a harmonized system for ozone monitoring, thresholds for health and vegetation protection, and public information duties. This framework has since been replaced by Directive 2002/3/EC (European Union, 2002) and is now consolidated under the Ambient Air Quality Directive (European Union, 2008), which sets binding standards for ozone and other pollutants across Member States. Compliance with these directives is critical for industries such as chemicals, paints, coatings, and pharmaceuticals (European Parliament Research Service. (2021)).
- Under the UNECE Gothenburg Protocol (to the Convention on Long-range Transboundary Air Pollution), signatory countries commit to reducing emissions of ozone precursors, including NO_x and VOCs, to mitigate cross-border smog and ground-level ozone formation (UNECE).
- In China, the Air Pollution Prevention and Control Law requires industries to reduce VOC emissions through strict standards, substitution of low-VOC materials, and the installation of treatment technologies. Compliance is monitored by the Ministry of Ecology and Environment (MEE) through real-time emission reporting and inspections, with penalties for exceedances. These measures, reinforced under China’s 13th and 14th Five-Year Plans, aim to curb ground-level ozone formation and reduce the health and environmental impacts of photochemical smog (Enviliance ASIA)

9.1.4. Importance for the Chemical Industry

Chemical processes such as the production of organic compounds, polymers, and pharmaceuticals are major sources of VOC emissions, releasing approximately 40,000 tons into the atmosphere annually (The Joint Research Centre: EU Science Hub, 2021). From production to processing, storage, and transportation, chemical plants emit VOCs that react with NO_x in the atmosphere to produce photochemical smog (Sanjh, S. 2023). Understanding and controlling POCP is essential for reducing ozone formation and complying with environmental regulations. Table 18 lists examples of the chemical industry where POCP is an important aspect.

Table 18: This is a non-exhaustive list of process steps that should be considered for data collection on POCP.

Process steps	Example
Raw Material Extraction	The extraction and processing of raw materials can release VOCs and NO_x, contributing to POCP.
Production and processing	Many industrial processes, such as distillation, cracking, and polymerization, emit VOCs.
Storage and Transportation	Storing raw materials and finished products in tanks can release VOCs, especially if they are not properly sealed.
Waste Management	Waste containing organic compounds can release VOCs if not properly treated.
Disposal & Recycling	Disposal and recycling processes can release VOCs and NO_x, influencing the POCP assessment.

9.2. Methodology of Characterization

Several methodologies can be employed to assess POCP in LCA. The choice of methodology depends on the goal and scope of the study, the available data, and the specific requirements of the assessment. Brief descriptions of existing LCIA methods and their considered characterization models are given below for the chosen EF method and for the other LCIA methods see the Appendix chapter 11.4.1.

9.2.1. Chosen method: EF

Hauschild et al. (2011) recommends Recipe as the default method at both the midpoint and endpoint level as it considers spatially differentiation based on the impact assessment methods existing in 2010. Recommendations to include natural ecosystem within the scope and to expand the CFs beyond Europe have been adapted with the update of ReCiPe method in 2016. In general, the model can be applied in other regions as well. This led to the consideration of POCP for both terrestrial ecosystem and human health (Huijbregts et al. 2017). Although ReCiPe 2016 offers a highly detailed quantification model and is widely regarded as the most comprehensive method for assessing POCP, we recommend using the EF method version 3.1. This recommendation is based on the need for consistency with other sustainability metrics presented in this guideline and alignment with the PEF reporting requirements.

Formula

Within the EF 3.1 method, the LOTOS-EUROS model is applied to calculate the POCP value. LOTOS-EUROS is a combination of Long-Term Ozone Simulation and European Operational Smog and calculates the CFs for human health damage caused by emitted substance *x* in Europe (Segers et al. 2025). The CFs is composed of three different factors: dimensionless intake factor ($IF_{pop,\,x}$), effect factor (EF_k in kg^{-1}) and damage factor (DF_k in yr) (Van Zelm et al 2008).

$$\mathrm{CF}_x = \sum_i \left(\mathrm{IF}_{\mathrm{pop},x,i} \sum_e (\mathrm{EF}_{e,k,i} \mathrm{DF}_{e,k}) \right)$$

Formula 9: Equation for "Characterization factor for compound x"

POCP values from Preiss (2015) and Derwent et al. (1998) und from updated work (Derwent et al. 2007a), (Derwent et al. 2007b) can be coupled with generic NMVOC CFs to calculate specific impacts per compound class:

$$CF_x = \frac{POCP_x}{POCP_{NMVOC}} \cdot CF_{NMVOC}$$

Formula 10: Equation for "Photochemical Ozone Creation Potential" calculation

Where:

- CF_x: characterization factor for compound x
- CF_{NMVOC}: midpoint CF for aggregated NMVOC emissions (e.g., in kg O_3 eq/kg)
- $POCP_x$: POCP of compound *x*
- $POCP_{NMVOC}$: average POCP across the NMVOC profile

Characterization Factors in EF Method

Table 19 below shows the POCP characterization factors (in kg NMVOC-eq. per kg) from EF 3.1 method. There are two relevant categories for POCP, 1) human health and 2) ecosystems. The relevant scope for this document and for sustainability metric is Human Health.

Table 19: Overview of selected NMVOC characterization factors

Compound	**CFs (kg NMVOC-eq. per kg) for Human Health**
Ethylene	1,69
Propylene glycol	0,772
1-Butene	1,82
trans-2-Butene	1,91
cis-2-Butene	1,94
trans-2-Pentene	1,89
Butadiene	1,44
Isoprene	1,84
p-Xylene	1,71
m-Xylene	1,87
o-Xylene	1,78
Toluene	1,08
Benzene	0,368
Pentane	0,667
Hexane	0,814
Heptane	0,834
Propane	0,297
Ethane	0,208
Acetaldehyde	1,08
Formaldehyde	0,877
Acetone	0,159
Methane	0,010
NO_x	1

The list of chemicals in the above Table 19 is non-exhaustive. To access the full list of characterization factors for POCP, please use the following link: EF 3.1

Selection guidance

Generally, EF 3.1 provides regionalized CFs for the POCP relevant elementary flows. However, depending on the database used (e.g., ecoinvent, Sphera MLC, CarbonMinds), the POCP is only assessed using averages provided by EF (like the water footprint with AWARE methodology, see Chapter Water use). Averages shall be used to increase consistency. The goal for the future should remain to switch from average to more regionalized CFs.

9.2.2. LCI Flows

Table 20 shows a few examples of LCI flows for POCP. For the full list see EF 3.1.

Table 20: Overview of LCI flows

Compound	**Description**
Ethylene	Produced from crude oil or natural gas. The feedstock (naphtha or ethane) undergoes steam cracking at high temperature, breaking large hydrocarbons into smaller molecules, yielding ethylene as a primary product.
Propylene glycol	Derived from crude oil or natural gas. Propane is converted to propylene, which is oxidized to propylene oxide. Hydrolysis of propylene oxide gives propylene glycol.
Toluene	Formed mainly from crude oil naphtha during catalytic reforming or recovered from coal tar distillation. Separation and refining yield toluene.
Benzene	Obtained from crude oil naphtha through catalytic reforming, or from pyrolysis gasoline (a byproduct of steam cracking). Extraction and purification yield benzene.
NO_x	Generated from air ($N_2 + O_2$) during high-temperature combustion in crackers, reformers, and furnaces. These conditions cause nitrogen and oxygen to combine into NO_x gases.

9.3. Assessment examples

Case Study:
A company conducted an analysis of its production processes to identify the main sources of VOC emissions and assess their POCP values using the EF method. Toluene (POCP EF: 1.08 kg NMVOC-eq/kg) was found to be the primary contributor to ground-level ozone formation.
The goal was to find an alternative that would reduce ozone formation without compromising product quality. Two options were evaluated:

- Methyl Ethyl Ketone (MEK): MEK has a POCP EF of 0.63. Advantages are good solubility as well as fast evaporation, but it requires 1.2 kg/kg for equivalent performance.
- Propylene Glycol Monomethyl Ether (PGME): PGME has a POCP EF of 0.60. It shows excellent solubility and moderate evaporation, but it requires 1.4 kg/kg for equivalent performance.

In this case study (see Figure 13), it is assumed that the solvent is completely evaporated, meaning that 100% of the solvent mass is emitted to air. The calculated POCP values therefore mainly represent the solvent's own contribution, based on its emission factor and the amount required for equivalent performance. In addition, a small "additional POCP emission" term (0.01–0.02 kg NMVOC-eq/kg) was included in the following calculations to account for other process-related NMVOC emissions such as handling, cleaning, or storage losses. These are not part of the solvent itself and therefore are not double-counted. The variation of this additional term between the scenarios reflects the differences in solvent volatility and quantity handled (e.g., 1.2 kg MEK vs. 1.4 kg PGME). This ensures that all relevant emissions are considered while keeping the calculation transparent and scientifically consistent.

Impacts were calculated according to the POCP guidelines:

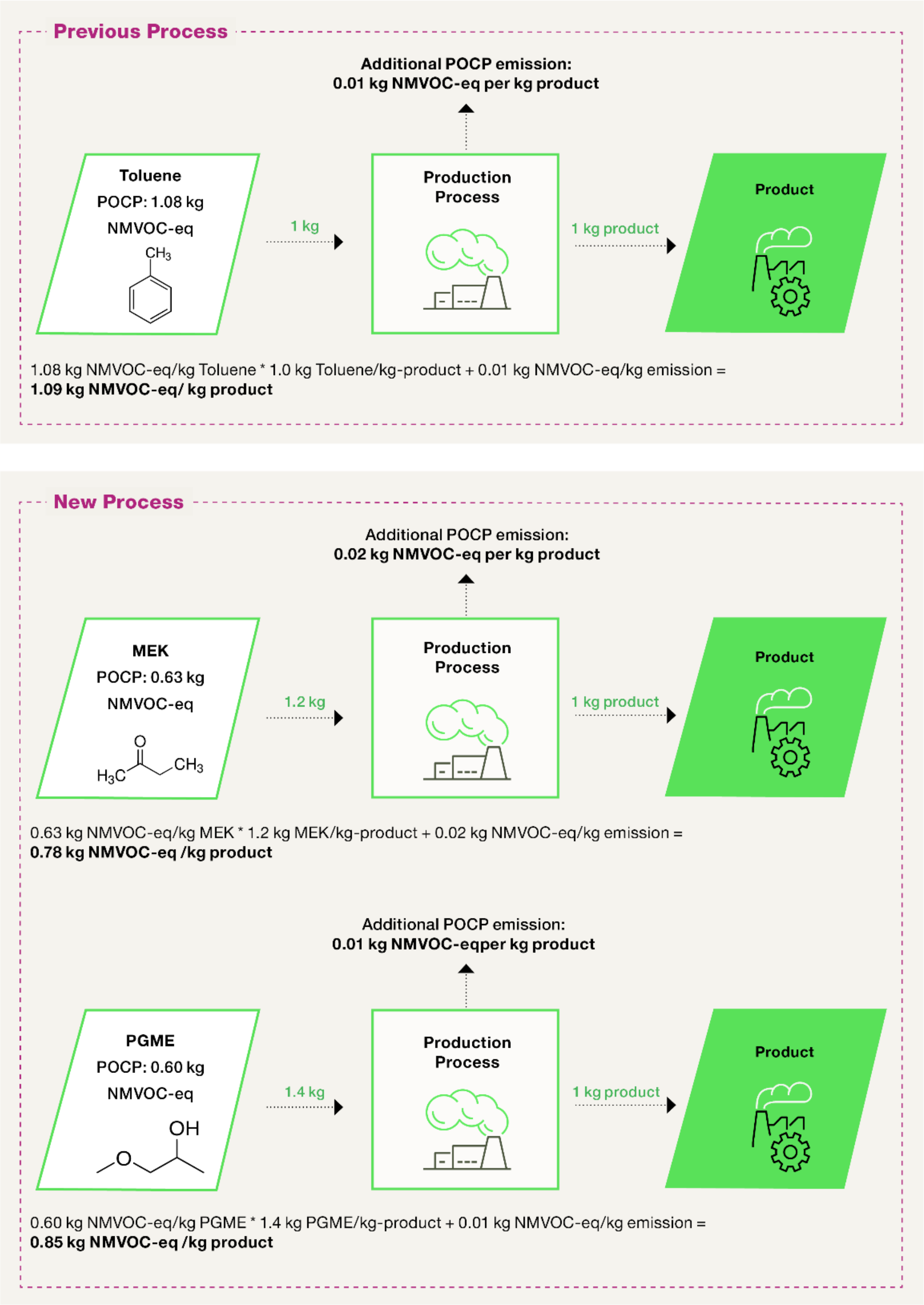

Figure 13: Comparison of previous and new process addressing POCP impacts

Switching to MEK reduced ozone formation and improved environmental compliance. VOC emissions dropped, product quality remained high, and stakeholder trust increased.

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10. Glossary

Abbreviation	Term	Definition	Source
	Activity data	“Activity data are quantified measures of a level of activity that results in GHG emissions or removals”[1]. Activity data can be measured, modeled, or calculated. There are two categories of activity data: process activity data and financial activity data. Process activity data are physical measures of a process that results in GHG emissions or removals. These data capture the physical inputs, outputs, and other metrics of the product’s life cycle (e.g. energy, mass, volume etc). Financial activity data are monetary measures of a process that results in GHG emissions.	TfS PCF Guideline v3.0
	Allocation	Partitioning the input or output flows of a process or a product system between the product system under study and one or more other product systems.	TfS PCF Guideline v3.0
	Background data	See also secondary data. Data that are linked to processes outside the operational control of the company.	TfS PCF Guideline v3.0
	Bill of materials (BOM)	A structured list of all the components, and their quantities that make up an assembly or product.	TfS PCF Guideline v3.0
	Biogenic carbon content	Fraction of carbon derived from biomass in a product.	TfS PCF Guideline v3.0

	Biogenic emissions	CO_2 emissions from the combustion or biodegradation of biomass.	TfS PCF Guideline v3.0
	Biogenic removals	The sequestration or absorption of GHG emissions from the atmosphere, which most typically occurs when CO_2 is absorbed by biogenic materials during photosynthesis.	TfS PCF Guideline v3.0
	Biomass	Material of biological origin excluding material embedded in geological formations and/or fossilized.	TfS PCF Guideline v3.0
CAS number	Chemical Abstracts Service Registry Number	A CAS Registry Number (CAS RN®) is a unique and unambiguous identifier for a specific substance that allows clear communication and, with the help of CAS scientists, links together all available data and research about that substance. Governmental agencies rely on CAS Registry Numbers for substance identification in regulatory applications because they are unique, easily validated, and internationally recognized.	TfS PCF Guideline v3.0 https://www.cas.org/cas-data/cas-registry
CCS	Carbon Capture and Storage	CCS involves the capture of carbon dioxide (CO_2) emissions from industrial processes, such as steel and cement production, or from the burning of fossil fuels in power generation. This carbon is then transported from where it was produced, via ship or in a pipeline, and stored deep underground in geological formations.	TfS PCF Guideline v3.0

CCU	Carbon Capture and Utilization	Carbon capture and utilization (CCU) involves the capture of the greenhouse gas CO_2 from point sources or ambient air and its subsequent conversion into valuable products.	TfS PCF Guideline v3.0
CFP	Carbon footprint of a product	See Product Carbon Footprint (PCF).	TfS PCF Guideline v3.0
CFCs	Chlorofluorocarbon	See Greenhouse Gas definition.	TfS PCF Guideline v3.0
CH_4	Methane	See Greenhouse Gas definition.	TfS PCF Guideline v3.0
CMP	Contract manufactured products	Contract manufacturing occurs when a company outsources part of the manufacturing process to a third-party company to reduce the expenses of production.	TfS PCF Guideline v3.0
	Characterization Factor	Factor derived from a characterization model which is applied to convert an assigned life cycle inventory analysis result to the common unit of the category indicator NOTE The common unit allows calculation of the category indicator result.	ISO 14044
	Cradle-to-gate	An assessment that includes part of the product’s life cycle, including material acquisition through the production of the studied product and excluding the use or end-of-life stages.	TfS PCF Guideline v3.0
	Cradle-to-grave	A cradle to grave assessment considers impacts at each stage of a product’s life cycle, from the time natural resources are extracted	TfS PCF Guideline v3.0

		from the ground and processed through each subsequent stage of manufacturing, transportation, product use, recycling, and ultimately, disposal.	
	Conformity assessment	Demonstration that specified requirements relating to a product, process, system, person or organization are fulfilled. Note 1 to entry: Adapted from ISO/IEC 17000: 2004, definition 2.1. ISO/TS 14441:2013(en), 3.13	TfS PCF Guideline v3.0
	Consumption mix	This approach focuses on the domestic production and the imports taking place. These mixes can be dynamic for certain commodities (e.g., electricity) in the specific country/region.	TfS PCF Guideline v3.0
CO_2e	Carbon Dioxide Equivalent	Carbon dioxide equivalent, or CO_2e is a metric measure representing all greenhouse gases by converting them to the equivalent amount of CO_2.	TfS PCF Guideline v3.0
	Endpoint characterization models	Estimate the ultimate effects (or “endpoints”) of environmental impacts on areas of protection, such as human health, ecosystem quality, and resource availability. These models extend the analysis further along the cause-effect chain, translating inventory data through midpoint categories into final damage categories. In this sense Human health (DALYs), ecosystem damage (species loss), resource	TfS PCF Guideline v3.0

		depletion are endpoint categories.	
C14-method	Radiocarbon dating	A form of radiometric dating used to determine the age of organic remains in ancient objects, such as archaeological specimens, on the basis of the half-life of carbon-14 and a comparison between the ratio of carbon-12 to carbon-14 in a sample of the remains to the known ratio in living organisms.	TfS PCF Guideline v3.0
DU	Declared Unit	Intermediate or final products, that is, products which will still be processed further to create a final product, can, however, have several functions based on their eventual end use. In this case (and where an LCA does not cover the full life cycle), the term Declared Unit – typically referring to the physical quantity of a product, for example “1 liter of liquid laundry detergent with 30 percent water content”– shall be used instead.	TfS PCF Guideline v3.0
DMP	Digital Material Passport	A structured digital record for a material that contains detailed information about sustainability and circularity, as well as required and potentially optional declarations, certificates, and additional material information. It focuses on intermediate materials in the value chain which may not be subject to regulation, but whose data are required to enable the issue of	Chem-X Definition

		regulated Digital Product Passports (DPPs). DMPs are designed to interoperate with one or more DPPs.	
DPP	Digital Product Passport	A structured digital record for a product that contains detailed information about sustainability and circularity, as well as required and potentially optional declarations, certificates and additional product information. It focuses on a regulated end product in the value chain. Both its information content and technical requirements follow regulatory requirements and/or standards delegated by the legislator to designated standardization bodies.	Chem-X Definition *Note 1: based on DPP definition in ESPR.*
DUNS	Duns and Bradstreet Number	The Dun & Bradstreet D-U-N-S Number is a unique nine-digit identifier for businesses.	TfS PCF Guideline v3.0
ECICS	European Customs Inventory of Chemical Substances	See table 4.2	TfS PCF Guideline v3.0
EEIO	Environmentally-extended input and output	Environmentally extended input–output analysis (EEIOA) is used in environmental accounting as a tool which reflects production and consumption structures within one or several economies.	TfS PCF Guideline v3.0
EF	Environmental Footprint	It is a multi-criteria measure to calculate the environmental performance of a product, service or	TfS PCF Guideline v3.0

		organization based on a life cycle approach.	
EoL	End of Life	End-of-life describes the end of the life cycle of a product. Here one can distinguish between different treatment methods: Recycling, landfill and incineration	TfS PCF Guideline v3.0
ERP system	Enterprise resource planning system	Enterprise resource planning is a system that helps automate and manage business processes across finance, manufacturing, retail, supply chain, human resources, and operations.	TfS PCF Guideline v3.0
EU	European Union	The European Union is a supranational political and economic union of 27 member states that are located primarily in Europe.	TfS PCF Guideline v3.0
	Functional unit	A functional unit describes the function of a product in question. For example, for a laundry detergent, the functional unit could be defined as “washing 4.5 kg of dry fabric with the recommended dosage with medium-hard water”. Understanding the functional unit is essential for comparability between products with the same function, as it provides the reference to which the input (materials and energy) and output (such as products, byproducts, waste) are quantified.	TfS PCF Guideline v3.0
GHG	Greenhouse Gases	Greenhouse gases constitute a group of gases contributing to global warming and climate change. The Kyoto Protocol, an environmental agreement adopted by many of the parties to	TfS PCF Guideline v3.0

		the United Nations Framework Convention on climate change (UNFCCC) in 1997 to curb global warming, nowadays covers seven greenhouse gases: The non-fluorinated gases: Carbon dioxide (CO_2) Methane (CH_4) Nitrous oxide (N_2O) The fluorinated gases: Hydrofluorocarbons (HFCs) Perfluorocarbons (PFCs) Sulphur hexafluoride (SF6) Nitrogen trifluoride (NF3) Converting them to carbon dioxide (or CO_2) equivalents makes it possible to compare them and to determine their individual and total contributions to global warming.	
GHG protocol	Greenhouse Gas Protocol Standard	International Standard on how to calculate Greenhouse Gases.	TfS PCF Guideline v3.0
GLO	Global		TfS PCF Guideline v3.0
GWP	Global Warming Potential	Global Warming potential is a term used to describe the relative potency, molecule for molecule, of a greenhouse gas, taking account of how long it remains active in the atmosphere.	TfS PCF Guideline v3.0
HCFCs	Hydrochlorofluorocarbon	See Greenhouse Gas definition.	TfS PCF Guideline v3.0
HEFs	Fluorinated ethers	Liquid Chemical.	TfS PCF Guideline v3.0

HFCs	Hydrofluorocarbons	See Greenhouse Gas definition.	TfS PCF Guideline v3.0
HS	Harmonized Commodity Description and Coding Systems	See table 4.2	TfS PCF Guideline v3.0
IEC	International Electrotechnical Commission	Founded in 1906, the IEC (International Electrotechnical Commission) is the world's leading organization for the preparation and publication of international standards for all electrical, electronic and related technologies.	TfS PCF Guideline v3.0
ILCD	International Life Cycle Data System	The International Reference Life Cycle Data System is an initiative developed by JRC and DG ENV since 2005, with the aim to provide guidance and standards for greater consistency and quality assurance in applying LCA.	TfS PCF Guideline v3.0
ISO	International Organization for Standardization	The International Organization for Standardization is an international standard development organization composed of representatives from the national standards organizations of member countries.	TfS PCF Guideline v3.0
ISOPA	European Diisocyanate and Polyol Producers Association	ISOPA is the European trade association for producers of diisocyanates and polyols, the main building blocks of polyurethanes.	TfS PCF Guideline v3.0
ISO 14067: 2018	ISO standard on Greenhouse gases — Carbon footprint of products — Requirements and guidelines for quantification	ISO 14067: 2018 specifies principles, requirements and guidelines for the quantification and reporting of the carbon footprint of a product (CFP), in a manner	TfS PCF Guideline v3.0

		consistent with International Standards on life cycle assessment (LCA) [ISO 14040 [ISO 14040: 2006] and ISO 14044].	
IT	Information technology		TfS PCF Guideline v3.0
kg	Kilogram		TfS PCF Guideline v3.0
kWh	Kilowatt-hour		TfS PCF Guideline v3.0
LCA	Life Cycle Assessment	The compilation and evaluation of the inputs, outputs, and the potential environmental impacts of a product system throughout its life cycle [ISO 14040: 2006].	TfS PCF Guideline v3.0
LCI	Life Cycle Inventory	The phase of life cycle assessment involving the compilation and quantification of inputs and outputs for a product throughout its life cycle [ISO 14040:2006].	TfS PCF Guideline v3.0
LCIA	Life Cycle Impact Assessment	The phase of life cycle assessment aimed at understanding and evaluating the magnitude and significance of the potential environmental impacts for a product system throughout the life cycle of the product [ISO 14040:2006].	TfS PCF Guideline v3.0
	Midpoint characterization model	Approaches that assess the potential environmental impacts of a product or process at an intermediate stage in the cause-effect chain. Examples are climate change, acidification, eutrophication, ozone depletion.	TfS PCF Guideline v3.0

LHV	Lower heating value	The lower heating value (LHV; *net calorific value*; *NCV*, or *lower calorific value*; *LCV*) is another measure of available thermal energy produced by a combustion of fuel, measured as a unit of energy per unit mass or volume of substance. In contrast to the HHV, the LHV considers energy losses such as the energy used to vaporize water. Lower heating value (LHV) is defined as the amount of heat released when a fuel is combusted, starting from 25°C and with the combustion products returned to 150°C, excluding the latent heat of vaporization of water.	Meherwan P. Boyce,10 - Combustors, Editor(s): Meherwan P. Boyce, Gas Turbine Engineering Handbook (Fourth Edition), Butterworth-Heinemann, 2012, Pages 427-490, ISBN 9780123838421, https://doi.org/10.1016/B978-0-12-383842-1.00010-X.
NACE	Nomenclature of Economic Activities	NACE (Nomenclature of Economic Activities) is the European statistical classification of economic activities. It is established by law.	TfS PCF Guideline v3.0
NF_3	Nitrogen triflouride	See Greenhouse Gas definition.	TfS PCF Guideline v3.0
N_2O	Nitrous oxide	See Greenhouse Gas definition.	TfS PCF Guideline v3.0
OCF	Organizational Carbon Footprint	Carbon Footprint of an Organisation.	TfS PCF Guideline v3.0
ODS	Ozone-depleting substance	It refers to gases containing either chlorine or bromine that are released to the atmosphere because of human activity and are controlled under Annexes A, B, C, or E of the Montreal Protocol. These include, among other CFCs, CCl4, CH3CCl3, halons, CH3Br and HCFCs. These ODSs typically have sufficiently long	WMO, 2022

		atmospheric lifetimes to reach the stratosphere after being emitted at the surface. Methyl bromide is the shortest-lived of the controlled substances and has natural and anthropogenic sources. Other substances contribute chlorine and bromine to the atmosphere but are not controlled under the Montreal Protocol for various reasons.	
	Primary data	Sometimes also called activity data. Data that concerns processes inside the operational control of the company or data from specific processes in the product life cycle. A partial LCIA is considered primary data if the measure of the activity data and the measure of the emission factor are based on data where the data generators have a direct access to via direct measurements or assessments where they have a direct control. “Data pertaining to a specific product or activity within a company’s value chain. Such data may take the form of activity data, emissions or emission factors. Primary data is site-specific, company-specific (if there are multiple sites for the same product) or supply chain–specific. Primary data may be obtained through meter readings, purchase records, utility bills, engineering models, direct monitoring, material or product balances,	TfS PCF Guideline v3.0

		stoichiometry or other methods for obtaining data from specific processes in the value chain of the company" [Path 2021:41]	
PCF	Product Carbon Footprint	The Product Carbon Footprint is the most established method for determining the climate impact of a product, considering the total greenhouse gas (GHG) emissions caused to produce a product, expressed as carbon dioxide equivalent. The PCF can be assessed from cradle-to-gate (partial PCF) or from cradle-to-grave (total PCF).	TfS PCF Guideline v3.0
PCR	Product Category Rules	Set of specific rules, requirements, and guidelines for developing Type III environmental declarations and footprint communications for one or more product categories. [ISO 14025:2006] . [ISO 14027]	TfS PCF Guideline v3.0
PFCs	Perfluorocarbons	See Greenhouse Gas definition.	TfS PCF Guideline v3.0
PFPEs	Perfluoropolyethers	Perfluoropolyethers (PFPE) are a group of plastics, usually liquid to pasty at room temperature, that are fluoropolymers consisting of fluorine, carbon and oxygen.	TfS PCF Guideline v3.0
PRODCOM	Production Communautaire (Community Production)	See table 4.1	TfS PCF Guideline v3.0
	Production mix	This approach focuses on the domestic production routes and technologies applied in the specific country/region and	TfS PCF Guideline v3.0

		individually scaled according to the actual production volume of the respective production route. This mix is generally less dynamic.	
	Programme operator	Body or bodies that conduct an environmental declaration programme or footprint communication programme. A programme operator can be a company or a group of companies, industrial sector or trade association, public authorities or agencies, or an independent scientific body or other organization. [ISO 14027]	TfS PCF Guideline v3.0
	Removal	The sequestration or absorption of GHG emissions from the atmosphere, which most typically occurs when CO2 is absorbed by biogenic materials during photosynthesis.	TfS PCF Guideline v3.0
	Secondary data	See also background data. Data that concern processes outside the operational control of the company or process data that are not from specific processes in the product life cycle. “Data that is not from specific activities within a company’s value chain but from databases, based on averages, scientific reports or other sources.” [Path 2021:41]	TfS PCF Guideline v3.0
SF_6	Sulphur hexafluoride	See Greenhouse Gas definition.	TfS PCF Guideline v3.0
SIC	Standard Industrial Classification	The Standard Industrial Classification (SIC) is a	TfS PCF Guideline v3.0

		four-digit classification system that classifies industries according to business activities.	
SMILES	Simplified Molecular Input Line Entry System	See table 4.2	TfS PCF Guideline v3.0
	Spot transaction	A spot transaction is the sale of a commodity, asset or right, under the terms of which delivery is scheduled to be made within the longer of the following periods: (a) 2 trading days; (b) the period generally accepted in the market for that commodity, asset or right as the standard delivery period.	TfS PCF Guideline v3.0
	System expansion	Expanding the product system to include the additional functions related to the co-products. System expansion is a method used to avoid co-product allocation.	TfS PCF Guideline v3.0
TÜV	Technischer Überwachungsverein (engl.: MOT)		TfS PCF Guideline v3.0
	Unit process	Smallest element considered in the life cycle inventory analysis (3.1.4.4) for which input and output data are quantified. [ISO 14040:2006], 3.34]	TfS PCF Guideline v3.0
UNSPSC	United Nations Standard Products and Services Code	See table 4.2	TfS PCF Guideline v3.0
	Utilities	The term “utilities” includes here: Electricity, process steam, excess steam, cooling water, demineralized water, process water, compressed air and nitrogen.	TfS PCF Guideline v3.0

	Validation	the process of evaluating a system or component to ensure compliance with the functional, performance and interface requirements. [ISO/IEC 14776: 2010]	TfS PCF Guideline v3.0
VAT	Value Added Tax		
	Verification	Confirmation, through the provision of objective evidence, that specified requirements have been fulfilled. [ISO 9000: 2005; ISO 14025:2006]	TfS PCF Guideline v3.0
	Waste	Substances or objects which the holder intends or is required to dispose of. NOTE This definition is taken from the Basel Convention on the Control of Transboundary Movements of Hazardous Wastes and Their Disposal (22 March 1989), but is not confined in this International Standard to hazardous waste. [ISO 14040:2006], 3.35]	TfS PCF Guideline v3.0
WBCSD	World Business Council for Sustainable Development	The World Business Council for Sustainable Development (WBCSD) is a business-led organization that focuses exclusively on business and sustainable development.	TfS PCF Guideline v3.0

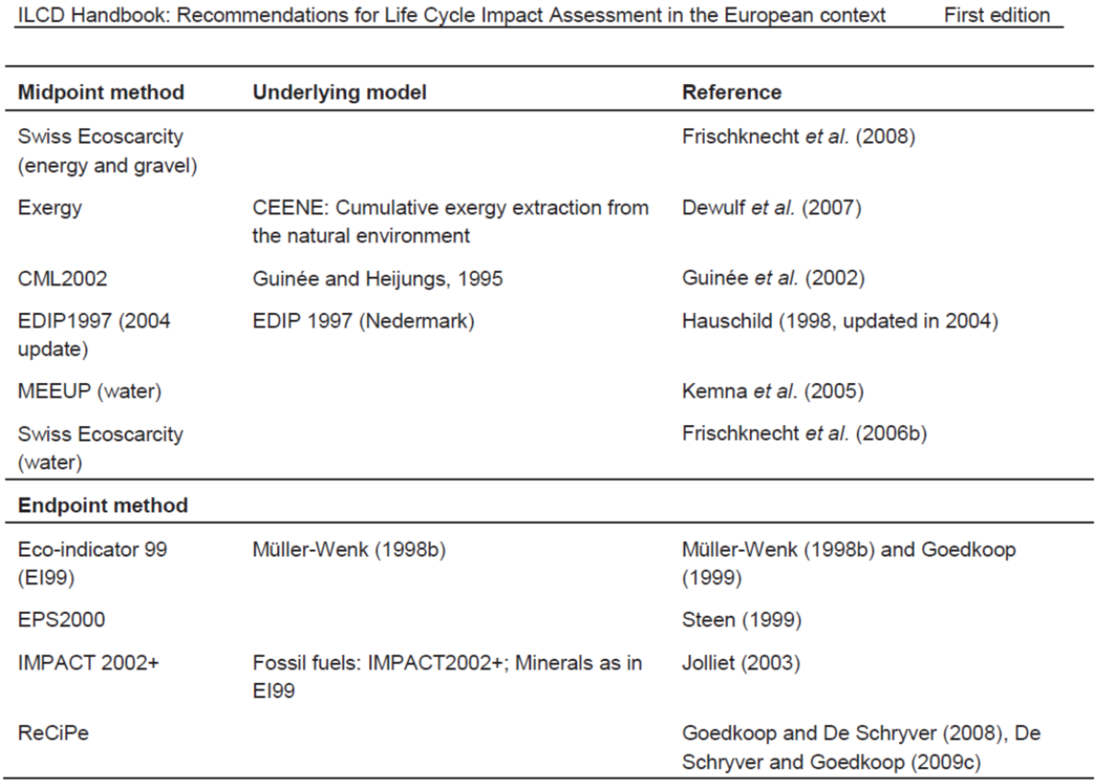
11. Appendix

11.1. Resource Use, fossils

11.1.1. Other LCIA methods: Resource Use, fossil

An overview of existing midpoint methods is given in Table 21. Drielsma et al. (2016) have compared the definitions as used by the Committee for Mineral Reserves International Reporting Standards (CRIRSCO) with definitions of reserves as used in the ADP (Resource use, fossils) (Van Oers et al., 2002).

Table 21: Overview of Midpoint assessment methods



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Midpoint method	**Underlying model**	**Reference**
Swiss Ecoscarcity (energy and gravel)		Frischknecht *et al.* (2008)
Exergy	CEENE: Cumulative exergy extraction from the natural environment	Dewulf *et al.* (2007)
CML2002	Guinée and Heijungs, 1995	Guinée *et al.* (2002)
EDIP1997 (2004 update)	EDIP 1997 (Nedermark)	Hauschild (1998, updated in 2004)
MEEUP (water)		Kemna *et al.* (2005)
Swiss Ecoscarcity (water)		Frischknecht *et al.* (2006b)
Endpoint method		
Eco-indicator 99 (EI99)	Müller-Wenk (1998b)	Müller-Wenk (1998b) and Goedkoop (1999)
EPS2000		Steen (1999)
IMPACT 2002+	Fossil fuels: IMPACT2002+; Minerals as in EI99	Jolliet (2003)
ReCiPe		Goedkoop and De Schryver (2008), De Schryver and Goedkoop (2009c)

Exergy

This method is based on Dewulf et al. (2007). They used Exergy as a key element in their assessment. Exergy, often referred to as "available energy" or "useful work potential", is a fundamental concept in the field of thermodynamics and engineering. It plays a crucial role in understanding and quantifying the quality of energy within a system and its potential to perform useful work. Exergy analysis has widespread applications in various fields, including energy engineering, environmental science, and industrial processes. Exergy values have been determined for a list of resources covering fossil fuels, minerals, nuclear energy, land resources, renewable resources (e.g. wind power and hydropower), atmospheric resources and water resources. The method addresses several shortcomings of earlier exergy methods, like double counting in bio-based fuels and confusing exergy loss in ores with exergy loss in the minerals that contain the metals being exploited.

Although this method involves the exergy concept thoroughly, it does not reflect the scarcity of resources. Exergy is a thermodynamic concept and simply put, it's used to measure the quality or usefulness of energy or materials. As such, for instance, fossil resources have high exergy values and release plenty of useful energy. Nevertheless, it doesn’t mean these resources are abundant or easily accessible. Even if this concept is interesting, we decided to follow the EF of the European Commission in sense of harmonization.

Swiss Ecoscarcity 2021 (energy)

The method of ecological scarcity – sometimes called Swiss Ecoscarcity or Swiss Ecopoints method – allows a comparative weighting and aggregation of various environmental interventions by use of so-called eco-factors. The method supplies these weighting factors for different emissions into air, water and top-soil/groundwater as well as for the use of energy resources. The eco-factors are based on the annual actual flows (current flows) and on the annual flow considered as critical (critical flows) in a defined area (country or region). The eco-factors were originally developed for the area of Switzerland (see references below). There, current flows are taken from the newest available statistical data, while critical flows are deduced from the partly scientifically supported goals of the Swiss environmental policy, each as of publication date. Later, sets of eco-factors were also made available for other countries, such as Belgium and Japan etc.

In the ecological scarcity method, an impact assessment of life cycle inventories is performed according to the 'distance-to-target' principle. The key metrics of this method are eco-factors, which indicate the environmental burden of an emission, resource use or other substance flows in the form of Ecopoints (UBP) per unit of quantity. An eco-factor is derived by relating the current situation to the tolerated maximum emission or use. The ecological scarcity method, for convenience also referred to as the eco points method, was first published in 1990.

This method is taken from Frischknecht et al. (2006), with adaptations by PRé as described below. The CFs have first been implemented by ESU-services Ltd. All files are provided without liability[14]. Ecological Scarcity 2006 is a follow-up of the Ecological scarcity 1997 method, which is called Ecopoints 97 (CH) in the SimaPro method library (superseded) and was lastly updated in 2021 (Federal Office for the Environment (FOEN) 2021).

The ecoinvent implementation contains seven specific impact categories, with for each substance a final UBP (environmental loading points) score as CF. This method only contains the impact category natural resources containing only water resources. The complete method can be found in the European methods category.

There are three important differences and reasons for not using it in the Chem-X methodology (SimaPro the methods library):

- The Ecopoint system does not use a specific classification. It assesses impacts individually. Although this allows for a detailed and very substance-specific method, it has the disadvantage that only a few impacts are assessed.
- The Ecopoint system uses a different normalization principle. It uses target values rather than current values.

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[14] Contact info: http://www.esu services.ch/address /

- The Ecopoint system is based on Swiss policy levels instead of sustainability levels. Policy levels are usually a compromise between political and environmental considerations.

The following data are necessary in calculating a score in Ecopoints for a given product:

- quantified impacts of a product;
- total environmental load for each impact type in a particular geographical area;
- maximum acceptable environmental load for each impact in that particular geographical area.

EDIP 1997

This method was updated in 2004 and includes non-renewable resources (fossil fuels and minerals). The amount of resources extracted is divided by the 2004 global production of the resource and weighted according to the quantity of resources in economically exploitable reserves. Effectively, this means that global annual production drops out, so that the characterization model is based on the economic reserves only. The CFs are expressed in person-reserve, meaning the quantity of the resource available to an average world citizen. That is not very often used in many LCA, so we do not use this method either. Furthermore, it is a normalized figure and not a clear midpoint-related approach. That does not fit with the other recommended methods. Due to harmonization, this method is not recommended to be used.

11.2. Water Scarcity

11.2.1. Example 1: Water scarcity impact for product with value chain in different countries

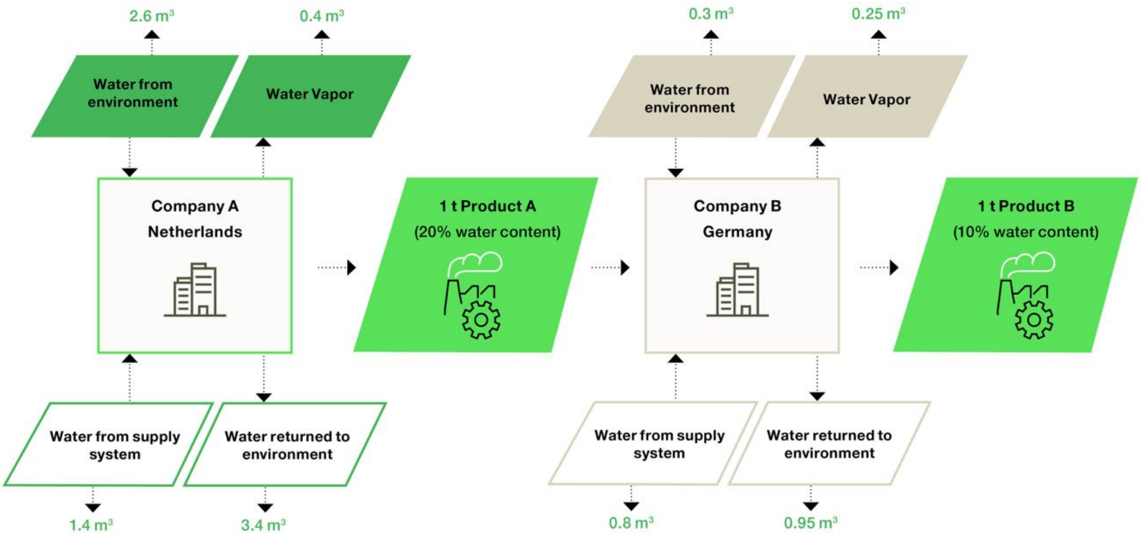


Figure 14: Example 1: Water scarcity impact for product with value chain in different countries.

Total Water Input Company A = 2.6 + 1.4 = 4 m^3
Total Water Output Company A = 3.4 + 0.4 + (0.2 x 1) = 4 m^3
Water Balance: Checked!

Consumptive Water Company A = 4 – (3.4) = 0.6 m^3
CF (NL) = 1.17 m^3 world eq./m^3
Water scarcity Impact Product A = 0.6 x 1.17 = 0.702 m^3 world eq. / ton

Total Water Input Company B = (0.2 x 1) + 0.3 + 0.8 = 1.3 m^3
Total Water Output Company B = 0.25 + 0.95 + (0.1 x 1) = 1.3 m^3
Water Balance: Checked!

Consumptive Water Company B = 1.1 – (0.95) = 0.15 m^3
CF (DE) = 1.36 m3 world eq./m^3
Water scarcity Impact Product B = 0.702 + (0.15 x 1.36) = 0.906 m^3 world eq.

11.2.2. Example 2: Water scarcity impact when input water country of origin is different from output water

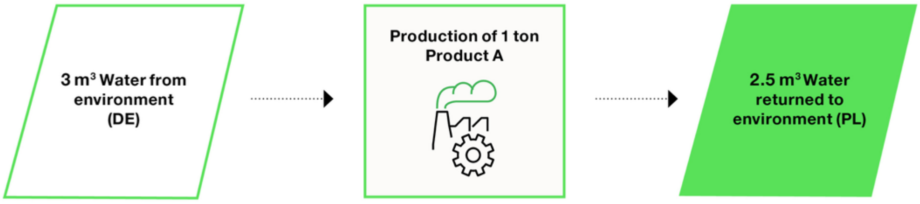


Figure 15: Example 2: Water scarcity impact when input water country of origin is different from output water.

CF_1 (DE) = 1.36 m^3 world eq./m^3
CF_2 (PL) = 1.96 m^3 world eq./m^3
Water scarcity impact = (Total water inputs x CF_1) – (Total water returned to environment x CF_2) = (3 x 1.36) – (2.5 x 1.96) = - 0.82
In this case, the water scarcity impact is negative because transferring the water from Germany to Poland even if not fully returned, it causes a credit due to different water stress level.

11.2.3. Examples on Corrective Considerations for Surplus Water Outputs

Table 22 represents the water inventory obtained after data collection.

Table 22: Input-output process water inventory before water balance correction (example 4)

Input				Output		
Raw materials	10	ton		Product	9	ton
Cooling materials	5	m^3		Steam condensate	1.5	m^3
Water for steam generation	2	m^3		Process water to WWTP	0.9	m^3
Process water	1	m^3		Cooling water returned to environment	5.5	m^3
				Water loss (evaporation)	1.6	m^3

Total Water Input = 5 + 2 + 1 = 8 m^3
Total Water Output = 1.5 + 0.9 + 5.5 + 1.6 = 9.5 m^3
Water Output Surplus = 9.5 – 8 = 1.5 m^3

- After confirming the water content of raw materials, 10% water content has been estimated to be included in raw materials.

- It has been also confirmed that due to having open facilities, rainwater has been entered into the network and returned into environment along with the cooling water. Therefore, the rainwater amount should be deducted from inventory based on the water imbalance.

The updated inventory is as follows:

Table 23: Input-output process water inventory after water balance correction (example 4)

Input				**Output**		
Raw materials (dry)	9	ton		Product	9	ton
Water content in raw materials	1	ton		Steam condensate	1.5	m^3
Cooling water	5	m^3		Process water to WWTP	0.9	m^3
Water for steam generation	2	m^3		Cooling water returned to environment (rainwater excluded[5])	5	m^3
Process water	1	m^3		Water loss (evaporation)	1.6	m^3
				Rainwater to be deducted!	0.5	m^3

Total Water Input = 5 + 2 + 1 + 1 = 9 m^3
Total Water Output = 1.5 + 0.9 + 5.5 + 1.6 – 0.5 = 9 m^3
Water Balance: Checked!

11.2.4. Examples on Corrective Considerations for Surplus Water Inputs

Table 24 represents the water inventory obtained after data collection.

Table 24: Input-output process water inventory before water balance correction (example 5)

Input				**Output**		
Raw materials (dry)	10	ton		Product	9	ton
Process water	4	m^3		Solid waste to incineration	2	ton
Water for steam generation	2	m^3		Steam condensate	1.5	m^3
				Process Water to WWTP	3	m^3

Total Water Input = 4 + 2 = 6 m^3
Total Water Output = 1.5 + 3 = 4.5 m^3
Water Input Surplus = 6 – 4.5 = 1.5 m^3

- After confirming the water content of solid waste, 50% water content has been estimated to be included in the solid waste.
- The water loss due to evaporation also has been confirmed for the steam. Therefore, evaporated water has been added to output flows based on the water imbalance.

The updated inventory is as follows:

Table 25: Input-output process water inventory after water balance correction (example 5)

Input		
Raw materials (dry)	10	ton
Process water	4	m^3
Water for steam generation	2	m^3
Output		
Product	9	ton
Solid waste to incineration	1	ton
Water content in the solid waste	1	m^3
Steam condensate	1.5	m^3
Water loss (evaporation)	0.5	m^3
Process water to WWTP	3	m^3

Total Water Input = 4 + 2 = 6 m^3
Total Water Output = 1 + 1.5 + 0.5 + 3 = 6 m^3
Water Balance: Checked!

11.3. Acidification Potential

11.3.1. Other LCIA methods: Acidification Potential

In the ILCD Handbook (Hauschild et al., 2011) different LCIA methods containing different models on midpoint level assessing the AP have been described and evaluated:

- **TRACI APs** are derived from Norris's (2003) model, which offers generic, spatially differentiated CFs for the U.S. It employs the ASTRAP fate model to connect emissions to land deposition, accounting for AP across all land and inland water areas, regardless of soil and ecosystem sensitivity. The model's dose-response curve is set to 1. While TRACI effectively evaluates acidifying chemicals, it is limited to terrestrial acidification in the U.S. and does not fully address soil sensitivity to acidifying deposition. Enhancing environmental relevance could involve adding soil fate factors to differentiate sensitive from non-sensitive areas. Additionally, the ASTRAP model used for atmospheric fate is considered outdated. (Hauschild et al., 2011)
- **MEEUP** (Kemna et al., 2005) is aligned with European legislation and the Gothenburg protocol, focusing on AP based on H^+ releases. It does not consider the chemical fate of emissions in air and soil, treating all emissions and depositions as equal in generating AP, with an implicit dose-response curve of 1. The method lacks environmental relevance due to its disregard for atmospheric fate and soil sensitivity, and it does not allow for regional differentiation (Hauschild et al., 2011).
- **CML 2002** employs the Hazard Index (HI) method (Huijbregts et al., 2001) to provide spatially specific CFs for acidifying and eutrophying air pollutants in Europe. These CFs indicate the marginal change in the hazard index across European ecosystems by comparing actual loads to critical loads, weighted by ecosystem and region. The European RAINS model (Amann et al. 1999) is used to assess atmospheric transport and deposition. The HI method assumes a dose-response slope that is inversely proportional to the critical load. While CML 2002 offers a solid evaluation, it is less current and holds less stakeholder relevance compared to other methods. (Hauschild et al., 2011)
- **ReCiPe** is a midpoint-endpoint method that utilizes the Base Saturation method developed by Van Zelm et al. (2007a) to assess atmospheric fate using the EUTREND model (Van Jaarsveld et al., 1997), focusing solely on terrestrial ecosystems. It employs the SMART 2 simulation model (Kros, 2002) to evaluate soil sensitivity at the midpoint level through changes in soil base saturation, with data currently available only for Europe. ReCiPe provides a solid foundation for future acidification methods based on the Base Saturation factor, offering an alternative to critical load approaches. However, the concept needs to be expanded to include ecosystems beyond forests, and further exploration is required to create consistent CFs for other continents, including potential proxies for effect factors. (Hauschild et al. 2011)
- **LIME** (Hayashi et al., 2004) is a midpoint-endpoint method that uses the Atmospheric Deposition Factor to express the SO_2 equivalency, indicating an increase in H^+ deposition per unit area due to additional acidifying emissions. The fate of these emissions is assessed using an atmospheric transport model or empirical data, depending on the chemical, and it focuses solely on terrestrial ecosystems. While LIME generally meets scientific criteria at

the midpoint level, its selected indicator lacks sufficient environmental relevance, as it only models the cause-effect chain up to the deposition of acid equivalents without considering sensitive and non-sensitive areas. (Hauschild et al., 2011)

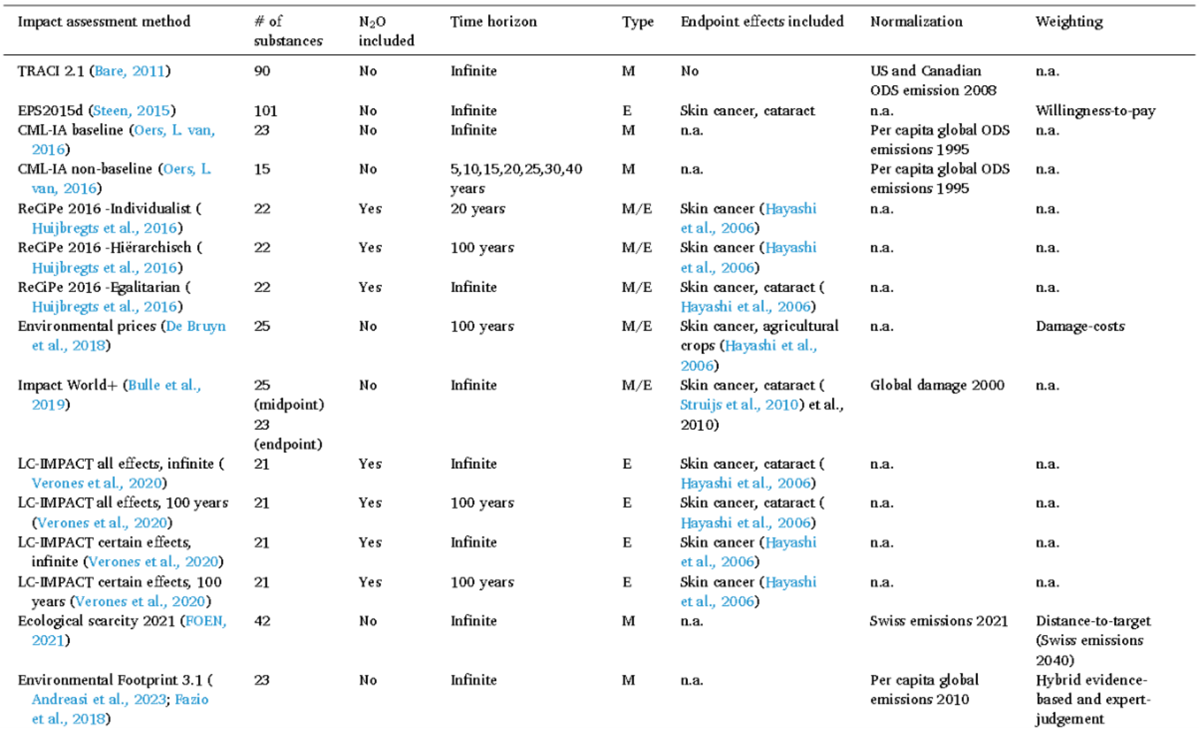
- **Payet** (2006) proposed a dose-effect relationship to evaluate changes in pH concentration in non-buffered water bodies, focusing on the fraction of affected or lost species, as part of the European NOMIRACLE project and IMPACT 2002+ developments. This method has not been operationalized or validated with field measurements and requires a fate model for further development. However, it could provide a valuable foundation for assessing the impact of acidifying chemicals on aquatic ecosystems. (Hauschild et al. 2011)
- **ImpactWorld+** enhances existing regional modeling capabilities by extending them to a global scale, enabling consistent evaluation of regional life cycle emission inventories within the framework of a global economy (Jungbluth, 2025). This methodology serves as an update to the IMPACT 2002+, LUCAS, and EDIP methods. ImpactWorld+ employs a midpoint-damage framework that offers four complementary perspectives to illustrate an LCIA profile: (1) midpoint impacts, (2) damage impacts, (3) damages affecting human health, ecosystem quality, and resource & ecosystem service areas of protection, and (4) damages related to water and carbon concerns. The assessment of terrestrial and freshwater acidification impacts combines global atmospheric source-deposition relationships with the sensitivity of soil and water ecosystems at a resolution of 2° × 2.5° (latitude × longitude) (Bulle et al., 2019). By utilizing more scientifically robust and advanced models, ImpactWorld+ delivers more accurate and environmentally relevant LCA results. Additionally, it incorporates uncertainties related to CFs and impact categories, employing cutting-edge characterization modeling. Notably, it is the first global regionalized method that allows for the assessment and differentiation of the same emission occurring in various geographical locations worldwide (Jungbluth, 2025).

11.4. Ozone Depletion Potential

11.4.1. Other LCIA methods: Ozone Depletion Potential

In a review of Oever et al. (2024) 15 LCIA methods covering ODP as impact category have been reviewed. An overview is shown in the following table:

Table 26: Description of the 15 LCIA methods selected for this review. Legend: M = midpoint, E = endpoint, n.a. = not available (Oever et al. 2024)



Impact assessment method	# of substances	N_2O included	Time horizon	Type	Endpoint effects included	Normalization	Weighting
TRACI 2.1 (Bare, 2011)	90	No	Infinite	M	No	US and Canadian ODS emission 2008	n.a.
EPS2015d (Steen, 2015)	101	No	Infinite	E	Skin cancer, cataract	n.a.	Willingness-to-pay
CML-IA baseline (Oers, L. van, 2016)	23	No	Infinite	M	n.a.	Per capita global ODS emissions 1995	n.a.
CML-IA non-baseline (Oers, L. van, 2016)	15	No	5,10,15,20,25,30,40 years	M	n.a.	Per capita global ODS emissions 1995	n.a.
ReCiPe 2016 -Individualist (Huijbregts et al., 2016)	22	Yes	20 years	M/E	Skin cancer (Hayashi et al., 2006)	n.a.	n.a.
ReCiPe 2016 -Hiërarchisch (Huijbregts et al., 2016)	22	Yes	100 years	M/E	Skin cancer (Hayashi et al., 2006)	n.a.	n.a.
ReCiPe 2016 -Egalitarian (Huijbregts et al., 2016)	22	Yes	Infinite	M/E	Skin cancer, cataract (Hayashi et al., 2006)	n.a.	n.a.
Environmental prices (De Bruyn et al., 2018)	25	No	100 years	M/E	Skin cancer, agricultural crops (Hayashi et al., 2006)	n.a.	Damage-costs
Impact World+ (Bulle et al., 2019)	25 (midpoint) 23 (endpoint)	No	Infinite	M/E	Skin cancer, cataract (Struijs et al., 2010) et al., 2010)	Global damage 2000	n.a.
LC-IMPACT all effects, infinite (Verones et al., 2020)	21	Yes	Infinite	E	Skin cancer, cataract (Hayashi et al., 2006)	n.a.	n.a.
LC-IMPACT all effects, 100 years (Verones et al., 2020)	21	Yes	100 years	E	Skin cancer, cataract (Hayashi et al., 2006)	n.a.	n.a.
LC-IMPACT certain effects, infinite (Verones et al., 2020)	21	Yes	Infinite	E	Skin cancer (Hayashi et al., 2006)	n.a.	n.a.
LC-IMPACT certain effects, 100 years (Verones et al., 2020)	21	Yes	100 years	E	Skin cancer (Hayashi et al., 2006)	n.a.	n.a.
Ecological scarcity 2021 (FOEN, 2021)	42	No	Infinite	M	n.a.	Swiss emissions 2021	Distance-to-target (Swiss emissions 2040)
Environmental Footprint 3.1 (Andreasi et al., 2023; Fazio et al., 2018)	23	No	Infinite	M	n.a.	Per capita global emissions 2010	Hybrid evidence-based and expert-judgement

For the DPP, only the midpoint categories are relevant. Therefore, the abovementioned endpoint including EPS 2015d and LC-IMPACT (incl. all the variations) will not be considered in the discussion.

The UNEP Handbook for the Montreal Protocol (UNEP, 2020) enlisted 93 CFs. Despite relying on relatively old data sources, the impact assessment method TRACI 2.1 contains the highest number of CFs with 90 substances, followed by Ecological Scarcity 2021 with 42 substances. While the majority of LCIA methods (e.g., CML-IA baseline, EF 3.1, Impact World+, ReCiPe 2016) only include 22 to 25 ODS.

Oever et al. (2024) discovered that of the 32 substances not regulated by the Montreal Protocol, which are instead reported in the WMO (2022) inventory, only 5 of them are very sparsely included in the LCIA (e.g., N_2O in ReCiPe). Oever et al. (2024) stated that up to now only the LCIA method EF version 3.1 (Andreasi et al., 2023; Fazio et al., 2018) provides the most recent factors based on a global inventory for 2010. The rest of the methods offer normalization factors, which mostly refer to global inventories dated before 2010. However, it should be noted that the completeness of the inventory used in EF 3.1 is estimated to be below 30% (Crenna et al., 2019). TRACI 2.1 contains normalization factors based on US and Canadian ODS emissions of 2008. (Oever et al. 2024)

Three different weighting methods were presented in the review of Oever et al. (2024). Ecological Scarcity 2021 provides a distance-to-target weighting factors, which express the normalized results relative to the Swiss policy targets for 2040, which limits the geographic representativeness. EF 3.1 incorporates a combination of public and expert panel-based weighting factors. (Oever et al., 2024)

Figure 16 illustrates the data sources and model assumptions for ODP considering the period of publication of the LCIA method. The graph shows EF 3.1. as the most recent methodology, which is based on Goedkoop et al. (2013) and WMO (2011 and 2014).

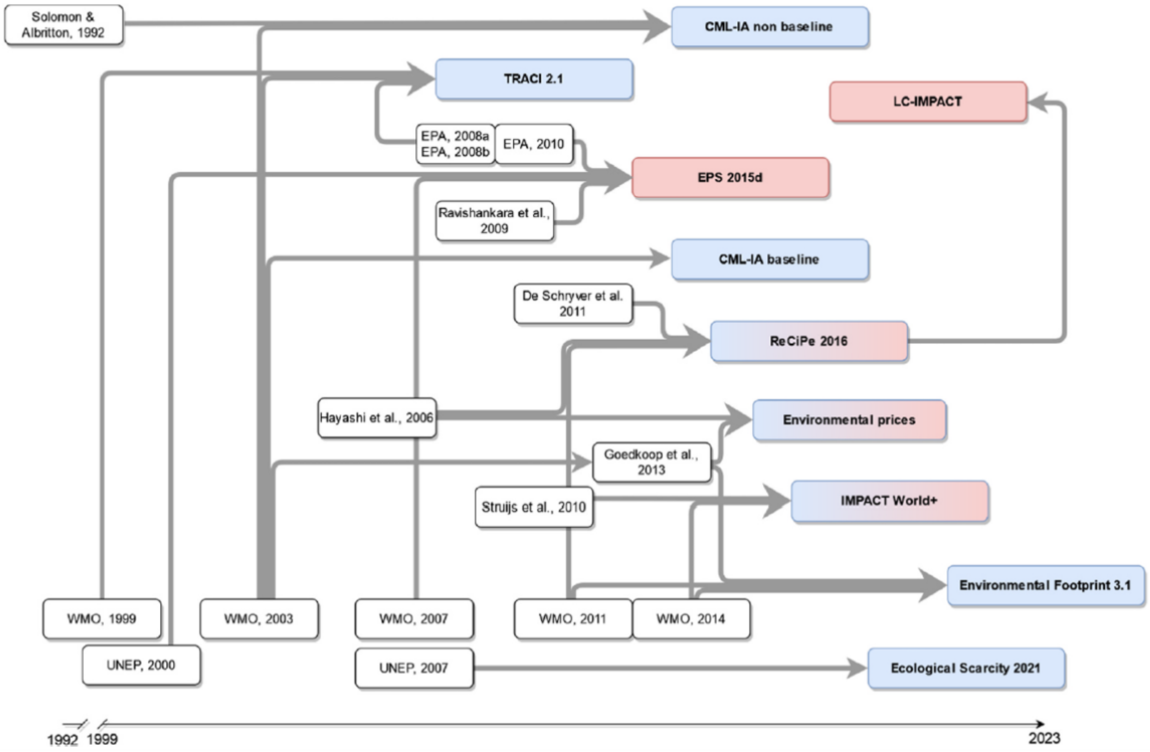


Figure 16: Overview of existing LCIA methods considering ODP in midpoint (blue ovals) and endpoint (red ovals) methods. White ovals represent data sources for ODP and model assumptions. (Oever et al., 2024)

11.5. Photochemical Ozone Creation Potential

11.5.1. Other LCIA methods: Photochemical Ozone Creation Potential

Table 27 compares several existing methodologies for assessing POCP.

Table 27: Overview of LCIA methods for POCP

Method	Midpoint/ Endpoint	Unit	Spatial resolution	Chemicals	Coverage	Models	Reference
CML 2002	M	kg ethylene-eq. per kg emitted	Country, Europe	NO_x, POCP-factors		POCP	Guinéeet al. (2002), Huijbregts et al. (2000)
ReCiPe 2016	M,E	Kg NO_x-eq	Europe but can be adapted for global	NO_x, NMVOC, N_2O	Terrestrial ecosystem, Human health	Global source-receptor model TM5-FASST	Van Zelm et al. 2016
TRACI 2.1	M	O_3 equivalent	North America and Mexico			Maximum Incremental Reactivity (MIR) scale	Sphera LCA Database Modelling Principles 2024
EF 3.1	M	Kg NMVOC-eq. per kg	Europe	NO_x, NMVOC,	Human health	LOTOS-EUROS model	Van Zelm et al. 2008
LIME	M,E	Kg ethylene eq. Into air per kg emitted	Japan	NO_x, NMVOC, POCP-factors	Human health, crops, wood and primary production		Hayashi et al. (2004)

As shown in the table above, the methods use different reference unit to measure POCP, consider different groups of chemicals and utilize different underlying models. These differences result in large variation in POCP values. This is also evident in the study conducted by Joseph, B et al., 2024 to assess the POCP during composting using three methodologies: ReCiPe, EF 3.0 and IMPACT WORLD+ as depicted in Figure 17.

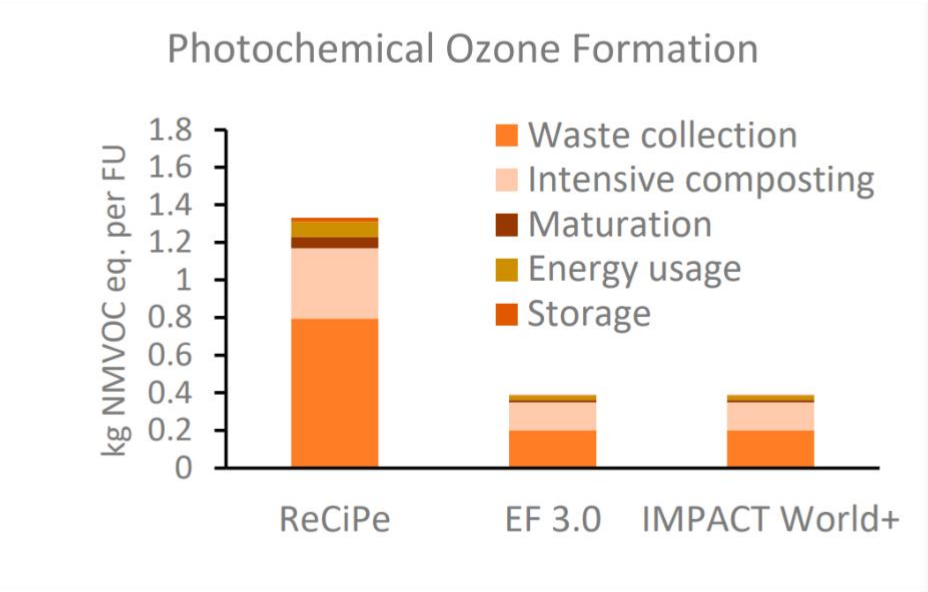


Figure 17: Comparison of photochemical ozone formation values (in kg NMVOC eq.) between the three methods: ReCiPe, EF 3.0 and IMPACT World+. (Joseph and Stichnothe, 2024)

Figure 17 highlights that the ReCiPe 2016 method yields the highest POCP value, while EF 3.0 and IMPACT WORLD+ methodologies results in a 76% lower value. As mentioned above, this is due to the differences in the characterization models used by the three methodologies. While LOTOS-EUROS model is used by EF 3.0 and IMPACT WORLD+ to characterize the impact of photochemical ozone formation, ReCiPe 2016 method uses global source-receptor model TM5-FASST. As a result, the coverage of the POCP causing substances has also varied. For instance, ReCiPe 2016 covers overall 134 substances, compared with 65 in EF 3.0 and 104 in IMPACT World+. Specifically looking at the individual NMVOC emissions, ReCiPe 2016 method covers nine ozone-forming substances compared to EF 3.0 and IMPACT World+, which covered only five and four substances, respectively.

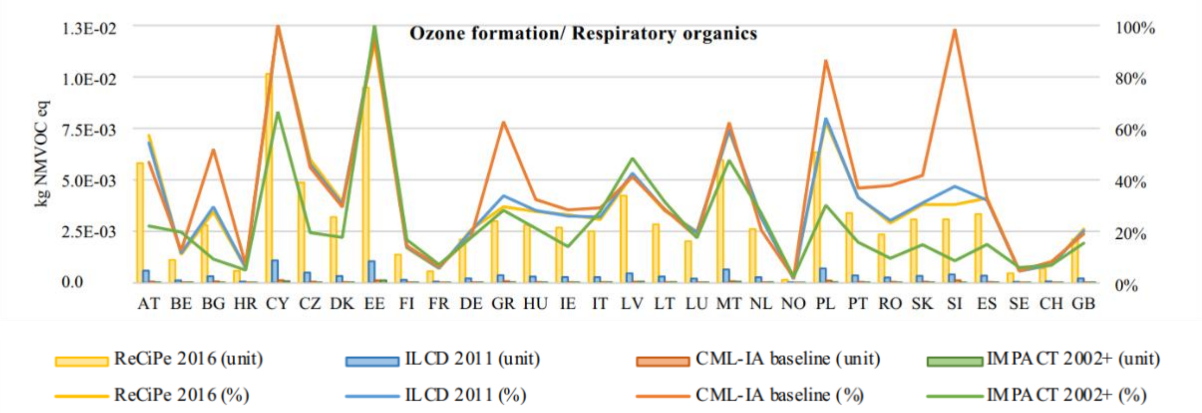


Figure 18: Comparison of photochemical ozone formation values (in kg NMVOC eq.) between the four methods: ReCiPe 2016, ILCD 2011, CML-IA baseline and IMPACT 2002+ . (Rybaczewska-Błażejowska and Jezierski, 2024)

Similar conclusion was also drawn by Rybaczewska-Błażejowska and Jezierski (2024) where results from ReCiPe 2016, ILCD 2011, CML-IA baseline and IMPACT 2002+ were compared for POCP at midpoint level of the electricity consumption mix across European countries. Figure 18 clearly presents the visible trend across the European countries, with ILCD 2011, CML-IA baseline and IMPACT 2002+ methods showing ~90% lower value on average in comparison to ReCiPe 2016.

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